Modelling, Identification and Control of Activated Sludge Plants for Nitrogen Removal

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prof.dr.Dipl.-Ing. H.A. Preisig
en
prof.dr.ir. G. van Straten

Aan Marion, Liza, Sharon en ons derde kindje

Contents

Summary

Stricter legislation on nutrient removal in wastewater treatment requires improved performance of activated sludge processes. The aim of this thesis is to study possible performance improvements of activated sludge plants for nitrogen removal through application of advanced modelling and control techniques and to develop methodologies to achieve improved operation. The emphasis is on continuously operated carrousel systems and pre-denitrification plants, which are the most important systems in The Netherlands. Different topics are addressed along successive steps in control system design, namely definition of the control goal, plant modelling and identification and controller design.

An inventory of the literature reveals that insufficient insight exists in the relationship between legislation and control goals. Artificial, indirect and vague control goals are applied that lead to time-consuming trial-and-error design procedures and that complicate judgement of particular controller designs. The availability of advanced modelling and control techniques argues to develop straightforward, optimisation-based controller design procedures to close the gap between legislation and controller specifications. Such a so-called analytic design procedure is characterised by mathematical modelling of goals, disturbances and plant and application of mathematical optimisation, where qualitative goals for activated sludge process operation are translated into formulation as (multi-criteria) optimisation problems. Trade-offs and selection of system boundaries must be carefully selected for an adequate goal definition.

Application of an analytic procedure for control system design requires reliable dynamic plant models, amongst others for control system evaluation. Modelling and identification of activated sludge plants is studied, focusing on Activated Sludge Model No.1 (ASM1) that describes the biological reactions in the plant. For accurate prediction of plant behaviour, calibration of ASM1 model parameters is required. However, still no clear, standard procedures for this task exist. An identifiability analysis is therefore carried out to reveal if sufficient ASM1 parameters can be uniquely estimated from a typical, realistic set of full-scale input/output measurements. A combined criterion for practical identifiability based on the determinant and the condition number of the so-called Fisher Information Matrix proves effective to detect identifiable parameters. Local and global identifiability analysis is carried out on a particular plant assuming perfect knowledge of the transport model. The results show that input/output measurements do not allow unique estimation of all required ASM1 parameters and that additional information is required. One such test to obtain additional information, namely for determination of biodegradable COD, an important quantity in ASM1 modelling, is refined and experimentally tested.

For identification in model-based control and for controller design, direct application of the full ASM1 is less suited, due to its size, identifiability problems and stiffness. Model order reduction by timescale separation with singular perturbation theory is therefore studied. Three procedures to test whether timescale separation through singular perturbation is possible are proposed, namely timescale estimation, direct scaling and analytical scaling. They are tested on a relatively simple model system. The timescale estimation procedure proves a very helpful tool in model reduction. It is more straightforward to apply than eigenvalue analysis, because it avoids an ambiguous state-to-eigenvalue association and it provides an error analysis. The analytical scaling procedure provides insight into the cause of time scale multiplicity. It is

successful only in a limited number of cases, however and is less generally applicable. The direct scaling procedure is not generally applicable.
For the test to determine biodegradable COD mentioned above, a reduced first-order model is derived by applying a quasi-steady-state assumption. The reduced model provides valuable insight, as well as quantitative relationships required for interpretation of this test.

The next step in control system design is control structure selection and the actual controller design. Control structure selection includes input/output selection (the selection of sensors and actuators) and controller configuration (their interconnections).

For input/output selection in activated sludge process control, a basic model analysis probably suffices once a correct selection of controlled variables has been made. Selection of controlled variables is more difficult. A possible methodology for their selection employs the minimum singular value of the plant transfer matrix, using a model such as ASM1. With respect to control configuration selection, several interactions occur in the activated sludge process. The need for non-interacting control from the perspective of the final control objectives remains to be established, however.

The actual controller design, especially the control law selection, is studied with Model Predictive Control as a prototype control technology. MPC performs model-based optimisation on-line, including feedback, and is best suited to deal with realistic optimisation problems under constraints. Linear MPC with constraints is applied to a pre-denitrification plant model and a carrousel model, which both are continuously operated systems. In both systems, stability problems occurred, caused by model mismatch. The results show that MPC with a nonlinear internal model is better suited for economic operation as the internal model can cope with a larger operational range. Moreover, the time-varying characteristics of the activated sludge process argue to include adaptation. To study the need for nonlinear and adaptive control, MPC robustness against state vs. parameter uncertainty is investigated on a simple model using a structured uncertainty description. The results show that state uncertainty has a larger effect than parameter uncertainty. Consequently, nonlinear control development should be given priority over parameter adaptation. However, these conclusions are drawn with caution, because the robustness analysis results are conservative.

At the current state-of-art in activated sludge modelling, one should avoid absolute quantitative conclusions when employing models tuned with existing calibration strategies. These do not yield unique parameters, so the physical interpretation of parameters is unclear and consequently prediction accuracy is limited. ASM1 calibration needs further development, as do transport models development and their calibration, especially for distributed systems such as carrousels.

Despite of this, models such as ASM1 are most helpful tools in developing straightforward controller design procedures. In combination with mathematical optimisation techniques, they provide a reference point for achievable performance and allow unambiguous evaluation of the effect of all design steps and of model uncertainty on overall process performance. Thus, modelling and optimisation are invaluable for improving process performance and for deciding on suitable control strategies.

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Stefan Weijers
May 2000

Chapter 1 Introduction

'What is your opinion? What modifications should we make to let our largest treatment plant comply with the new standards on effluent nitrogen? Should we extend the plant volume or can we save money by installing only an ammonia sensor that are claimed to be reliable now? Or should we apply these advanced, multivariable model based control schemes this control engineer presented today?' asked the manager of the Water Board Central Research office on returning from the workshop on Monitoring and Control for Nutrient removal from Wastewater. The chief process engineer replied: 'We have not yet studied all the alternatives, but the simulations up till now with the calibrated plant model show that DO control based on ammonia does quite a good job in several cases. However, effluent nitrate incidentally becomes very high, so we are still working on the values for the ammonium setpoints for the different influent scenarios. We are not sure however how certain the predictions with the calibrated model are under the extreme weather scenarios'.

This fictive dialogue illustrates several problems typical to present practice of wastewater engineering, which are the subject of this thesis. The thesis deals with mathematical modelling and process control of activated sludge plants for domestic wastewater treatment, with emphasis on nitrogen removal. This introductory chapter sketches the impact of the more stringent legislation on wastewater treatment technology, identifies the need for modelling and control and indicates some important scientific and technical developments that stimulate progress in both areas (Section 1.1). Then, the problem statement and the scope of the thesis are formulated (Section 1.2), followed by the research methodology (Section 1.3) and the research delineation (Section 1.4). The problem statement will be specified according to the major steps in control system design. The structure of the thesis is outlined in Section 1.5.

1.1 Need for dynamic modelling and control of activated sludge plants

1.1.1 History of and introduction to wastewater treatment

In the industrialised, western society, wastewater treatment has become a prerequisite to maintain satisfactory surface water quality. This is largely a consequence of the historical development through which sewers have become the predominant sanitation system, transporting waste to surface water. In the 19th century, industrialisation and urbanisation gave rise to a dramatic increase in population density and lack of proper sanitation led to several epidemics in different countries. After the Great Plague in London in 1857, the British government decided to use water to transport the pathogen containing waste from the cities to the sea, with the introduction of water closets and sewers ('seawards'). In the decades after the introduction of the London sewer system, in many western cities sewer systems were constructed and became favoured over other competing sanitation systems, such as the Liernur vacuum system in several Dutch and German cities, and barrel collection systems e.g. in Sweden, Germany and The Netherlands (Oremus 1990, Lange and Otterpohl, 1997).

The increased pollution load to surface water after the introduction of sewers led to a severe deterioration of water quality in many surface waters. In Table 1.1, the most important groups of pollutants in domestic sewage are indicated (Metcalf & Eddy, 1991), together with effects on surface water quality, and an indication of the associated time scale of the effects (Lijklema *et al*., 1993, Schilling *et al*., 1997). It should be noted that this table applies to domestic wastewater. Significant industrial discharges into the sewer may have a strong influence on wastewater composition, while the nature of the pollutants is very industry specific. For

industrial wastewater, source control is the preferred solution, and industrial wastewater is not considered further in this thesis.

Table 1.1: Pollutants in domestic wastewater and effects

Pollutant group	Time scale	Effect on surface water
Solids	Acute/	Aesthetic
Organic material	Delayed	Oxygen depletion through microbial oxidation
Ammonia		Toxic
		Oxygen depletion through microbial oxidation
Pathogens		Hygienic
Nutrients (N, P)	Accumulating	Eutrophication leading to algal blooms
Organic micropollutants		Ecotoxic
Heavy metals		Ecotoxic
Chlorides		Ecotoxic

In the first half of the 20th century, many rivers, streams and other surface waters were so heavily polluted that they could be qualified as stinking open sewers (Dirkzwager and Kiestra, 1995). Mainly acute problems from solids and organic material became manifest. The naturally occurring ecosystems had been seriously distorted and in many cases normal aquatic life had almost disappeared as a result of oxygen depletion due to biological oxidation of organic compounds. In addition, stench resulting from anaerobic conditions was frequently a problem.

It took until the second half of the 20th century before legislation on wastewater treatment became effective in most western countries. The focus was initially on reduction of acute problems, especially the reduction of oxygen depletion problems through removal of biodegradable organic compounds, and, to a lesser extent, ammonia. In The Netherlands, the Law on Surface Water Pollution (WVO) became effective in 1970.

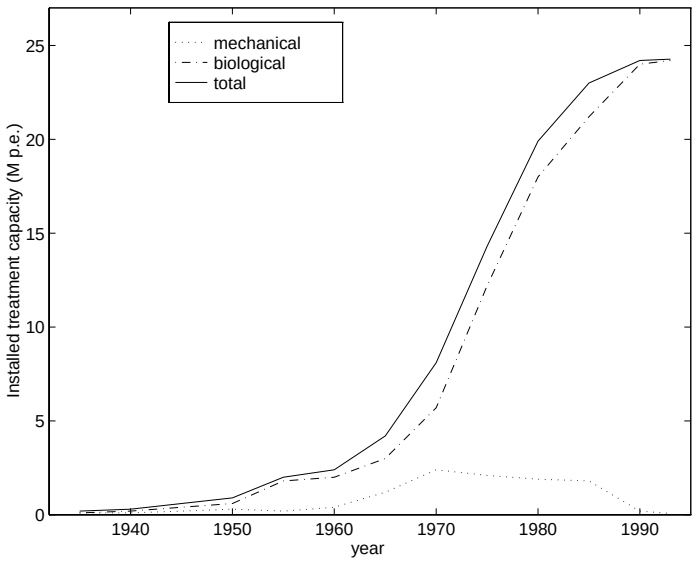


Figure 1.1: Installed sewage treatment capacity in The Netherlands. In 1970, the WVO became effective (Dirkzwager and Kiestra, 1995). Biological treatment is applied most frequently. (Capacity is expressed as M p.e., millions of person equivalents)

Because of legislation, over the past few decades wastewater treatment has been introduced on a large scale. In terms of treated raw material, wastewater treatment can now be considered the largest process industry, with an average flow of approximately $40 \cdot 10^6$ m^3 being treated daily in Western Europe (Vanrolleghem, 1994). Sewage treatment is accomplished most economically

by biological oxidation, and the activated sludge process with its variants is the most commonly used process. Figure 1.1 illustrates the progress of different treatment technologies in The Netherlands over the past decades, which shows the predominance of biological treatment.

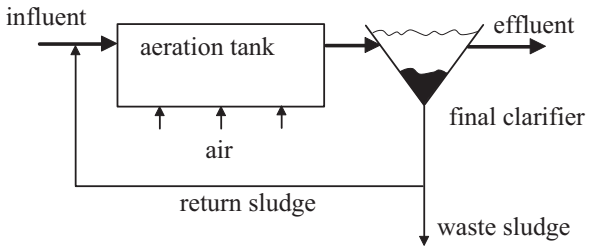


Figure 1.2: Archetypal flow scheme of conventional activated sludge plant

Figure 1.2 shows an archetypal flow scheme of an activated sludge plant. In the aeration tank, air is mechanically imparted, and different types of micro-organisms in the so-called activated sludge oxidise pollutants to less harmful compounds whilst producing new biomass. So-called heterotrophic bacteria oxidise carbonaceous organic compounds to carbon dioxide and autotrophic bacteria partially oxidise ammonia to nitrate, a process referred to as nitrification. After biological treatment, the activated sludge is separated from the wastewater in the final clarifier. The treated wastewater is disposed into the surface water and the sludge is partly recirculated to the activated sludge tank and partly wasted as excess sludge.

The process scheme depicted in Figure 1.2 shows only the biological treatment of a typical wastewater treatment plant. In general, wastewater treatment also includes mechanical treatment to remove floating and settleable solids as a first step and other operations such as sludge treatment and chemical treatment. Several modifications of the conventional activated sludge system are described in Chapter 2.

1.1.2 Legislation with respect to nutrients and biological nitrogen removal

Over the past decades, also long term effects resulting from eutrofication of surface water as a result of nutrient discharges became manifest. Occurrence of elevated levels of nitrogen and phosphorus in various chemical forms gives rise to algal blooms, which cause oxygen depletion, odour problems, aesthetic problems (green water), excretion of toxins and serious disturbance of aquatic ecosystems.

Legislation with respect to nutrients on a European level became effective in the late eighties. Initially, the Northsea Action Plan and the Rhine Action Plan in 1987 aimed at an emission reduction of 50 % in 1995 compared to 1985. The EC Guideline ‘Urban Wastewater’ in 1991 imposed a further reduction of N and P by 75% at the end of 1998. In some countries, nutrient removal had been started earlier; e.g. in Sweden, where P removal started in the early seventies (Olsson *et al.*, 1998).

Phosphorus removal can be accomplished relatively simply in existing wastewater treatment plants by adding a chemical precipitation step[1]. Consequently, in The Netherlands the 75 % removal demand with respect to phosphorus was met in 1995 (Hofstra and Leentvaar, 1995, Gaastra *at al.*, 1996).

[1] Chemical precipitation has the disadvantages of introducing chemicals into the environment and increasing sludge production, whilst P removal can also be achieved biologically. Eventually, biological P removal may become the preferred option as it is already at some Danish plants (Olsson *et al.*, 1998).

Upgrading plants for nitrogen removal on the contrary is more difficult to accomplish. Like conventional treatment, economical nitrogen removal is achieved biologically, and proceeds in two steps. The first step is nitrification (Eq. 1.2). This process requires an aerobic environment, that is, presence of abundant molecular oxygen. Under aerobic conditions, also organic carbonaceous material is biologically oxidised (Eq. 1.1). A commonly used total measure for organic compounds in wastewater is the Chemical Oxygen Demand, COD, which is a standardised method for wastewater characterisation. The second step is reduction of nitrate to molecular nitrogen, referred to as denitrification, requiring abundant COD (Eq. 1.3). Here, the environment is anoxic, that is, without oxygen, with nitrate. The biological processes can be written as follows.

Step 1: Aerobic environment:

$$\text{COD removal:} \qquad \text{COD} + O_2 \rightarrow CO_2 + H_2O + \text{activated sludge} \tag{1.1}$$

$$\text{Nitrification:} \qquad NH_4^+ + O_2 \rightarrow NO_3^- + 2H^+ \tag{1.2}$$

Step 2: Anoxic environment: (denitrification includes COD removal)

$$\text{Denitrification:} \qquad \text{COD} + NO_3^- + H^+ \rightarrow N_2 \uparrow + \text{ activated sludge} \tag{1.3}$$

As an example, Figure 1.3 shows a scheme of a predenitrification system, a frequently applied system for biological nitrogen removal. The influent enters the anoxic reactor for maximal COD utilisation for denitrification, and a high recirculation ratio is required to provide sufficient nitrate for denitrification. Other systems for nitrogen removal are discussed in Section 2.2.

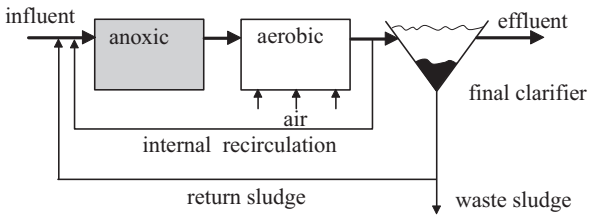


Figure 1.3: Scheme of predenitrification plant

1.1.3 Need for control

In comparison with conventional activated sludge plants, nitrogen removal plants are more complicated. More process steps are present, and several additional conditions have to be met for successful N removal. The interdependent, interacting process steps must be mutually tuned, while the steps proceed under different rates. Nitrification is the slower step due to the low growth rate of nitrifying organisms and exhibits a stronger temperature dependency. Moreover, the COD/N ratio must be sufficiently high (>7) and sufficient nitrate must be available for successful denitrification.

Consequence of this increased process complexity is that the process is much more vulnerable to disturbances. The disturbances in sewage treatment are in general so large, that the activated sludge process must be regarded to be in unsteady operation. The main disturbances are due to

large variations in flow, load and temperature. Several factors contribute to these variations. Flow and load typically exhibit a diurnal pattern, because of variations in water consumption in the households. In addition, many sewers are of the mixed type, where urban drainage and urban sanitation are combined in one system. For example, in The Netherlands, approximately 90 % of the sewers is of the mixed type (Oremus, 1990). Consequently, enormous flow and load variations may occur during rain events, occasionally giving rise to plant overloading with possibly serious plant malfunction. In addition, seasonal temperature variations occur, because of seasonal influence on influent temperature and ambient temperature. As the rates of the various biological processes exhibit a very different temperature dependency, and especially nitrification decelerates at low temperatures, temperature variations constitute a significant disturbance factor to the nitrogen removal process.

Because of increased process complexity and vulnerability, upgrading for nitrogen removal is much more involved than for phosphorus removal, both economically and technically. Upgrading existing plants requires significantly higher investments. For complying with the new standards in The Netherlands, a required investment between 1.5 and 2 Billion Dutch Guilders has been estimated, partly for building new plants, but mainly for upgrading existing plants, with operation costs amounting up to approximately 300 Million Dutch Guilders yearly (Gaastra *et al*., 1996).

Wastewater treatment plant design has become more difficult. In the past, wastewater treatment plants were designed as continuous processes in steady-state operation. For nitrogen removal processes, dynamics and operation require much more consideration in the design stage. In general, process control is considered a prerequisite for reliable operation. Moreover, because of the enormous investment costs involved, extensive plant optimisation through process analysis and improved process control is a very interesting option, because of possible savings when compared to costly extension of the plant volume (Gaastra *et al*. 1996).

Summarising, stricter demands on effluent nutrients require a more complex treatment process, which is more vulnerable to the large variations that are typical in sewage systems. Process dynamics require both dynamic modelling to provide insight in process performance under dynamic conditions and process control to achieve reliable and improved process operation.

1.1.4 Stimulation of control

Thus, Instrumentation, Control and Automation (ICA) of wastewater treatment plants are becoming increasingly more important.

Table 1.2: Identified bottlenecks, and stimulating developments for increased ICA

Bottleneck	Stimulating development
- insufficiently strict requirements	stricter regulations
- insufficient economic motivation for wwtp automation (non-profit process)	discharge levies, high investment costs for upgrading
- expensive sensors (investment and/or maintenance)	stronger economic incentive for ICA
- inadequate instrumentation: lack of reliable sensors	new, robust sensor types
- plant constraints: actuators not sufficiently suited for control	more emphasis on control in design phase
- lack of process understanding	increased understanding through modelling
- education/training of operators	decision support systems and telemetry
- communication	modelling, computer visualisation

Table 1.2 summarises identified bottlenecks for applying enhanced ICA in wastewater treatment, which has been observed to lag behind the chemical process industry (Olsson, 1993; Vanrolleghem, 1994; Jeppsson, 1996). In the table, factors that currently stimulate increased ICA are also indicated.

Stricter regulations and stronger economic incentive through forced investments and discharge levies form a major motivation for enhanced ICA, as indicated above. Maybe equally important have been several scientific and technical developments stimulating ICA in wastewater treatment:

- *Mathematical modelling of activated sludge processes*.
  A milestone in this area has been the publication of the so-called IAWQ Activated Sludge Model No. 1 (ASM1) in 1987 (Henze *et al.*, 1987). This model has now become accepted internationally and has significantly stimulated the use of mathematical modelling and dynamic simulation, which are now becoming routinely used by wastewater engineers and consultants since commercial software for dynamic simulation with the model has become available. In The Netherlands (STOWA 95-01), standardisation has also stimulated application of modelling. Likewise, several clarifier models describing the sludge sedimentation behaviour (Ekama *et al.*, 1997) are becoming commonly used.

- *Sensor development*.
  While until recently lack of sensors was a major obstacle for process control in wastewater treatment, nowadays sensors are available for many important process variables. Examples are sensors based on flow injection analysis for ammonia, nitrate and phosphate, which have become sufficiently robust and reliable for use in practice. This is recognised both internationally (Wacheux *et al.*, 1993; Vanrolleghem, 1994; Lynggaard-Jensen and Harremoës, 1996) and in The Netherlands after several field tests (Mulder, 1993; van Dalen, 1993). Another example are sensors based on respirometry, which monitor the biological activity in the plant (Spanjers, 1993; Vanrolleghem, 1994; Spanjers *et al*. 1998). Several other interesting sensor types are available or under development.

- *Systems Engineering, Control Engineering and related scientific fields.*
  Several promising control methods have been developed over the past decades. As an incomplete list, we mention digital control, optimal control, adaptive control, nonlinear control, Model Predictive Control, robust control, expert system control and fuzzy control, and combinations of these methods. In addition, there has been important progress in several other related fields relevant for modelling and simulation, such as systems theory providing several methods for analysis of dynamical systems, linear and nonlinear system identification for extracting model parameters from experimental data (Eykhoff, 1974; Ljung and Söderström, 1983; Ljung, 1987), experimental design methods for efficient experimentation (Himmelblau, 1970; Zarrop, 1979), methods for model structure selection and model discrimination, identifiability theory, singular perturbation theory (Kokotovic *et al.*, 1986) for model order reduction and several other order reduction methods.

- *Computer hardware and software and Numerical Mathematics*.
  Computing hardware has shown an amazing progress with the tremendous miniaturisation in microelectronics. This in turn motivated development of numerical methods, amongst others for optimisation (Gill *et al*., 1981; Fletcher, 1987), integration (e.g. Shampine, 1994) and linear algebra (Dongarra *et al*., 1979; Golub and Van Loan, 1983). The availability of

cheap computing power and availability of powerful numerical methods in high level languages and general-purpose modelling and simulation environments have greatly influenced engineering science including wastewater engineering. Nowadays, application of mathematical models and controllers of considerable complexity to real-life problems is possible.

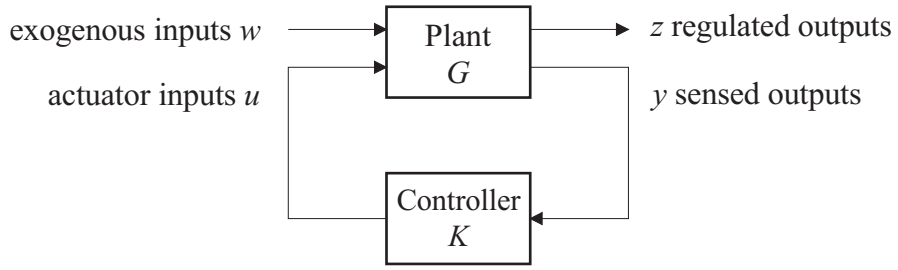
Summarising, both an economic pull through legislation and a technology push by availability of several tools are stimulating increased instrumentation, control and automation in wastewater treatment.

1.2 Problem statement and scope of the thesis

The developments described above stimulated the scientific and professional community to put significant efforts into the area of modelling and control of activated sludge plants over the past few years. This thesis also aims at contributing to improvement of wastewater treatment in nitrogen removal plants, which is formulated in the following problem statement.

Problem statement:
Study possible performance improvements of operation of activated sludge processes for nitrogen removal through application of advanced modelling and control techniques and develop methodologies to achieve improved operation.

The problem statement relates to several relevant aspects in modelling and control system design. These aspects are systematically discussed by considering the different steps or stages that can be distinguished in control system design, which are shown in Figure 1.5. In the discussion, the general closed loop system set-up, which is shown and explained in Figure 1.4, is used.



This set-up is now commonly used in modern control. The exogenous inputs *w* include all external inputs, including reference trajectories and setpoints, disturbances, but excluding manipulated variables. In *w* also constraints are included. The actuator inputs *u* coincide with the manipulated variables of the plant, and are exactly the signals leaving the controller. The measured outputs *y* are the process variables which are actually measured by sensors and input into the controller. The regulated outputs *z* include all variables considered important, which can be the measured outputs, but also the actuator inputs or other variables of interest.

Figure 1.4: General closed loop control system set-up (Boyd and Barratt, 1991)

Stage	Action	Refers to
1	Definition of the goal	*w, z*
2	Modelling of the plant	*G*
3	Input/output selection	*u, y*
4	Control configuration	*K*
5	Controller design	*K*
6	Controller evaluation	Closed loop system with plant model
7	Implementation, testing and commissioning	Closed loop system with plant

Figure 1.5: Control system design scheme

The different aspects of the problem statement will now be discussed along the successive steps of the control system design scheme and selected issues for research will be indicated[2].

1. Goal definition

As the starting point in control system design, usually there is the important and nontrivial task to translate qualitative, often poorly defined goals into quantitative, clearly defined control system specifications. This step is most important as it determines subsequent steps, including the evaluation of the designed system where achieved performance is evaluated against required performance (see below).

In wastewater treatment, legislation has to be translated into operational goals, which in turn must be translated to control system specifications. Several causes complicate straightforward control goal specification. For example, a given legislative framework can be interpreted into different operational goals. Moreover, the choice of controlled variables is relatively complicated, as several sensor types are available and the selection of type, number and location is nontrivial.

Because of the importance and difficulties of control goal formulation, **this thesis aims to contribute to a more straightforward control system design approach by analysing and systemising goal formulation**.

2. Modelling of the plant

Modelling of the plant is the second important task in control system design. In this thesis, 'model' is restricted to 'mathematical model'. This is considered a logical choice in view of the currently available knowledge in mathematical form, while we realise that also linguistic and other models can be of value for control.

The goals to be achieved in the respective stages of control system design require models of different complexity. Consequently, modelling does not completely precede but rather is part of (several of) the other stages.

In the controller evaluation stage, physical (or mechanistic) nonlinear models of high order are usually applied. ASM1 is the state-of-art model for activated sludge processes. To reliably simulate the real plant, the model must be accurately calibrated. This also holds true for other important applications such as process analysis, for example to decide whether operation must be improved. Considerable research activities have been devoted to ASM1 calibration,

[2] Control system design is not a straightforward procedure but rather an iterative learning process. Results at any of the stages may give rise to redefinition of preceding stages. Especially, modelling and process analysis will help to find clear opportunities for process improvement and to state well-defined control system specifications, whereas controller design and evaluation may indicate process and model limitations and lead to control system respecification or model improvement.

and it has become clear that good calibration is a difficult task, amongst others due to the identifiability properties of the model, and needs further study. For these reasons, **modelling and identification of wastewater treatment plants has been chosen as a research topic in this thesis**.

For controller design, the full ASM1 model is too complicated and models of lower complexity are required. The degree of complexity including the model structure and order of these simpler models depend largely upon the particular methods selected for these stages. In several cases, models applied at later stages are derived from rigorous models used at preceding stages. For this reason, and because of the identifiability problems with the full model, development of reduced models for the purposes of control and observer-based process monitoring is an important task. Therefore, **model reduction has been selected as another topic in this thesis**.

3. Input/output selection

Control structure design consists of control configuration and input/output selection. In the control literature, much more attention has been paid to controller design than to control structure design. Nevertheless, a wrong control structure may put fundamental limitations on performance, which advanced control cannot overcome.

In input/output selection, one decides upon the number, place and kind of manipulated variables u and measured variables y. In addition, decisions with respect to the control scheme can be part of this step, such as for example selection of the number of degrees of freedom (1-DOF or 2-DOF) (van de Wal, 1998). The possible set of choices grows combinatorial with the number of candidates for u and y. Therefore, in theory the set is huge if the number of candidates is large. In practice, heuristic guidelines may significantly reduce the number of candidate choices, but typically, a large number remains. For large sets, it is impossible to design and test all possible combinations, and methods to select good candidate choices are required.

Recently, several new types of sensors have become available improving the ability of directly measuring wastewater quality. This increased the number of candidates for measured variables y for control. At the same time, the possible types of manipulated variable increased in wastewater treatment systems for nitrogen removal. In principle, the number of possible candidate IO sets is therefore very large. Therefore, **the need for IO selection methods in wastewater treatment is studied**.

4. Control Configuration

At this stage, one decides upon the structural interconnections between y and u. A MAMS (Multiple Actuator, Multiple Sensors) system does not necessarily lead to a MIMO (Multiple Input, Multiple Output), completely centralised design. Decentralised control is easier to design, implement and maintain than fully centralised control. A trade-off must be made between costs of fully centralised control against performance loss when using fully decentralised control. Partially decentralised control often offers an attractive alternative. An example of a partially decentralised controller (one SISO loop and one 2x2 MIMO loop) is the following system. Here y_1 is controlled by u_1, and y_2 and y_3 are controlled by u_2 and u_3 (x means interconnection, 0 means no interconnection).

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} x & 0 & 0 \\ 0 & x & x \\ 0 & x & x \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

In wastewater treatment plants for biological nitrogen removal, several interactions occur. Nevertheless, relatively little attention has been paid to application of multivariable control. Therefore, we will **explore the need for centralised control**.

5. Controller design

This stage includes control law selection, modelling for control, and controller tuning. With respect to the control law selection, it has been indicated above that many control methods are available. Few of them, however, are being applied to the activated sludge process. The activated sludge process is nonlinear, time variant (because of changing parameters), multivariable, stiff, uncertain and ill-defined, subject to large disturbances and relatively slow. Therefore, one might expect that application of advanced control techniques developed for one or more of these characteristics might lead to advantages over classical control. Thorough comparative studies addressing this question yet have to be done. Therefore, **obtaining more insight into possible improvement by advanced control techniques is an aim of this thesis work**[3].

Controller tuning often requires several iterations before a satisfactory tuning is achieved. This should be avoided through a straightforward design procedure. **It is a goal to contribute to a systematic design methodology**, especially through clear goal definition and application of model based and optimisation-based type of controllers.

It must be assessed how reliable control is compared to expensive concrete hardware. In view of the listed process characteristics, control system robustness under uncertainty is an important requirement. Therefore, **control system robustness is studied**.

6. Controller evaluation

The closed-loop performance of the designed controller is evaluated on a simulated plant before implementation on the real plant. Typically, different input sequences are applied, and robustness tests are carried out. Especially the evaluation stage may lead to re-iteration through one or more preceding design stages. In wastewater treatment, typically ASM1 and related models are used for simulation of the activated sludge part, eventually combined with other mechanistic models for other process units, such as the clarifier or sludge treatment.

This thesis contributes to control system evaluation by studying control goal formulation, to provide a clear performance measure for evaluation. Moreover, calibration of ASM1 to obtain reliable mechanistic models for the evaluation stage is studied.

7. Implementation, testing and commissioning

Finally, the designed controller is implemented on the real plant, together with related hardware, like sensors, actuators, cabling and processors. Often, retuning is required, depending upon the accuracy of the plant models applied at the various design stages. After successful testing against various criteria, such as reliable and robust operation, the designed controller can be commissioned for daily operation. It can then be evaluated for improved performance against the defined goal in the real plant. The implementation stage is not addressed in this thesis however.

1.3 Research methodology

The problem statement is approached by investigating the different stages of control system design discussed above. For each design stage, a state-of-art assessment is carried out. The aim

[3] The ultimate goal of the research in this thesis is improved plant operation; to achieve this goal efficiently, increased insight is an important prerequisite and thus constitutes a valuable product in itself.

is to obtain insight in a broad sense, rather than focussing on one particular technique or design aspect. For the modelling and controller design stages, a more extensive study is carried out as summarised below, together with a brief description of the methodologies applied.

Modelling
Modelling methodology of biotechnological processes is summarised to put into perspective modelling of activated sludge plants with Activated Sludge Model No. 1. For identification of ASM1 to describe existing plants, strategies in the literature are critically assessed. Identification of kinetic and stoichiometric parameters are studied in more detail in order to determine what parameters can be estimated from input/output data and which have to be determined separately. This is done by testing different criteria for parameter identifiability of the model, all based on the Fisher Information Matrix. Numerical studies and full-scale experiments are used to test the results obtained.

Model reduction focuses on order reduction through timescale separation. Singular perturbation theory is studied on a simple model system to obtain better understanding of timescale properties of ASM1 and to develop a systematic reduction procedure. A quasi-steady-state assumption is applied to obtain a specific ASM1 reduction for interpretation of a batch test.

Control
Studies with respect to control are based on ASM1, assuming that this model reflects typical activated sludge process behaviour, at least in a qualitative sense. Linear MPC with input constraints is applied to study possibilities and limitations of advanced, model-based control, starting with linear control.

Controller robustness is tested by simulating the nonlinear plant models for different influent scenarios. In addition, stability robustness of MPC controlled plants is analysed with a simple model system, using the structured singular value. For this purpose, a structured uncertainty model is developed.

1.4 Research delineation

The focus of this thesis is on nitrogen removal. Phosphorus removal is not considered for reasons discussed in Sections 1.1.2 and 1.1.3. The emphasis is on continuously operated carrousel systems and pre-denitrification plants, which are the most frequently applied systems in The Netherlands.

With respect to modelling, emphasis is put on the application of ASM1, including model tuning and model reduction. Only the standard ASM1 is used; dialects of ASM1 or more recently developed models such as ASM2 (Henze *et al*., 1994) and ASM3 (Gujer *et al*., 1999) are not, with the exception of the dialect of the Simba implementation (Ifak, 1995). This dialect is used in the simulations in Section 5.4. In the study on model reduction, a procedure for reduction is developed. The procedure was not applied to ASM1 reduction.

The study is restricted to the biological process. It does not cover sedimentation or plant wide-control. Consequently, no sedimentation model calibration is considered.

With respect to control, model-based control is chosen as the preferred method. This choice is motivated by the current state-of-art of mathematical models and control techniques. Consequently, no rule-based systems such as expert systems or fuzzy control are studied. The study is restricted further to application and analysis of linear MPC with constraints. This provides a good starting point for control, which can be extended to nonlinear MPC.

Focus is on control of the nitrogen concentrations. This requires good control of the dissolved oxygen (DO) concentration. In this thesis, however, DO control will not be considered in detail, as many studies have already been carried out on this topic. Instead, it will be assumed that the local DO controller is perfect, e.g. when applied in a cascade control configuration.

The control goal formulation and model calibration that are studied are also relevant for control system evaluation. Other aspects of control system evaluation, such as deciding on suitable scenarios for testing the designed controller, which is not a trivial task, are not studied.

Controller implementation, testing and commissioning are not part of this study. Control studies carried out here are restricted to simulation studies.

The focus of this thesis is on operation. The design phase is very important, as a poorly designed plant will exhibit intrinsic limitations that cannot be compensated for by advanced control. Dynamics and control must become an intrinsic part of process design of wastewater treatment plants to avoid such performance limitations by poor design. Although design is not the focus here, dynamic models and structured control design will also be helpful in plant design.

1.5 Structure and main contributions of the thesis

The thesis structure follows largely the stages of control system design described in Section 1.3 and is outlined in Table 1.3.

Table 1.3: Thesis structure

Step	**Chapter**
1. Goal	2: Control goal formulation
2. Modelling	3. Modelling , model calibration and identifiability 4. Model reduction
3. IO selection 4. Control configuration 5. Controller design	5. Controller design
6. Controller evaluation	2: Control goal formulation 3: Model calibration 5: Controller design
7. Controller implementation, testing and commissioning	Not studied

All chapters contain an introduction, state-of-art assessment of the literature, discussion and conclusions. Chapter 3, 4 and 5 are more elaborate and cover the research issues described in Section 1.3. Most new contributions of this thesis are within these chapters. Besides these new contributions, the integrated coverage of different aspects through the control design scheme is believed to be a valuable contribution in itself, as is the link between modelling and control through analysis of model (parametric) uncertainty.

The main topics and contributions of this thesis are as follows:

Control goal formulation is discussed in Chapter 2. It is analysed why goal formulation for control of wwtp's is nontrivial. Formulation as optimisation problem is presented as a

framework for control system specifications. A proposal for cost minimisation is given as well as directions to develop an integrated approach for the complete wastewater system.

Chapter 3 deals with mechanistic modelling for controller system evaluation. Modelling of wwtp's and calibration of Activated Sludge Model No. 1 (ASM1) are discussed. A procedure for detecting identifiable parameters is developed. It is applied to determine how many and which parameters of ASM1 can be obtained from full-scale plants under normal operation. A procedure using batch tests for determination of biodegradable COD, required in ASM1 calibration, is proposed and experimentally tested.

Chapter 4 focuses on model reduction to obtain reduced models for controller design and as internal model for model based control. Three procedures to detect timescale multiplicity, required for reduction by singular perturbation, are studied on a simple model system.

For the batch test to determine biodegradable COD, a specific reduced model of ASM1 is derived. This reduced model provides an analytical relationship as a function of ASM1 parameters for a conversion factor that is required for interpretation of this test.

Control structure design and controller design and evaluation are the topic of Chapter 5. With respect to control structure selection, a procedure to for input/output selection is suggested. With respect to controller design, applicability of linear MPC with constraints is studied for two important types of wastewater treatment plants, a predenitrification system and a carrousel system. A robustness analysis is carried out on a simple model to distinguish between the influence of model mismatch due to model parametric uncertainty and due to linearization errors.

Finally, conclusions with respect to the various aspects of the problem statement are given in Chapter 6.

Chapter 2 Control goal formulation for wastewater treatment

'MPC allows you to operate the process at its quality constraints, which enables more economical process operation. That is why it is so successful in petrochemical industries, and that's why it is interesting to apply to wastewater treatment also', the control engineer claimed in his lecture at the meeting of wastewater engineers. During the lunch, a vivid discussion took place. 'We should save money by operating exactly at the discharge permits', the head of the process department of the Eastern Water Board said, 'and the law does not demand us to do more than that'. His colleague of the South-eastern Water Board opposed: 'I disagree. It is not our task to make profit. The law only gives an upper limit on discharges, and we must do the best we can to ensure that this is never exceeded. Quality, not cost, should be our prime concern and the law demands us to apply the Best Available Technology.' The head of the research department of the Eastern Board said: 'I think that focussing too much on quality leads to excessive costs. We are currently looking more closely at our discharge goals for nitrogen and are convinced that we can save considerable energy while achieving even better total N removal if we put less emphasis on effluent ammonia than we do now.' 'That's interesting, can you tell me more about the expectations and implications', asked another person at the table and the discussion continued for the remainder of the lunch.

Goal formulation for control of wwtp's is nontrivial and deserves considerable attention of the scientific and professional community, and therefore this issue is analysed in this chapter. In the introduction, a framework for systematic control system specification that should facilitate straightforward control system design is presented. Wastewater treatment systems that are relevant for this thesis are presented in Section 2.2. Section 2.3 discusses the translation of legislation on an international level to plant-specific control specifications. An assessment of the state-of-art of control goals for wastewater treatment in Section 2.4 shows that in current practice goal definition is rather heuristic, leading to indirect design procedures and suboptimal solutions. Section 2.5 illustrates the crucial role of trade-offs in operation with several examples. Section 2.6 proposes possible approaches for rational goal definition as a multi-criterion problem that enables a transparent trade-off between different objectives, including costs. Section 2.7 formulates conclusions.

2.1 Introduction

The goal definition is the most important issue in control system design as it determines all subsequent steps in the design process. In many application areas, qualitative, vaguely defined goals must be translated into quantitative, clearly defined control design specifications. Consequently, for successful control system design specification, a good interaction between engineers from the specific application area and control engineers is required. This also holds true for wastewater treatment. In wastewater treatment, legislation has to be translated into plant goals. These in turn must be translated to control system specifications, such as reference signals, criteria and constraints. Section 2.3 discusses the different steps in the translation process, which can be viewed as a multi-level water pollution control problem.

Section 2.4 discusses the state-of-art of goals applied in current practice and research of wastewater treatment plant control. This reveals the following problems in the formulation of control goals and associated design procedures:

1. Insufficient insight in relationship between plant goals and control goals: a large variety of control goals are applied for similar plant goals. For example, for respirometry based control alone, Spanjers *et al.* (1998) report a list of 18 controlled variables in 77 references, most of which for comparable plant goals, namely reliable effluent quality despite disturbances against reasonable cost.
2. Trial-and-error design procedures: most reported control designs are done by trial-and-error with typically much iteration leading to time-consuming designs. Even worse, these design procedures are unable to recognise inconsistent specifications.
3. Insufficiently detailed specification of plant goals: there is a lack of standard, consistent criteria for evaluating plant performance. Consequently, it is difficult to objectively assess performance improvement and thus to judge on the success of selected control goals or particular designs.

Apparently, while a vague, qualitative plant goal is verbally easily defined, its translation into practically useful specifications is more difficult. As an example of such a verbal goal we cite (Dirkzwager and Kiestra, 1995): "Maximise treatment efficiency against minimal cost". If we analyse this goal formally, it appears to be a contradiction in terms, as it expresses two goals that cannot be achieved simultaneously: treatment is maximised at infinite costs and costs are minimised if there is no treatment at all. Imposing constraints on treatment and costs leads to two extreme possibilities, namely to maximise treatment with given budget on one hand or minimise cost at given permits on the other hand. Intermediate solutions between these extremes represent different acceptable trade-offs between cost and quality. Besides this trade-off between cost and quality, also important trade-offs between other objectives must be made. Thus, a good trade-off between the different conflicting demands is essential in the translation of plant goals to control goals and characterises a good control system design.

Concluding, there is a need both for objective criteria for performance evaluation and for straightforward, systematic design procedures that enable transparent trade-off between objectives.

The point of view in this thesis is that possible improvements in operation can be assessed unambiguously through a rational, quantitative design procedure by formulating the design problem as a mathematical, multi-criterion optimisation problem. In this approach, all plant objectives and constraints are explicitly formulated in quantitative way. The trade-offs between different objectives in control system design can then be analysed through mathematical optimisation. Moreover, formulating all desired system performance objectives as well-defined design specifications will avoid trial-and-error in the design procedure, will enable a more straightforward assessment of limits of performance and allow to unambiguously conclude whether a desired performance can be achieved through (improved) control or not[4].

Besides performance specifications, design specifications may include robustness specifications (against model uncertainty) and control system specifications.

The concept of such a so-called analytic design procedure, discussed in the textbook of Boyd and Barratt (1991) provides a methodological framework for such systematic design. The analysis in this thesis is inspired by their work, while the concept is extended to nonlinear systems on one hand and limited to the application of wastewater treatment on the other hand.

[4] Applying such an optimisation-based approach does not mean that only one optimum or one such formulation exists. Rather, the approach helps to make decisions more straightforward and transparent.

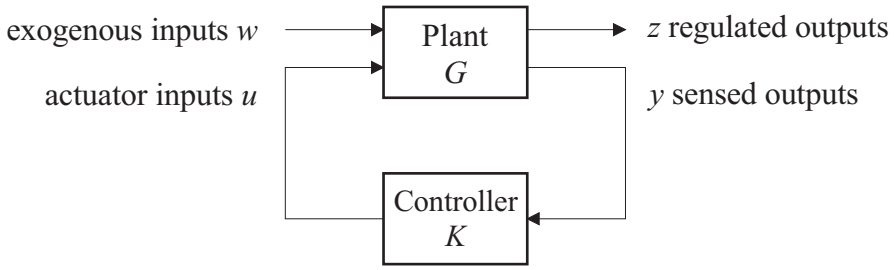


Figure 2.1: General closed loop control system set-up (Boyd and Barratt, 1991)

Required for such an analytic procedure are reliable mathematical models of (See Figure 2.1):

1. Design specifications *z* and references *w*.	These are discussed in this chapter.
2. Disturbance and noise signals *w*.	The influent characteristics must be well known (amongst others);
3. Plant model *G*.	This is the topic of Chapters 3 and 4.

The availability of well-accepted mathematical models such as ASM1 strongly argues for abandoning trial-and-error design procedures and applying straightforward analytic design procedures.

After the analyses and reviews in Sections 2.2 - 2.5, Section 2.6 presents possible approaches to formulate the control system goal as a cost optimisation problem or as a multi-criterion optimisation problem.

The emphasis in this chapter is on which goals are to be achieved rather than on how the goals can be achieved. Different aspects of the 'how' are topic of the subsequent chapters[5], where Chapters 3 and 4 will focus on modelling, whereas Chapter 5 will concentrate on how to deal with optimisation in practice, under model uncertainty and unknown disturbances and with the optimisation and controller design methods currently available. The aim is to stimulate the application of a structured design approach rather than providing an exhaustive inventory of detailed specifications for control of sewage treatment plants.

2.2 Biological wastewater treatment systems

The activated sludge process is by far the most predominant process for sewage treatment. Several process configurations exist. Those configurations that are relevant for the state-of-art assessment are discussed here. Biological phosphorus removal is not treated. More details can be found in Metcalf & Eddy (1991), Henze *et al.* (1995) and Jeppsson (1996).

[5] In general, realistic optimisation problems are nonlinear and non-convex, for which the global optimum cannot be found efficiently nor guaranteed. Frequently, randomised approaches (Vidyasagar, 1997) are applied. These methods are also of interest for identification problems and robustness analysis. In Chapters 3, a type of randomised approach will be applied for global identifiability analysis. The large computational requirements of nonlinear optimisation put restrictions on problem size. To develop solution strategies for realistic engineering problems through mathematical optimisation, model reduction is a possible path. Model reduction will be treated further in Chapter 4.

2.2.1 Conventional activated sludge systems

In conventional activated sludge plants, the reduction of oxygen consuming compounds COD and, often partly, ammonia is the main objective. The involved biological processes are written in Eqs. (1.1) and (1.2). An archetypal process scheme is given in Figure 1.2.

The process scheme depicted in Figure 1.2 only gives the most essential part of a typical wastewater treatment plant. Normally, the wastewater is first fed through a grit chamber to remove crude solids. Then in many cases the medium sized particles sediment in a primary clarifier. Also important is the waste sludge treatment. In many cases, the sludge is thickened in a thickener and stabilised in a digestion tank by anaerobic digestion, in which process methane is produced. Supernatant of the digestion process often is fed back to the aeration tank. This gives an internal load that cannot be neglected, because the concentrations in this supernatant, especially of ammonia, are very high.

Several variants and modifications of the conventional activated sludge system exist. In some cases, the aeration basin is designed as a mixed reactor. More often, however, one tries to realise plug-flow-like behaviour by making the reactor relatively long or by using several tanks in series. In some cases the wastewater is introduced at several points in the aeration tank; this configuration is called step aeration or stepped feed (Metcalf & Eddy, 1991).

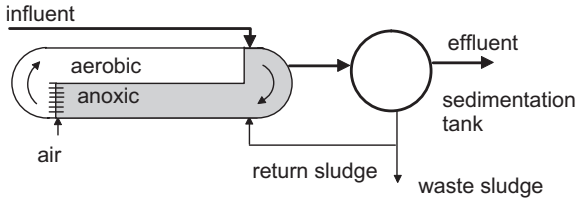


Figure 2.2: Oxidation ditch (top view)

Another variant is the oxidation ditch, developed especially for small wastewater streams by Pasveer in The Netherlands during the 1950s (Figure 2.2) (Pasveer, 1971). This system was originally designed for cyclic operation, including a sedimentation phase, so without the need for a separate sedimentation tank. The oxidation ditch has been applied frequently in the Netherlands, in most cases however operated continuously with a separate sedimentation tank.

2.2.2 Nitrogen removal

Biological nitrogen removal has been discussed in Section 1.1.2, and a scheme of predenitrification has been presented in Figure 1.3. Another important system, which is being applied in many places in the Netherlands, is the carrousel, an example of which is shown in Figure 2.3.

The carrousel is a modification by a Dutch consulting company (DHV) of the oxidation ditch. Instead of brush aerators, turbine aerators are being used, which allow using deeper reactors (up to 4 m) with a large internal recirculation flow (Koot and Zeper, 1972). In the oxidation ditch and in carrousel systems, oxygen is depleted after some distance from the aeration point, resulting in part of the reactor being available for denitrification. Therefore, these systems can be used for nitrogen removal.

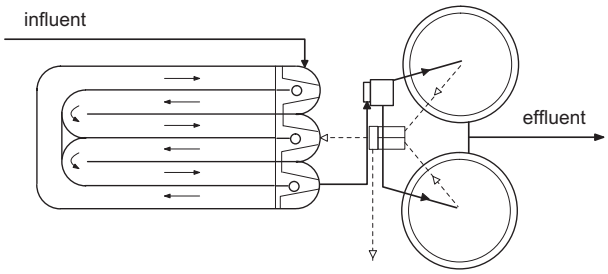


Figure 2.3: Carrousel

The pre-denitrification system and the carrousel system described above are operated continuously. Several other variants exist were the alternation of aerobic and anoxic conditions is created not in space but in time. The most important systems are the following. In intermittent aeration, the aeration is switched on and off intermittently with some interval in the range of at most a few hours. This way of operation is possible because the hydraulic residence times are relatively long. In alternating systems, several parallel reactors are operated alternating in a discontinuous fashion. Examples are the oxidenitro system, a modification of the oxidation ditch to achieve nitrogen removal, and the biodenitro system, a Danish modification (Christensen,1975; van den Oever, 1991).

Recently, Lukasse *et al.* (1998a) compared continuous and intermittent aeration. It would be interesting to also compare continuous operation (pre-denitrification and carrousels) with alternating operation (biodenitro systems); this is however not further pursued here.

2.2.3 Inputs and outputs for activated sludge process control

This section lists possible process inputs and outputs for control of wastewater treatment plants. Table 2.1 summarises possible inputs or manipulated variables for different wastewater treatment systems.

Table 2.1: Manipulated variables in wastewater treatment

Manipulated variable	Conventional	N-removal
Influent flow rate Q_{in} (storage)	∃	∃
Return sludge flow rate Q_r	∀	∀
Internal recycle flow rate Q_{ic}		pdn
Excess sludge flow rate Q_w	∀	∀
Flow rate to clarifier	∃	∃
Aeration intensity k_La	∀	∀
Volume fraction aerobic		∃pdn
Distribution of aeration	∃	∃
Phase lengths		cari, bdn
Distribution of influent flow α	∃	∃
Distribution of return sludge β	∃	∃
External carbon addition		∃
Precipitants to improve sludge sedimentation	∃	∃

Legend: ∃: at some plants, ∀: at all plants, pdn: in predenitrification systems, bdn: in biodenitro systems, cari: in oxidation ditches and carrousels with intermittent aeration

Several indicators exist of wastewater quality and process condition. This paragraph lists the most important indicators together with methods for their measurement, while Section 5.2 gives an overview of the quantities that can be measured on-line. Chemical Oxygen Demand (COD)

is a measure of total organic pollution and is analysed by chemical oxidation. Biodegradable COD, COD_{BD}, is the biodegradable part. No standardised method exists for its measurement. One method is to use prolonged BOD tests, which is investigated in Chapter 3.5. The Biological Oxygen Demand (BOD) is a measure of biodegradable pollution, and is measured by oxygen consumption in closed bottle tests. Most frequently used is BOD_5^{20}, which is the BOD determined after 5 days of incubation at 20°C. For control, short term BOD, BOD_{st}, measured with respirometry, is a better measure of available BOD. Other quantities measured with respirometry are the maximal, actual and endogenous respiration rate (Spanjers *et al*., 1998) and the Total Area Under Curve (STOWA 97-w02). Another measure of pollution is the (volatile) suspended solids concentration, (V)SS. The sludge concentration is often expressed as Mixed Liquor Suspended Solids (MLSS). For this quantity, also sensors exist. The ammonia and nitrate concentration can be measured with sensors besides wet-chemical analysis in the laboratory. As a cheap alternative for nitrate sensors, sometimes the Oxidation-Reduction Potential (ORP) is used. Its application relies upon the detection of an inflection point ('nitrate-knee') in a curve of ORP vs. time that indicates exhaustion of nitrate (Charpentier *et al*., 1991, 1998). Total organic nitrogen including ammonia is measured with the so-called Kjeldahl analysis, and expressed as Total Kjeldahl Nitrogen, TKN (or N_{KJ}). Sludge sedimentation is usually measured as the sludge volume index (SVI) in a standardised sedimentation test.

2.3 Legislation and translation to plant goals and control goals

Water pollution control can be viewed as a hierarchical, multi-level control problem (Figure 2.4), comparable with plant-wide control schemes applied in the (petro-) chemical industries (e.g. Backx, 1987, Prett and García, 1988, Rijnsdorp, 1991). In this scheme, the different control levels are associated with different geographic scales (from broad (Europe) to narrow (via nation to area)) and with different approaches in legislation and goal definition, as well as with different time scales.

On the highest level, level 6, legislation on a supra national, e.g. European level is formulated. In Europe, for nitrogen removal a requirement of 75 % removal has been defined. This is implemented into national legislation, level 5. In this implementation step, political forces and administrative and economical feasibility considerations play an important role besides scientific and technical arguments. Consequently, legislation is implemented differently in different countries[6].

In the Netherlands, legislation with respect to nutrients was implemented through two AMvB's (Abbreviation of Algemene Maatregel van Bestuur, translated as General Enactment of Administration). The AMvB N-removal, published in 1992, imposes a maximal effluent total nitrogen concentration of 10 mg/l as a yearly average of weekly grab samples (15 mg/l for plants smaller than 20,000 p.e.) as from the beginning of 1998 for existing plants (immediate for new plants). Alternatively, a total N-removal efficiency of 75 % over each water management area is demanded. The AMvB P-removal, published in 1990, is comparable, imposing an effluent concentration of 1 mg/l (typically, moving average over 10 weekly grab samples) as from the beginning of 1995 (2 mg/l for plants smaller than 100,000 p.e.).

[6] On the supra national as well as on the national levels, an evolution of objectives takes place over time. Objectives are adapted to the state of knowledge, insight, technology and social priorities. From this observation, legislation itself can be regarded as an adaptive control system.

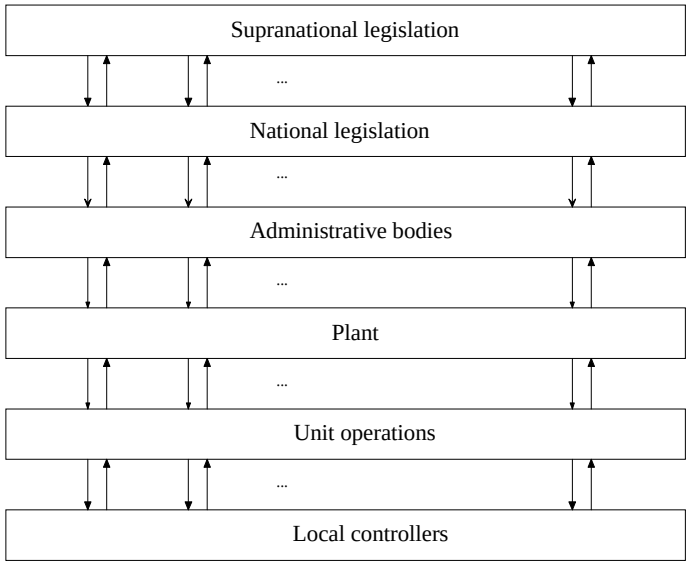


Figure 2.4: Water pollution control as a multi-level hierarchical control system

A given national legislative framework is translated to the level of responsible administrative bodies in the respective countries, level 4. The administrative organisation varies considerably over different countries. In some countries, administrative bodies are responsible for the complete wastewater management of a catchment area or river system, whilst in other countries the responsibilities are much more scattered, often due to historical reasons. In The Netherlands, most responsibilities for the water quality management have been concentrated into all-in Waterboards, where the areas roughly correspond with provinces (Ijff, 1995). Within each of these areas, a nitrogen removal efficiency of 75 % is required over the total area, however not for individual plants.

Consequently, in The Netherlands in the different administrative areas, the legislation can be interpreted into different plant goals, level 3, for individual plants thus incidentally leading to a more-or-less site-specific implementation of permits. At many plants, one aims at achieving low effluent ammonia concentrations in addition to fulfilling total N permits. A variety of desired or maximal values for effluent ammonium and nitrate corresponding to different trade-offs between these components are consequently applied.

Goals for plants in turn are translated into goals for operation of unit processes, level 2. Alternatively, if interactions between unit operations are taken into account and decomposition into unit processes is not applied, plant goals are translated into operational goals and constraints for the plant as a whole (this is used by Spanjers *et al.*, 1998). On the lowest level, we finally have the local control loops, which may be SISO or MIMO, and the actually manipulated and controlled variables. The next section reviews plant goals and control goals.

2.4 Goals, criteria and constraints for wwtp's: practice and possibilities

Control goal definition includes the selection of relevant controlled variables and the specifications for these variables, including setpoints or reference trajectories *w*. Specifications can refer to for example the setpoint, average value or peak deviation of a signal. In addition, other possibilities exist.

In this section, goal formulations applied in control of wastewater treatment plants are reviewed, which shows that control goal formulation is indirect and ambiguous. For similar

plants with similar goals, different variable(s) to be controlled are chosen as well as different selections of setpoints or ranges for the selected controlled variable.

After treating conventional treatment (2.4.1) and nitrogen removal with emphasis on pre-denitrification and carrousel systems (2.4.2), Section 2.3 gives a summarising discussion of these sections. The importance to consider the whole plant and the system boundaries is discussed in Section 2.4.4. Section 2.4.5 summarises recent research efforts aimed at integrated management of the complete wastewater system.

2.4.1 Conventional activated sludge

Cases where the goal is directly related to effluent quality have been few. Busby and Andrews (1974) used a performance index with the BOD load from the sewage treatment plant (STP) integrated over 1 day in a simulation study. Effluent quality expressed as BOD or COD however is difficult to measure on-line, and reliable sensors have become available only recently. Therefore, control has been done mostly by imposing operational constraints as discussed in Section 2.6.2. In this approach, in fact one tries to achieve quality via reliability as a goal.

The best known example of using reliability as a goal by imposing operational constraints is DO control, which has been used by far the most frequently for control of conventional activated sludge plants. Early reports are Maier (1974), Woodruff (1974), Lewin (1974). Evaluation of 413 test findings on 38 municipal wastewater treatment plants in Western Germany showed the need for automatic DO control to ensure sufficient nitrification (Eisele, 1987).

Other authors have emphasised the importance of control of the sludge concentration, e.g. via control of MLSS. For example, von Sperling and Lumbers (1989) denoted MLSS as the most important variable to be controlled in oxidation ditches, as did Bernard (1974).

MLSS and DO control were studied in a pilot plant by Ruider and Schopper (1974). Control of MLSS and sludge height in the clarifier was studied by Vawser *et al*. (1974), and more recently by Van Impe *et al*. (1991) and Vanrolleghem (1994).

Sludge loading has been indicated as a key parameter for control, e.g. the F/M (Food to Mass) ratio was suggested by Armiger *et al*. (1991). Another suggested key parameter is activity or specific activity of biomass: Marsili-Libelli (1989) denoted SCOUR (Specific Oxygen Uptake Rate) as the most important process variable (it is noted that for this variable two measurements required, namely OUR and MLSS). Vitasovic and Andrews (1989) controlled the SCOUR profile in a step-feed configuration, together with control of DO and MLSS. Andrews (1974) and Busby and Andrews (1974) suggested step-feed control to improve sludge settling.

Van Straten *et al*. (1993) showed in a steady-state analysis that it is better to aim at effluent quality control than to use DO control and thus apply reliability control. With the absence of reliable sensors for effluent quality (BOD or COD), efforts have been undertaken to estimate substrate and/or biomass concentration from DO measurements. An early effort was to apply state estimation in LQG (Hamalainen, 1974). Recently, Ryckaert (1998) investigated observability and identifiability for relatively simple activated sludge models for different sensor combinations. If such a state and/or parameter estimation approach is adapted, several associated problems must be accounted for. Some of such problems are discussed in Chapter 3.

A robust alternative to state estimation of substrate (BOD) is application of respirometry, which is increasingly being used as a substrate sensor in control. For example, regulation of short-term

BOD measured by respirometry has been suggested as a control goal (Spanjers and Klapwijk, 1990; Spanjers *et al*. 1993). Klapwijk *et al.* (1993) suggested control based on actual respiration rate (by influent flow rate), maximal respiration rate (by sludge waste flowrate) and instantaneous respiration rate. The report on respirometry (Spanjers *et al*., 1998) clearly indicated ambiguity in translating plant goals to control goals as discussed in Section 2.1.

Most examples above were limited to the bioreactor or to SISO control loops. An early study towards plant-wide control of activated sludge plants was the optimisation study by Bowden and Wright (1974). Von Sperling and Lumbers (1991) performed an integrated control study on a carrousel with overall system objectives. The objective could be set to either maximise treatment with given either budget or minimise cost at given permits. This approach contained many elements of an analytic design procedure advocated in this thesis, namely 1. Overall, quantitative objective, 2. Mathematical models of process and disturbances; 3. Plant-wide control (all manipulated variables were optimised simultaneously, thus considering interactions); 4. Mathematical optimisation; 5: Time-scale separation to reduce the computational complexity; 6. Randomised approach to assess system robustness under different influent scenarios. The optimal control approach[7] aiming at minimal costs was compared with five classical, decentralised control structures for sludge inventory control with the sludge recycle rate and the sludge wastage rate. Monte-Carlo simulation was used to enable a statistical analysis of the results. The optimal control gave in general a significantly better effluent quality, although in some cases at higher operating cost.

2.4.2 Nitrogen removal

This section focuses on recent studies, including practical evaluations on full-scale plants. For pre-denitrification and carrousel systems, control based on ammonia, nitrate, ammonia and nitrate and other controlled variables are discussed respectively.

Predenitrification

Ammonia: In several cases, focus is placed on ammonia. Control of effluent ammonia (by aeration with cascaded DO control) was suggested by Kayser (1990) for small plants (<100,000 p.e.), besides effluent turbidity as a measure of BOD. Both and Neef (1991) aimed at control (by aeration with cascaded DO control) of the ammonia concentration after the bioreactor below 2 mg N/l of one street of a 160,000 p.e. plant. In evaluation of fuzzy control in simulation studies (STOWA 97-32), an ammonia setpoint of 2 mg N/l was applied. The goal Brouwer *et al*. (1998) used in a pilot plant was to have no violation of ammonia effluent permits. For control of a 60,000 p.e. treatment plant of the Lippeverband, a target range for effluent ammonia between 0.8 – 1.2 mg N/l was the primary goal, with minimisation of effluent nitrate as a secondary goal (Husmann *et al.* , 1998). Nielsen and Önnerth (1996) achieved much improvement in overall N-removal after changing trade-off in a recirculating plant. Increase of ammonia from below 0.1 to 0.3 resulted in a decrease of nitrate from 8 to 4 mg N/l, with no longer need for chemical dosage and with less energy consumption.

Nitrate: The second stage of the two-stage (AB) Utrecht STP was adjusted to operate like a predenitrification reactor (STOWA 97-W05). Control of nitrate in the denitrification zone was done with the internal recirculation (as in Figure 1.3). Tuning in practice appeared difficult. A

[7] From the details given, it is not clear whether the optimisation was done in a receding horizon fashion, as is done in Model Predictive Control. Rather, it seems that open-loop control has been applied. Influence of model mismatch was not studied.

calibrated simulation model (based on ASM1) was used to support controller tuning. The dynamics of the model were different from practice however[8]. Several tests had to be performed on the plants for adequate tuning. As the internal recirculation had an adverse effect on SVI, the internal recirculation had to be minimised by control. In addition, the SVI was decreased by substrate dosage in the form of waste sludge from the first stage. Increased nitrogen removal (11 %) was observed after modifications and with nitrate control.

Ammonia and nitrate: Kayser (1990) suggested control of effluent ammonia between 1 and 3 mg N/l (by aeration with cascaded DO control) and nitrate in the denitrification zone close to zero (by internal recirculation), for large plants. Lukasse *et al*. (1997a) minimised the time averaged weighted sum of deviations of effluent ammonia and nitrate from zero, both in simulations and on a pilot plant. In a pilot plant study, Lukasse (1999) minimised the l_1-norm (integrated absolute sum) of deviations from the setpoints 2 and 0 mg N/l for ammonia and nitrate respectively. The weights in the optimisation criterion were tuned such that ammonia was controlled to its setpoint. Lindberg (1997) used in simulation studies the objective to control effluent ammonia at setpoint 0.5, and effluent nitrate setpoint of 6 mg N/l. Hoen *et al*. (1996) used an effluent ammonia setpoint of 5, and effluent nitrate setpoint of 16 mg N/l.

On a 405,000 p.e. plant, combined ammonia control (on-off with a range of 1-3 mg N/l) and nitrate control with a nitrate setpoint of 2 mg N/l in the denitrification zone (STOWA 97-w04) was tested (using cascade control on internal recirculation). Total N decreased from 23 mg/l to 14 mg/l. No influence on sludge sedimentation properties was observed.

Other controlled variables: The oxidation-reduction potential (ORP) was not a satisfactory to control the second stage of the two-stage Utrecht STP configured as predenitrification plant (STOWA 97-W05).

Carrousels

Ammonia: For the 25,000 p.e. carrousel Reeuwijk-Randenburg, the plant goal was to achieve effluent total N below 10 mg N/l. Aeration was adjusted based on ammonia in the reactor (one aerator continuously) and DO measurements (other aerator on-off). During a first test period, aeration was adjusted with switching values for ammonia of 1.0 and 2.7 mg N/l (Mulder, 1993). The resulting average ammonia and nitrate effluent concentrations were 2.7 and 1.7 mg /l (80% of design load) and 2.2 and 4.5 mg/l respectively (>100% of design load). Peaks in ammonia concentration during peak loads could not be avoided. Compared to DO control, comparable effluent total N was achieved, with higher effluent ammonia and lower nitrate, and with more constant effluent quality (DO control resulted in high nitrate concentrations during winter, which were compensated by lower concentrations in summer).

In a later test period, the control configuration was slightly changed to on-off control on ammonia and continuous DO control with the other aerator (De Vente, 1993). This led to a trade-off between ammonia and nitrate with slightly higher effluent ammonia with lower total-N when compared to DO control. To solve problems with the sludge volume index (SVI), another adjustment of the control configuration was applied using a weighted NH_4 and DO signal for both aerators, with weight factors as tuning parameters. The trade-off was changed to higher nitrate (incidentally in winter 10 mg N/l).

[8] This is likely to be caused by the fact that (ASM1) calibration focused on fitting correct effluent concentrations and did not focus on the input/output process dynamics for the specific control loop (effect of internal recirculation on the nitrate concentration in denitrification zone)Apparently, calibrating ASM1 to an overall (influent/effluent) process behaviour does not automatically describe correctly dynamics of internal processes.

Goals at the 300,000 p.e. Kralingseveer STP (STOWA97-W01) were to have effluent total N below 10 mg N/l (on a yearly basis), with good sludge sedimentation, Kjeldahl-N < 8 and ammonia < 6 mg N/l. This was implemented with control of ammonia and DO with 4 aerators, using logic (rule-based) control with 6 ammonia setpoints, 2 DO setpoints and 2 switching-time lengths as tuning parameters. Re-tuning by increasing ammonia setpoints was required to avoid initial problems with high SVI values. Improved effluent quality was obtained when compared to the situation with only DO control. Kjeldahl-N decreased from 7.8 to 4.6 mg N/l while nitrate increased from 6.8 to 7.2 mg N/l, leading to a decrease in total N from 14.6 to 12.2 mg N/l. It was concluded that still better N removal could only be achieved through decrease of the sludge load.

Spies and Seyfried (1988) aimed at not exceeding effluent ammonia 5 mg N/l at 15 ºC despite very large load variations through ammonia measurement inside the aeration tank and cascade DO control at a 110,000 p.e. plant. This control gave good effluent quality with respect to ammonia, as its concentration never exceeded 4 mg/l, even at low temperatures of 3.5 ºC. This was partly due to the lower load during winter. To achieve sufficient (simultaneous) denitrification, retuning was required.

Nitrate: To achieve an effluent total N of maximally 10 mg N/l on the 90,000 p.e.Hattem STP, a half intermittent aeration (one aerator on, one aerator on-off) based on nitrate was applied, switching aeration on at nitrate below 3 and off at nitrate above 5 mg N/l (van Dalen, 1993). The resulting effluent total N concentration was 7.8 mg N/l, with much smaller variation in effluent nitrate than in the reference situation with only DO control (1.5-5.3 vs. 0.3-34). Total energy consumption increased by 18%, but energy consumption per kg N removed decreased by 10%.

Ammonia/nitrate: At the 38,000 p.e. Gennep STP, combined NH_4/NO_3 control (with the aeration valve using two PD controllers) was compared with DO control (one PD controller) (de Man, 1995, STOWA 97-33). Several setpoints for NH_4 and NO_3 in the mixed liquor were applied (both 5, 3 and 2 mg/l) and several setpoints and locations for DO (0.5, 1.2 and 0.8-1.2 mg/l). The average N removal with DO control was 80%, with NH_4/NO_3 control 84% (this difference was not significant). No adverse effect on sludge sedimentation was observed.

At the 96,000 p.e. Beemster STP, the plant goal was to achieve total N < 8 mg/l (STOWA 97-w03). Different control goals to achieve this were tested: 1) DO control (PI); 2) ammonia/DO control (cascade, setpoint DO control (PI) determined by NH_4 controller (PI)) and 3) nitrate/ammonia/DO control (cascade, setpoint DO controller (PI) determined by NH_4 controller (PI), setpoint NH_4 controller determined by nitrate controller (P)). With these different control goals, comparable, good effluent qualities were achieved (between 2 and 7 mg N/l). Tuning was done using a (calibrated) simulation model; however, application of the tuned controller settings to the real plant was not straightforward and manual retuning was required in most cases. No adverse effects on sludge sedimentation, sludge production or sludge composition were observed.

At the Hildesheim plant, mixed liquor ammonia and nitrate were controlled with aeration with a type of split-level control. Control was based on nitrate at ammonia concentrations below 8 mg/l to achieve a high level of denitrification and was based on ammonia when ammonia superseded 8 mg/l, until again ammonia < 3 mg N/l (reference by Kayser, 1990).

Other controlled variables: For the Beemster STP, also control based on respirometry was tested (STOWA 97-w02). The area of the respirogram (TAUC, Total Area Under Curve) measured in the carrousel was used as controlled variable, as a substitute for ammonia measurements. Logic control using a lookup-table with switching values for the 4 aerators as a function of measured TAUC was applied. The tuning was supported by simulation. Good effluent quality was achieved (between 6 and 8 mg/l) with slightly lower energy consumption (3%) than with DO control. No effect on sludge sedimentation was observed.

To improve nitrogen removal, simulation studies using multivariable control based on LQG were performed in comparison with DO control, NH_4/DO cascade control and NO_3/NH_4/DO cascade control (van Schagen *et al*., 1995; Meinema *et al*., 1995). Here, in the controller criterion an explicit trade-off was made between effluent qualities and control effort. To enable comparison with the other studies, an ammonia setpoint of 3 mg/l was selected. Simulation studies indicated that improved effluent quality might be achieved with less energy consumption.

In the full-scale cases discussed in this section, control of sludge recycle flow rate and control of sludge waste flow rate were not explicitly considered, and used in separate control loops.

2.4.3 Discussion and conclusions on control goals

For conventional plants, the overview shows that few control goals directly aim at effluent quality. Instead, most goals are indirect and focus on control of a process variable (or indicator) that is (supposed to be) related to process reliability. There is no agreement on which indicator to select. Only one study aimed at optimal operation considering cost and effluent quality of the plant as a whole and showed superior performance to classical control in terms of effluent quality. No robustness to model mismatch was investigated in that study.

In plants for nitrogen removal, often a more direct control of effluent quality is applied, especially through application of ammonia or nitrate sensors. Here, however, in most cases an (implicit) trade-off is made between ammonia and nitrate. This occurs for example if only a sensor for ammonia is installed and ammonia is used as controlled variable. In that case, ammonia is given priority over nitrate. The same holds *mutatis mutandis* if only a nitrate sensor is installed. Lack of directness of goals is also observed from the fact that in some cases a setpoint for a selected controlled variable (e.g. ammonia) is used, while in other cases an upper limit is applied, and in still other cases a range is used. Moreover, the setpoints and ranges are sometimes used as tuning parameters, which is not a transparent way to trade-off between different variables.

From the cases described, it is clear that goal definition is not straightforward and rather ambiguous. For similar plants and plant goals, many different approaches are applied with respect to sensor selection and selection of setpoints or ranges for the selected controlled variable. In several cases, not only controller settings but also setpoints are used for tuning, which illustrates the lack of relationship between plant goal and the selected control goals. In some cases, the selection of the control goal is determined by preferences for specific (or cheap) sensors that have no well-defined relationship with the plant goals.

2.4.4 Choice of system boundaries

In most of the studies in Sections 2.4.1 and 2.4.2, emphasis has been on bioreactor performance. However, the bioreactor is only one, be it important, part of the treatment plant. Consideration of other unit operations and the interactions between them is very important for

the operation for the plant as a whole, as has been emphasised already by Bernard (1974). The whole plant was considered in the optimisation study of von Sperling and Lumbers (1991). More recently, Olsson and Jeppsson (1994) made a qualitative inventory of interactions and cause-effect relationships. Especially, interactions between bioreactor and clarifier are important, but also sludge treatment and other internal recycle streams cannot be neglected.

Besides considering system boundaries within the plant, definition of adequate, realistic objectives for operation requires adequate choice of the system boundaries of the plant as a whole. While it is not so common to use overall financial costs as an indicator of process performance in municipal wastewater treatment, still, to come to a quantitative design procedure, it is necessary to express operating costs realistically. It is insufficient to consider only influent and effluent quantities and qualities to evaluate plant performance. Instead, the complete interaction of the plant with its environment must be considered. In Figure 2.5, an overview of the inputs and outputs in operation of a treatment plant is shown. It is noted that maintenance costs and materials are not considered in this scheme.

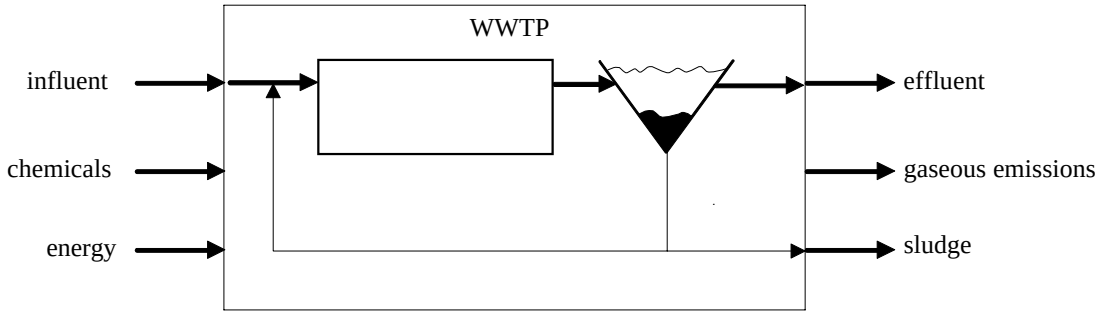


Figure 2.5: Inputs and outputs of a wastewater treatment plant

Inputs to the system include, besides influent, energy for aeration and pumping, chemicals e.g. for sedimentation, precipitation and chemical analyses; outputs are, besides effluent, gaseous emissions and sludge. All these interface variables should be considered. Contributions to total operating costs are shown in Figure 2.6.

a: Average for industrial plants b: Municipal wastewater, from benchmark

Figure 2.6: Operating costs of wastewater treatment (see text).

The costs in Figure 2.6.a are averages of activated sludge plants for different types of industrial wastewater (Vanderhagen *et al.*, 1994). Figure 2.6.b is based on results of simulation studies of a municipal wastewater treatment plant (Debuscher *et al.* 1999). The plant is defined in the

benchmark that is discussed in Section 2.6; the benchmark does not include investment costs, maintenance, manpower and chemicals. An overview of the costs for municipal wastewater treatment made in 1989 (Vanderhagen *et al*., 1994) showed a much larger portion of the investment cost than for industrial wastewater treatment.

For both types of plants, sludge treatment has a relatively large contribution to total cost, several times larger than energy. It is remarkable that levies are much more significant in municipal treatment than in industrial treatment, where they have a minor contribution only. This is probably the case because for the levies for municipal treatment recent legislation was used. It is noted that investment costs for sludge treatment also form a significant part of the investment cost of the treatment plant, so sludge treatment is a large contribution to total costs. Objective functions for operation that consider different costs are discussed further in Section 2.6.

Finally, it is important to note that the wastewater treatment plant is only one part of the complete wastewater system, which consists of sewer, treatment plant and receiving water. Currently, legislation for sewers and legislation for WWTPs have been developed and implemented separately. The permits are mainly emission based and technology oriented, and do not consider total emissions or impacts on receiving water quality (e.g. Rauch *et al*., 1998).

Considerable improvement is expected when sewer, treatment plant and receiving water are jointly considered, with objectives for the overall system aiming at total emissions or even receiving water quality (Lijklema and Tyson, 1993; Lijklema *et al*. 1993; Capodaglio, 1994; Otterpohl, 1994; Harremoës *et al*., 1994). Here, a trade-off between the different subsystem objectives or final water quality objectives can be made through multi-criterion optimisation. Thus, an integrated approach can lead to optimal utilisation of wastewater infrastructure; this is further discussed in Section 2.4.5.

2.4.5 Integrated approach to wastewater management

Recently, several studies of the urban wastewater system have aimed towards more integration. Models, tools and approaches have recently been discussed extensively by Schuetze (1998), which is referred to for more information. As different conceptions of integration exist, it is useful to distinguish between:

1. Integration of objectives: subsystem's objectives include objectives of another subsystem;
2. Integration of information: (control) decisions in one subsystem are based on state information from another subsystem[9].

Many of the reported integrated studies have been design oriented rather than control oriented. These studies typically involve only integration of objectives and one can speak of an *integrated approach*. Some examples are the following (these examples focus more on system design than on control but are helpful to illustrate the importance of an integrated approach). Hansen and Pedersen (1994) did an integrated assessment for a catchment in western Greater Copenhagen, where different modifications on sewer and/or STP were evaluated on total pollution discharge of phosphorus.

[9] This is a slightly modified definition of Schuetze (1998).

Bauwens *et al*. (1996) studied effects of different design and control measures (storm tank installation, step feed, ratio control of recirculation flowrate) on emissions and river quality. A statistical approach based on historical rain series was applied. The acute effect of (short) CSO events on DO was demonstrated. Control measures against CSO's through installation of storage basins was beneficial even though emissions from the STP increased by 50%.

Rauch and Harremoës (1995) studied the impact of rain events on total nitrogen loading and on the DO concentration at three locations in the receiving water, using statistical evaluation. For accumulative pollution of nitrogen, sewer overflows played a minor role; detention basins had a limited effect on acute pollution. Oxygen depletion and ammonia peak concentration in the river were statistically assessed as measures of acute pollution by Rauch and Harremoës (1996). Positive effect of detention basins was compensated by prolonged high hydraulic loading of the treatment plant. This study confirmed the need for integrated analysis of the system.

Integrated control in urban wastewater management is characterised by integration of information in addition to integration of objectives (Schuetze, 1998). Application of integrated control thus creates *integrated systems* (Weijers, 1996). Some recent studies are discussed here.

Nielsen *et al*. (1996) used flow predictions from the sewer and a new control concept in the treatment plant, aeration tank settling, to increase hydraulic peak capacity of the plant and successfully tested this concept on full scale.

CSO reduction through real time control in the sewer was investigated by Rauch and Harremoës (1998). Nonlinear MPC using genetic algorithms with a perfect model were employed to achieve optimal control. Hardly any influence on water quality measured as DO concentration level was observed. In (Rauch and Harremoës, 1999), the control objective was to maximise the minimum DO concentration in the river. The resulting optimal strategy was suboptimal with respect to CSO reduction. These results show that currently applied, artificial performance criteria (control goals) for individual subsystems such as CSO's are not appropriate.

Schuetze (1998) considered control of both sewer and STP, aiming at optimising a combined criterion with respect to the DO concentration in the receiving water (maximise minimal DO and minimise duration of DO below a given level). An integrated control approach was compared with a base case. This base case consisted of optimal, fixed settings for local control loops in the sewer system and the treatment plant. The integrated case consisted of a simple rule-based override control during extreme events. The optimisation of all settings was performed off-line. A Controlled Random Search proved the most appropriate optimisation algorithm. In the cases studied, the DO in the receiving water was improved, be it at the expense of higher ammonia concentrations. Results of simulations on individual events strongly suggest applying on-line, dynamic optimisation of setpoints instead of off-line, fixed setpoints. Future improvement suggestions were to apply a multi-objective criterion, and to put more effort into selection of the control structure and the control law[10].

Within the COST-682 action on integrated wastewater management, one working group has concentrated on developing an integrated, water quality objective oriented approach. The main points are summarised here. Schilling *et al*. (1997) indicated that only a few impacts typically dominate the ecological status of the particular receiving water and outlined a procedure to define such water quality oriented objectives. These would then be the objectives to focus on. Moreover, the impacts can be classified into acute, delayed and accumulating, and system

[10] In Schuetze (1998), the term Control framework denotes Control structure and Control law.

decomposition in timescales can be applied, thus possibly leading to large simplifications in modelling. A procedure for such goal oriented modelling and some examples were described in Rauch *et al*. (1998). Vanrolleghem *et al*. (1999b) described a procedure for setting-up measurement campaigns for calibration and validation of integrated models of wastewater systems. While the last three mentioned papers aim at integrated approaches for system design, the approach and procedures constitute a good starting point for developing a rational, integrated approach in control, which will be outlined in Section 2.6.

2.5 Trade-offs in translation of legislation to control goals

Trading-off between different objectives is crucial in translation of legislation to wastewater treatment plant operation. This is illustrated here with different types of trade-off examples.

The first example deals with trade-off between effluent ammonia and nitrate, which is a trade-off between different quality objectives. Trading-off between these components is crucial for nitrogen removal. To illustrate this, the effect of trade-off between these components on removal efficiency is considered here in a qualitative sense. Figure 2.7 shows effluent ammonia, nitrate and total nitrogen as a function of the DO setpoint for two temperatures. The case has been inspired by Veersma *et al*. (1995), who studied the influence of (only) the DO setpoint on effluent nitrogen in a carrousel system under static operation. More details of the system are given in Appendix B[11].

At many plants, one aims at achieving low effluent ammonia concentrations besides fulfilling N total permits. Consequently, a higher priority is typically placed on effluent ammonia than on effluent nitrate. Two possibilities to implement this are depicted in Figure 2.7: 1) A weighted sum of effluent ammonia and nitrate, where the weight factor on ammonia is four times that on nitrate, and 2) Selection of a low setpoint for ammonia to guarantee sufficient nitrification.

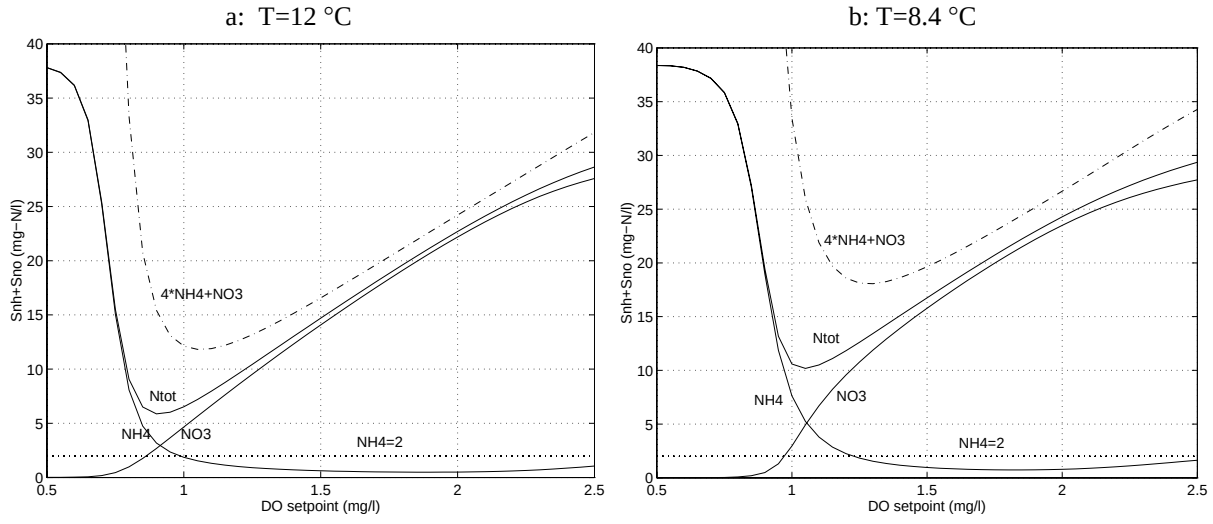


Figure 2.7: Dependency of optimum in N-removal on weight factors and disturbances

[11] Figures 2.7a and b were produced applying equal sludge ages at both temperatures. The sludge concentration at lower temperature is slightly higher (see Appendix B). Therefore, the difference in performance would probably be more pronounced when using equal sludge concentrations.

In Figure 2.7.a, it can be seen that at T=12 °C, the selection of the goal has a minor effect on total N-removal. The optimum N-removal corresponding to effluent total nitrogen Ntot of 6 mg N/l is achieved at a DO setpoint of approximately 0.9 mg DO/l. The ammonia setpoint of 2 mg/l is achieved at 1 mg DO/l with higher Ntot of 6.2 mg N/l while the weighted sum is optimal at 1.1 mg DO/l with a higher Ntot of 6.5 mg N/l, so at the cost of slightly higher nitrate.

If we now consider Figure 2.7.b, with a lower temperature of 8 °C, which approximately corresponds to winter conditions, the selection of the goal has a significant effect on total N-removal. It is possible to achieve the permit on total N of 10 mg-N/l at an optimum DO setpoint of approximately 1.1 mg DO/l. The ammonia setpoint of 2 mg/l is achieved at 1.25 mg DO/l with higher Ntot of 12.5 mg N/l while the weighted sum is optimal at 1.3 mg DO/l with a higher Ntot of 13 mg N/l. Now, a small improvement in ammonia (from 5 to 2) is achieved at the cost of large increase in nitrate (from 5 to 11) and of total N. Thus, the process operates very suboptimal from the point of view of total N removal. This phenomenon would be even more pronounced for higher loaded plants.

Moreover, if the DO setpoint for optimal total N-removal at 12 °C would be applied at 8 °C, this would lead to a very high effluent ammonia of approximately 18 mg-N/l and almost no denitrification. A fixed DO setpoint can thus lead to poor process performance.

Additional simulations showed that, besides temperature changes, other changes in process conditions like load changes and parameter changes lead to similar observations.

This shows that different process conditions require different trade-offs that cannot be achieved through fixed weight factors for ammonia and nitrate or fixed setpoints on DO or ammonia. The optimal trade-off has to be established in a more flexible manner. A logical approach is to implement a higher level of optimising control, with optimisation objectives that more directly reflect the actual plant objectives and that are not restricted to fixed trade-offs. This was the motivation for the scheme in Figure 2.4 and the proposal to adopt the integrated view discussed later in this chapter.

The second example is trade-off between economy and quality. There is considerable design freedom to trade-off between cost and quality between two extremes: one can maximise treatment under budget constraints or minimise cost with permit constraints. For example, von Sperling and Lumbers (1991) developed an optimisation system for oxidation ditches that could be set to optimise either operational costs or process performance. Between these two extremes, there is a continuous set of acceptable solutions that may well represent a more satisfactory solution than either of the extremes. This set can be found through formulation as a multi-objective problem and investigating the so-called trade-off surface (consisting of so-called Pareto optimal solutions) using the objective weights as design parameters.

A third trade-off example is between reliability and quality. As an illustration, the sludge concentration is considered. A high sludge concentration is advantageous for treatment performance. In addition, investment costs might be kept low if a high sludge concentration could be maintained. However, the sludge concentration is restricted by the clarification process, as this is hampered by too high concentrations. In practice therefore, operational constraints are placed onto the sludge concentration to ensure reliable operation. In this trade-off, system boundaries within the plant become important and there is a trade-off between different unit processes.

A final trade-off example, which addresses the choice of the system boundaries of the system with its environment, is the trade-off between sewer and wastewater treatment plant. In many

mixed sewer systems, during storm flow it is possible to trade-off between wastewater treatment plant loading and Combined Sewer Overflows. The maximum plant load is here mainly limited by clarifier capacity and too high loading may cause sludge loss leading to a deterioration of effluent quality. On the other hand, receiving water quality may be dramatically affected by CSO's. A transparent decision can only be made by trading-off between the two systems considering interactions.

2.6 An approach for goal formulation

This section presents a possible approach for goal formulation. Section 2.6.1 describes a rational goal formulation based on operating costs. Section 2.6.2 argues to approach the control system design problem as a mathematical optimisation problem. This makes design trade-offs transparent. Moreover, a possible methodology for an integrated approach oriented directly at water quality objectives is indicated.

2.6.1 Benchmark for control system performance evaluation

An objective goal formulation is required for control system evaluation and testing. To enable a more objective comparison of control system designs, both the Task Group on Respirometry of the IAWQ and the European COST Actions 682 and 624 developed a platform independent simulation benchmark (Vanrolleghem *et al*. 1996; Spanjers *et al*., 1997, 1998). The benchmark definition includes a plant layout, realistic influent patterns and a test protocol with an objective performance assessment through a concise goal formulation. These are briefly described here; a concise description is given in Alex *et al*. (1999a).

The performance assessment is done by considering two sets of criteria:

1. The set refers directly to plant performance in terms of financial costs, namely:
   - Costs of effluent quality, computed with load-averaged costs and constraints as follows:
     - Criterion function:

$$EQ = \frac{1}{t_e \cdot 1000} \int_{t=0}^{t_e} (w_{SS} SS(t) + w_{COD} COD(t) + w_{TKN} TKN(t) + w_{NO} S_{NO}(t) + w_{BOD} BOD_5(t)) \cdot Q_e dt$$

     with: t_e : end of influent pattern (see below)
     w_{---}: costs or weight on effluent quality parameters
     SS: suspended solids, TKN: Total Kjeldahl nitrogen
     Q_e : effluent flow rate.

     - Constraints on effluent quality, which are set to the flow-weighted average concentrations over three influent patterns:
       COD < 100 mg/l, BOD_5 < 10 mg/l, suspended solids < 30 mg/l,
       ammonia < 4 mg N/l, Total N < 18 mg N/l.
   - Costs of operation[12]
     - Sludge production (kg d^{-1})
     - Controller output variations (peak loads and variation indicative of mechanical weir)
     - Aeration energy (AE) and pumping energy (PE) (kWh d^{-1}).

No other operational constraints are given.

[12] No chemical addition including external carbon dosage for denitrification is considered in the benchmark and therefore costs of chemicals are not included in the performance assessment.

2. The second set of criteria refers to the local control loops, for which the IAE (Integral of Absolute Error) and ISE (Integral of Squared Error) are computed.

Three two-week influent patterns are applied (disturbance signals), with typical diurnal variations and a load decrease during weekend. The second file has a sustained rain event in the second week, the third file has two storm events, which are shorter but more intense than the rain event. The temperature is 15 ºC. It is noted that no test on temperature variation is included.

The plant configuration consists of a predenitrification plant with 5 ideally mixed compartments, and a clarifier modelled with 10 layers. The models used are ASM1 for the biological processes and Takács double-exponential model (Takács, 1991) for the clarifier.

The test protocol includes open-loop and closed-loop simulations. In the basic configurations, two local control loops are defined: setpoint control on DO in last compartment and nitrate setpoint control in second (anoxic) compartment.

Thus the benchmark goal is a combination of cost optimisation and quality optimisation, where the levies are used as weight factors on quality parameters.

Recently, the benchmark was used to test two biomass loading control strategies (Debusscher *et al*., 1999). This test showed that when all relevant effluent quality parameters and overall costs are considered, none of the proposed strategies led to an improvement. This result confirmed the importance of overall performance assessment. Interestingly, also the lack of proper controller tuning procedures was indicated.

In addition to the criteria described above, other evaluation tools are considered within COST Action 624, such as (microbial) risk assessment and LCA (Life-Cycle Assessment). One can argue if this is important for control or rather for Decision Support in treatment system design.

Effluent costs are relatively ad-hoc and are politically determined weight factors as described in Section 2.1. They can be used in micro-economic approach (plant operation), but for planning on a larger national, macro-economic scale, a more rational approach is required. A rational alternative for using costs to weight different objectives would be to apply an integrated approach as discussed in the next subsection.

2.6.2 Defining goals and constraints and trade-offs

This section departs from the following working definition of the qualitative plant goal for wastewater treatment plant operation to show that goals can best be expressed as a multi-criterion optimisation problem:

‘Maintain reliable effluent quality despite disturbances against reasonable costs’.

This definition reflects the plant goal definitions employed by Olsson and Jeppsson (1994) (‘Satisfy effluent requirements consistently and minimise costs while maintaining water quality’) and Spanjers *et al*. (1998) (‘Keep the plant running, while meeting the effluent standards and minimising costs’), with the adjustment that in this definition ‘reasonable cost’ replaces ‘minimal costs’, for reasons that will become clear below.

The definition encompasses three aspects of plant operation, which are:

1. Reliability - the plant must be kept running, and process upsets such as sludge washout or loss of biological activity must be avoided;
2. Quality – the legal permits and eventually plant-specific effluent quality objectives must be met;
3. Economy - the costs to achieve reliability and quality should be kept low.

These aspects can be assigned a priority ranking with in the order of decreasing importance: reliability, quality, and economy. This is because aiming at quality makes sense only if the plant is running properly and economic optimisation only makes sense if the quality specs are met.

In the definition however, it is not obvious what is the goal, and what are constraints. To arrive at an analytic design procedure based on mathematical optimisation, several optimisation problems might be formulated to quantify or specify the qualitative plant goals into quantitative operational goals and constraints, for example the following:

P.1: min cost
subject to constraints on reliability and quality

P.2: max quality
subject to constraints on reliability and cost

P.3: max reliability[13]
subject to constraints on quality and cost

This ambiguity in problem specification illustrates that it is rather artificial here to distinguish between goals and constraints. Consequently, one might as well formulate the problem as a multi-criterion optimisation problem, for example with a weighted-sum objective P.4.

P.4: min $\{w_{rel} \cdot -\text{reliability} + w_{quality} \cdot -\text{quality} + w_{cost} \cdot \text{cost}\}$
subject to hard constraints

with the weight factors $w_{...}$ to account for relative importance of the different aspects, and the minus-signs on reliability and quality to define maximisation[14].

Several factors complicate translation of operational objectives into quantitative design specifications formulated as a mathematical optimisation problem.

A first difficulty is that selection of weights $w_{...}$ is not straightforward. One main cause is that it is not so easy to use overall financial cost as an indicator of process performance in municipal wastewater treatment. This is more logical for production processes in profit organisations, where it is rational to express objectives in term of financial cost and aim at profit maximisation (although also here many indirect costs may be difficult to express accurately). In wastewater treatment, this is less straightforward. This is partly caused by the fact that regularly plant goals are kept lower than legal permits to ensure reliable operation (which is an implicit trade-off),

[13] Reliability is more difficult to quantify. Often it is expressed qualitatively, e.g. ‘prevent sludge bulking’ or ‘prevent sludge loss from the clarifier’. It is argued below that, typically, operational constraints are introduced to ensure reliability. These can then be used to quantify reliability. Of course, this is somewhat artificial.

[14] min -a = max a

partly by the fact that (in The Netherlands) municipal wastewater treatment is (still) a non-profit operation.

The weights can therefore be used in control system design as design parameters to trade-off between different performance specifications.

A second problem is that limited knowledge and model complexity necessitate a pragmatic approach through the introduction of artificial operational constraints. In principle, P.1 – P.4 might be formulated as overall optimisation problems expressing the actual operational goals (including reliability), without unnecessary artificial constraints on the system states and with only hard constraints on the decision variables (especially the manipulated variables). Optimal state trajectories (corresponding to optimal process conditions) might then be computed via dynamic optimisation using mathematical models of all phenomena relevant for reliability, quality and economy. This might be implemented either on-line or off-line, in the latter case with on-line feedback control to ensure realisation of the optimal trajectories. However, current knowledge is too limited for such an approach, because not all cause-effect relationships and interactions are sufficiently well-known, such as, for example, the relationship between aeration intensity and sludge sedimentation behaviour. On the other hand, several existing models are too complex for dynamic optimisation and control. To circumvent these problems, the operational problem is in general drastically simplified by putting operational constraints on several process variables. It has been observed that often such constraints are mixed up with the actual operational objectives (Olsson and Jeppsson, 1994).

A third problem is that not all variables that correspond to the actual plant objectives can be measured on-line, and consequently a selection of suitable measured variables must be made. This is treated in more depth in Chapter 5.

Finally, an issue of a more technical nature is that it is sometimes necessary to circumvent hard constraints, especially with respect to state variables. This so-called constraint softening is usually achieved through adding terms to the sum-weighted objective with appropriate weighting factors.

Thus, control system design for wastewater treatment plants can be approached as a multi-criterion optimisation problem. Weights of the different objectives and eventually constraints can be used as design parameters to trade-off between different objectives.

It is noted that multi-criterion optimisation requires user interaction. Therefore, it typically is performed off-line, where it allows a transparent trade-off in the controller design to choose weights in a criterion function to be applied in on-line control.

Summarising, minimisation of total operating costs of the plant can be used as a starting point in control goal definition, where the trade-offs with reliability and quality can be transparently assessed by multi-criteria optimisation.

In the benchmark and in the discussion until now, the system boundaries have been drawn around the treatment plant. However, while minimisation of treatment plant operating costs may be rational from a micro-economic viewpoint, from a macro-economic viewpoint it is less attractive. This is because current legislation is technology oriented, segmented and neglects total impacts from the wastewater system and consequently leads to suboptimal usage of the wastewater system (sewer-treatment plant- receiving water), as was argued in Sections 2.4.4

and 2.4.5. The suggested procedures for integrated modelling can *mutatis mutandis* be translated to integrated control as follows. For receiving waters, generally a limited set of objectives can be selected. Such a limited set of water quality objectives constitutes a good starting point for a multi-criterion objective function for integrated control. For implementation of this integrated control, on-line optimisation using nonlinear Model Predictive Control is a conceptually appealing method. Application of artificial, fixed setpoints or weight factors can then be abandoned. Application of simple, goal oriented models and decomposition into timescales may further reduce required model and computational complexity. However, it remains to be investigated how large the performance improvements of such a model-based control approach would be when compared to heuristic approaches, such as rule based control. Especially important in implementation will be the impact of model uncertainty on control system stability and performance, which has until now been hardly addressed at in the studies in integrated control.

2.7 Conclusions

An inventory of control goals in the literature reveals that insufficient insight exists in the relationship between legislation and control goals for wastewater treatment plants. A heuristic controller design approach is typically adopted, employing indirect and vague control goals that lead to time-consuming trial-and-error design procedures and that complicate judgement of particular controller designs.

The availability of advanced modelling and control techniques argues to develop a straightforward, optimisation-based controller design procedure to close the gap between legislation and controller specifications, instead of a heuristic approach. In such a so-called analytic design procedure, the control system design problem is formulated as a mathematical optimisation problem, where all plant objectives and constraints are explicitly formulated in a quantitative way. Trade-offs can then be made explicit during design through mathematical optimisation and cumbersome trial-and-error and artificial objectives can be avoided. Such an analytic design procedure requires reliable mathematical models of goals, disturbances and the plant and their uncertainties.

This chapter dealt with modelling of goals, thus focusing on which goals are to be achieved rather than on how the goals can be achieved. One possibility was discussed, namely to define the control goal as a minimisation problem of operating costs for the plant as a whole, treating quality and reliability as constraints. The operating costs should include costs of effluent disposal as imposed by national legislation, costs of energy consumption, costs of consumption of chemicals and sludge disposal costs.

A multi-criterion optimisation formulation that includes cost, quality and reliability as objectives is a more suitable paradigm for realistic definition of control goals than cost minimisation. Trade-off between different conflicting objectives is crucial, which can be done more transparently via multi-criterion optimisation than with single-criterion optimisation.

Considering the treatment plant alone may lead to suboptimal solutions. This can be avoided in an integrated approach that aims directly at water quality objectives for the receiving water and considers joint operation of sewer system and treatment plant. A possible methodology for such an integrated control approach was indicated

Different aspects of the ‘how’ to achieve the formulated goals are topic of the subsequent chapters that contribute to developing an analytic design procedure for control of activated sludge plants. The results in Chapter 5 show that aiming at economic operation and abandoning

setpoint control results in operation over a larger range, and consequently requires nonlinear control. While the analytic design procedure is relatively well developed for linear controller design, for nonlinear control this is not the case. Consequently, an analytic procedure cannot directly be applied and both control methods and models need development.

Chapter 5 will investigate development of control methods and will concentrate on how to deal with optimisation under model uncertainty and with the controller design methods currently available. Model Predictive Control is studied as a model-based control method to carry out on-line optimisation of activated sludge plants. The cost function approach that was suggested in this chapter is however not applied yet, as this needs further development. Instead, linear MPC employing different control goals is applied to study applicability of the method to activated sludge plants. Robustness against model uncertainty is also studied.

Chapter 3 treats physical, mechanistic modelling of activated sludge plants. Mechanistic models are important especially for control system evaluation, where the control system is typically tested under several conditions. For control system design for specific plants, the model must reliably reflect real plant behaviour. The larger operational range due to economic operation imposes stronger requirements with respect to model validity than operating with fixed setpoints. Model identification therefore deserves considerable attention and this topic is studied in Chapter 3.

Chapter 4 deals with models for controller design or as internal model in model based control, focusing on nonlinear models for application in nonlinear control. The mechanistic models based on Activated Sludge Model No. 1 studied in Chapter 3 are not directly suited for control. If these mechanistic models accurately describe the process dynamics, however, reduced models can be extracted for controller design thus re-using the knowledge in the mechanistic models. Chapter 4 especially studies nonlinear model reduction through separation into different timescales with the technique of singular perturbation. For application of this technique, the model must be in the so-called standard form, which means that it can be separated into slow and fast states. A methodology to make this separation is developed, because existing methods are insufficiently straightforward. A relatively simple model is used to test this methodology. Application of the technique to ASM1, however, was beyond the scope of this thesis.

Chapter 3 Modelling, model calibration and identifiability

Once more, he looked at his monitor with simulation results, which were obtained with another set of parameter values. The consultant had now already been working several days on calibration of the main activated sludge plant of the Southern Wastewater Board. Different combinations of parameter values gave similar results in the effluent concentrations. Which parameters should he use for calibration? He still was not certain how much confidence he could place on the calibrated values for the rate constants and the affinity constants. Moreover, he asked himself 'How reliable are the simulations with the calibrated model with the different test scenarios?'

This chapter concentrates on mechanistic modelling of activated sludge plants for control system evaluation. Section 3.1 introduces reactor model-building, model calibration and the issue of model identifiability. Section 3.2 gives a state-of-art assessment in model-building, model calibration and model identifiability of activated sludge plants and ASM1. This provides the motivation for the research described in the Sections 3.3 - 3.5. These sections consider different aspects of model calibration including identifiability and influent characterisation.

3.1 Introduction

The availability of activated sludge models has greatly stimulated research in dynamics and control of the activated sludge process. The availability of these mathematical models argues to apply an analytic design procedure for control system design, as was discussed in Chapter 2. The different design stages of the procedure, e.g. the controller design stage and the control system evaluation stage, require plant models of different complexity. This chapter focuses on modelling of activated sludge plants for control system evaluation.

In control system evaluation, mechanistic nonlinear models of high order are usually applied to test the control system under several conditions. The mechanistic model should reliably reflect real plant behaviour under these conditions. Achieving this takes two steps. First, a model must be built that adequately captures the relevant process characteristics for the intended purpose, which is here to simulate plant behaviour under the different test conditions[15]. Secondly, the model must be accurately calibrated to the real plant. While the emphasis in this chapter is on calibration, and, more specifically, of ASM1 parameters, both steps are discussed in this chapter. This is done to provide, through an overview of modelling methodology, a correct perspective of the role of ASM1 in plant modelling, which is desired for adequate plant model calibration and subsequent application of the model.

The focus is on the bioreactor part of activated sludge plants. Modelling methodology of bioreactors is summarised as far as relevant for activated sludge modelling. Figure 3.1 gives an overview of modelling of bioreactors and outlines where the different issues are discussed.

The basis for reactor modelling is constituted by conservation laws and transport phenomena on one hand and chemical thermodynamics and reaction kinetics on the other hand (Figure 3.1). A reactor model is a mathematical, macroscopic model describing the overall behaviour of the reactor, the so-called macro-kinetics. Central in modelling is the use of balance equations.

[15] In fact, this is the reason that usually mechanistic models are preferred over black-box models, as they are better suited for extrapolation.

Balances can be written for extensive variables. In homogeneous systems, no concentration gradients occur. In that case, in mathematical form the balance equation for an extensive property E with intensive quantity e over a reactor can be written as follows:

$$\frac{deV}{dt} = F_{in,E} - F_{out,E} + r_E V \tag{3.1}$$

In (3.1), r_E is the volumetric reaction rate, the so-called micro-kinetics, V the reactor volume, $F_{in,E}$ and $F_{out,E}$ are the transport terms into respectively out of the reactor.

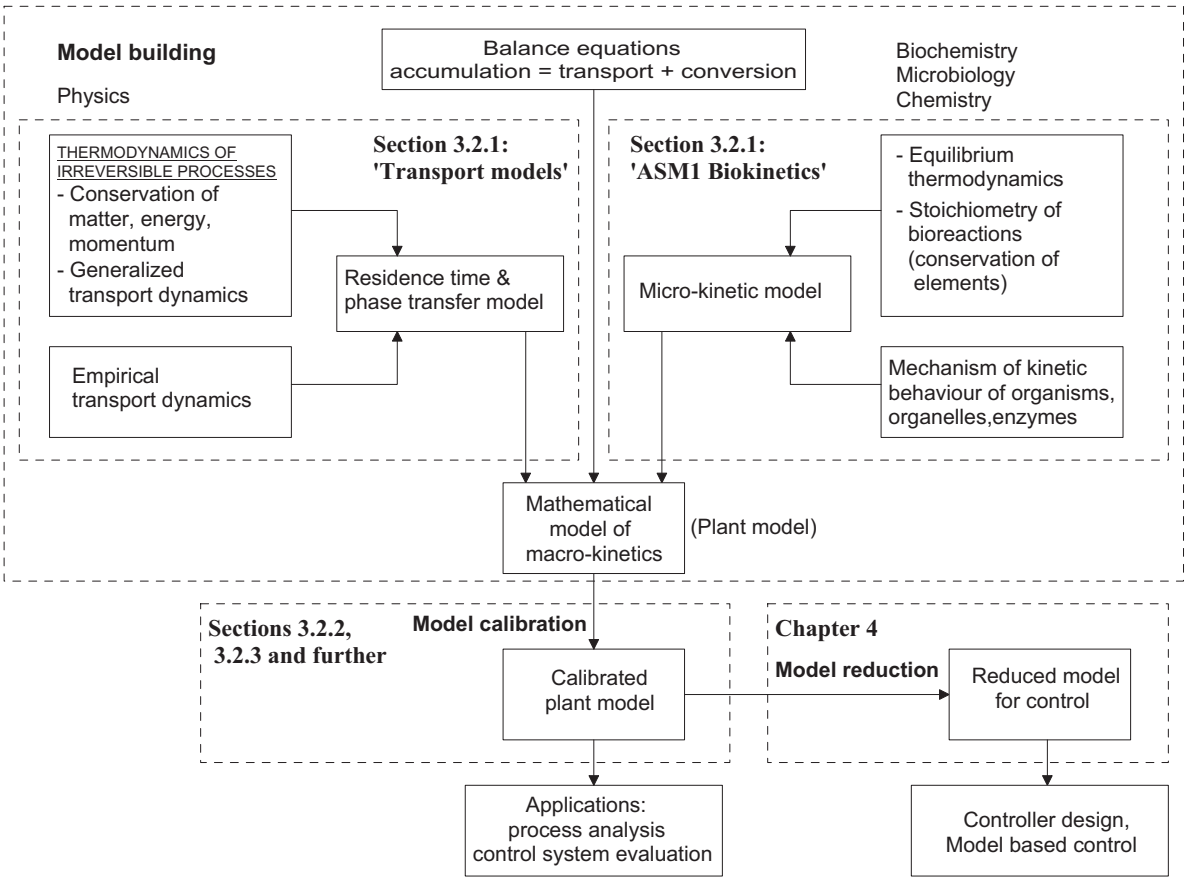


Figure 3.1: Bioreactor modelling consists of model-building (Roels, 1983) and model identification or calibration.

In non-homogeneous systems, transport within the reactor and place-dependency of the reaction rate r_E must be taken into account, which is expressed in the following balance equation:

$$\frac{d}{dt}\int_V edV = F_{in,E} - F_{out,E} + \int_V r_E dV \tag{3.2}$$

In practice, systems are often non-homogeneous, because of gradients through non-perfect mixing and existence of multiple phases. Consequently, for reactor modelling both micro-kinetic models (r_E in Eq. 3.2) as well as models for internal transport (describing place dependency) are important. In the sequel, the latter will be referred to as transport-physical models. Section 3.2.1 will describe modelling of the micro-kinetics and transport-physical

modelling for activated sludge plants. The discussion of micro-kinetics will focus on Activated Sludge Model No. 1 (ASM1) that is the state-of-art model for the micro-(bio)kinetics of activated sludge processes.

The plant model thus built must be accurately calibrated to the real plant if the model is used for control system evaluation for a particular plant. Accurate calibration is important also for other model applications such as process analysis, to decide whether and how operation must be improved. Moreover, if the mechanistic model accurately describes the real process dynamics, reduced models can be extracted for controller design thus re-using the knowledge in the mechanistic models (see Figure 3.1; model reduction for control is treated in Chapter 4).

From the introduction on reactor modelling above, it is clear that plant model calibration[16] must include calibration of transport-physical models as well as calibration of ASM1 model parameters. Calibration is a nontrivial task, in which one has to decide on the selection of parameters to be used in calibration and on the design of experiments required for their determination. Section 3.2.2 discusses state-of-art of model calibration of activated sludge plants, which shows that, while considerable efforts have been put into calibration of ASM1 parameters, calibration still needs further development.

An important issue in model tuning is identifiability of the model parameters. A correct calibration should enable physical interpretation of the calibrated parameters and allow prediction with the model beyond the experimental conditions of calibration. This is only possible if the model parameters can be uniquely determined from the available data, that is, if the model is identifiable. Thus, the identifiability properties of applied models determine the success or failure of calibration. Consequently, understanding of the model's identifiability is essential for analysing and developing calibration procedures. Section 3.2.3 discusses identifiability in model calibration of activated sludge plants. In the subsequent sections, identifiability is investigated further, to increase insight in the identifiability of plant models that are based on ASM1 to guide development of calibration strategies.

The chapter is set up as follows. Section 3.2 describes state-of-art in modelling, calibration and identifiability of activated sludge plants with emphasis on ASM1. Section 3.3 investigates local identifiability of the model's biological parameters from input/output data. Section 3.4 applies a randomised approach to study its global identifiability properties. The studies show that additional information is required to input/output data, e.g. in the form of lab-scale experiments. Therefore, one such lab-scale test is studied in Section 3.5. Section 3.6 summarises the main results in the form of concluding remarks.

3.2 State-of-art

3.2.1 Model-building of activated sludge plants

ASM1 Biokinetics

In 1986, the Task Group on Mathematical modelling of Activated Sludge Processes published Activated Sludge Model No. 1. This model represented a consensus concerning the simplest model with the capability of realistic predictions of single sludge systems carrying out oxidation

[16] The plant model consists of a micro-kinetic model (ASM1) and a transport physical model. Both the transport-model and ASM1 parameters need calibration to calibrate the plant model. In the literature and in this thesis, the term 'ASM1 model calibration' is used not only to refer to calibration of the ASM1 biokinetic model, but also to calibration of plant models based on ASM1 by calibrating ASM1 parameters in these models.

of carbonaceous material, nitrification and denitrification. In the development of the model, primary consideration was given to prediction of activated sludge concentrations during selection of process stoichiometry and to estimation of electron acceptor requirements during development of process rate expressions.

This model defines components, stoichiometry and kinetics of activated sludge processes, which are briefly described in this section. The equations are given in Appendix A. For more details is referred to (Henze *et al.*, 1987 and 1987a; Dold and Marais, 1986).

In ASM1, 13 components are defined, which are given in Table 3.1. Some of these components (S_{NH}, S_{NO}, S_O and S_{ALK}) correspond to existing chemical species that can be measured directly. The other components are conceptual and cannot be measured directly. Most important is the COD fractionation. A distinction is made between biodegradable COD and inert COD. Inert COD consists of soluble (S_I) and suspended inert COD (X_I), including inert products from biomass decay (X_P) (see below). Biodegradable COD consists of the other four COD fractions. Rapidly biodegradable COD, S_S, is supposed to be the substrate for growth of heterotrophic biomass X_{BH}; this biomass carries out carbon oxidation (Eq.1.1) and denitrification (Eq. 1.3). Slowly biodegradable COD cannot be directly consumed. The autotrophic biomass X_{BA} carries out nitrification (Eq. 1.2).

Table 3.1: Overview of components in ASM1 ($S_{...}$: soluble, $X_{...}$: suspended components)

Organic (COD)
soluble inert S_I
suspended inert X_I
suspended inert products X_P
readily biodegradable substrate S_S
slowly biodegradable substrate X_S
heterotrophic biomass X_{BH}
autotrophic biomass X_{BA}

Nitrogen (N)
ammonia S_{NH}
nitrate S_{NO}
soluble organic nitrogen S_{ND}
suspended organic nitrogen X_{ND}

Other
oxygen S_O
alkalinity S_{ALK}

The model distinguishes 8 processes. These are 1) aerobic growth, 2) anoxic growth and 3) decay of heterotrophic biomass, 4) growth and 5) decay of autotrophic biomass, 6) hydrolysis of X_S to S_S, 7) hydrolysis of X_{ND} to S_{ND} and 8) ammonification of S_{ND} to S_{NH}.

The model includes a so-called death-regeneration concept, which supposes that biomass decay produces slowly biodegradable X_S (and inert products X_P), which is subsequently regenerated through hydrolysis to S_S, which can serve for new biomass growth. While decay is a well-accepted concept in biotechnology, regeneration is not. Consequently, the decay rate in ASM1 has a physical interpretation different from the traditional decay rate.

Stoichiometric model parameters are the heterotrophic yield Y_H, autotrophic yield Y_A, N-content of biomass i_{XB} and inert products i_{XP} and the fraction of biomass yielding inert products, f_p. For most processes, Monod kinetics are applied. Appendix A and the symbols list contain a complete list of the parameters. Here we mention the following. Heterotrophic parameters are the maximal growth rate μ_H, decay rate b_H, affinity constants for S_S K_S, for S_O K_{OH}, for S_{NH} K_{NHH}, for S_{ALK} K_{ALKH} and a correction factor for anoxic growth η_g. Autotrophic parameters are the maximal growth rate μ_A, decay rate b_A, affinity constants for S_O K_{OA}, for S_{NH} K_{NHA}, for S_{NO} K_{NO}, for S_{ALK} K_{ALKA}. Hydrolysis parameters are the hydrolysis rate k_h and affinity constant K_x and a correction factor for anoxic hydrolysis η_h. Ammonification

parameters are the rate k_a. For several parameters, usually also a temperature dependency is included (Gujer, 1985).

The model contains some serious simplifications of reality. Important simplifications are the following: 1) The influent consists of thousands of chemical components, which are lumped into only a few hypothetical groups. 2) Rapidly biodegradable COD is supposed to be soluble, which is not necessarily the case. 3) Many micro-organism species are present that degrade COD and that constitute an ecological system of enormous complexity. These are lumped into one biomass species X_{BH}. 4) The heterotrophic biomass is modelled as unstructured biomass. It is known that such unstructured models may exhibit bad predictions in highly dynamic environments as they do not take into account changes in biomass composition (Roels, 1983). This is probably partly compensated for with the death-regeneration concept)[17]. 5) The biomass grows in flocs with concentration gradients because of diffusion limitation; this may cause simultaneous denitrification in the flocs while the solution is aerobic.

Because of the underlying simplifications, the model parameters are macroscopic parameters into which many processes are lumped, which has to be kept in mind in the physical interpretation of model parameters. Thus, the model can be regarded as a mechanistic, white model when compared to completely black-box models such as artificial neural nets. When compared to the complexity of reality of the biological and biochemical processes, however, one would rather still call it a black-box model.

Transport models

If the mixing timescale in a reactor is not much smaller than the reaction timescales, mixing is not perfect and gradients occur, which affect the macro-kinetics. In large-scale reactors, it is generally difficult to obtain perfect mixing. While in aerobic bioprocesses and in activated sludge systems reactions are relatively slow, still, however, typically gradients occur in the dissolved oxygen concentration. Moreover, in many activated sludge plants one intentionally aims at creating a plug-flow like behaviour to obtain higher reactor efficiency. Consequently, gradients must often be accounted for in activated sludge modelling.

One might try to solve Eq. (3.2) through integration of microscopic balances, including micro-impulse balances. However, this would be a tedious task on one hand while the level of detail is not required for macroscopic modelling on the other hand. Common practice to model mixing instead is to build so-called *combined models* (Himmelblau and Bischoff, 1968) with idealised model reactors as building blocks with flow streams between one another. The most frequently used building blocks are the Continuous Stirred Tank Reactor (CSTR), the plug-flow reactor, the tanks (CTRSs) in series and plug-flow with diffusion (Himmelblau and Bischoff, 1968; Levenspiel, 1972).

In activated sludge modelling, mostly CSTR or CSTR in series are applied as building blocks. In models for control design, often only one CSTR is used. Carrousel systems are usually modelled as CSTRs in series (e.g. van Rooij *et al*., 1993, van der Kuij *et al*., 1993), although also plug-flow, or plug-flow with dispersion (Stamou *et al*., 1999) or other combined models are used occasionally. For example, Cook (1984) applied a CSTR combined with plug-flow. More complicated flow patterns such as shortcuts and backflow occur in practice, that can have

[17] In the successor of ASM1, ASM3 (Gujer *et al*., 1998), the death-regeneration concept has been abandoned. Instead, storage products in the cell are now modelled thus constituting a structured biomass model.

a large influence on reactor performance, as was illustrated already by Ottengraf (1971) for a full-scale plant.

Transfer between phases such as oxygen transfer modelling is not considered here and we refer to standard textbooks (Metcalf & Eddy, 1991) and papers (van 't Riet, 1983; Kissel, 1986).

3.2.2 Calibration of activated sludge plants

Introduction

For simulation of activated sludge plants with ASM1 based models, data are needed of the micro-kinetic model and the transport-physical model. The following data are required:

Micro-kinetic model:
- Model components: influent characterisation of the COD and nitrogen fractions distinguished in the model (in this thesis, component fractions are viewed as parameters);
- Model (biological) parameters: kinetic and stoichiometric parameters;
- Initial conditions (for dynamic simulation).

Transport-physical model:
- Reactor design data, such as reactor volumes and pump capacities;
- Operational data (averaged for static simulation, as a function of time for dynamic simulation): influent flow and concentrations, other (internal) flows and loads, temperature and aeration intensity;
- Mixing model.

In calibration of models that are based on ASM1, values for these data are chosen or determined from experiments for the plant to be modelled. This is not a trivial task. In the first place, several important ASM1 model components are conceptual quantities that cannot be directly measured. Consequently, COD characterisation is difficult and not all the initial conditions can be directly measured. Secondly, the number of biological parameters is large (approximately 20) and one has to decide which parameters must be determined and one must design experiments that provide information to identify these parameters. Thirdly, it takes effort to obtain accurately all operational data such as flows. Finally, an adequate mixing model must be developed. Many research efforts have therefore been put into developing calibration strategies for calibrating ASM1 based models, which are discussed below.

ASM1 biokinetics calibration

After the publication of ASM1, in the literature initially much emphasis has been placed on determination of biological parameters and of influent COD fractions. Some of the ASM1 model parameters appeared to be relatively constant for different system configurations and wastewaters and can be assumed known and constant. Other parameters however show a stronger dependency upon the plant and wastewater and their values must be fit to the plant and the conditions in the plant.

Several strategies to determine ASM1 parameters have been proposed, which differ in selection of experiments, of measurements and of parameters to be determined. The most important are the Task Group proposal, calibration based on full-scale input/output data and calibration using respirometry and dedicated experiments. These strategies are discussed here.

Finally, some remarks with respect to determination of initial conditions and estimation algorithms are made.

Summary Task Group proposal

In its report, the Task Group proposed a provisory procedure for calibration of the model COD fractions and biological parameters. This procedure included 6 CSTR experiments (for S_S, X_I, μ_A, μ_H, K_S, k_h, K_X and k_a), 5 batch tests (for S_I, Y_H, b_H, η_g and η_h) and 1 fed-batch test (K_{NH}). For application to full-scale plants, this procedure is too laborious and expensive. Moreover, no fit is made to the full-scale plant input/output behaviour, so accurate simulation of full-scale behaviour is not guaranteed.

Full scale input/output data

Several strategies have been used to calibrate the model to input/output behaviour of full-scale plants. In view of the macroscopic meaning of the model parameters, it is necessary to use at least some model parameters as lump parameters of the macroscopic behaviour of the process. This can be done by fitting the model to the observed overall plant behaviour. It can not be expected that correct predictions of the full-scale behaviour can be extrapolated from parameters determined on laboratory or pilot scale alone, unless the transport-physical model is perfect. Even with perfect transport-physical models, the transfer of parameters determined on lab-scale to full-scale can be problematic. This will be discussed below, under respirometry.

In this full-scale calibration, decisions have to be made with regard to experiment duration, sampling frequency, choice of measurements, outputs to be fitted, parameters to be determined and fitting procedure to be used. One approach is steady-state calibration. In steady-state calibration, data obtained from the plant are averaged under the assumption that this average represents a steady-state. This approach is regularly applied, for example, two full-scale plants were calibrated this way (Lesouef *et al*., 1992). Shortcomings of steady-state calibration are the following. If the input variations are faster than the process dynamics, which is usually the case, then the process does not operate in steady-state. When fitting with averaged data one attempts to fit a steady-state of the model to an unsteady plant, this may result in biased parameter estimates. Because the system is nonlinear, averaging can also introduce bias. Another disadvantage of steady-state calibration is that the number of parameters that can be estimated is equal to or smaller than the number of outputs.

Better results can be obtained by fitting the dynamic behaviour of the process. Dynamic data contain more information than static data and in principle, the number of parameters that can be determined is larger than the number of outputs. For many plants, routinely collected data is available. It is therefore tempting to use historical data for dynamic calibration. The achievable accuracy is limited however, due to low sampling frequency, which is typically once per week. Because of the resulting uncertainty in the influent load and the limited number and frequency of outputs to be fitted, calibration in this way was reported to be unsatisfactory (Witteborg *et al*., 1994, Weijers *et al*., 1994).

Special monitoring exercises are required for accurate modelling. The experiment duration and sampling frequency must be chosen in relation to the time constants of the process and the frequency spectrum of influent variations. An important time constant of the process is the hydraulic residence time, which is typically several hours to half a day. Experiment duration must therefore be at least in the order of days. Several calibrations of the IAWQ Model on full-scale plants have been reported. The experiment duration and the sampling frequency chosen range from 6 h to 10 days and 0.3 to 3 per hour respectively.

A crucial decision is which outputs are to be fitted and which parameters are to be determined. Table 3.2 summarises different choices for parameters and outputs.

If the recommendations of the Task Group (Henze *et al.* (1987)) are combined with the parameters used in full scale calibration experiments in Table 3.2, the following set of parameters is obtained: μ_H, K_S, K_{OH}, μ_A, b_A, K_{NHA}, K_{OA}, η_g, k_h and (S_S+X_S). Jeppsson (1993) reported the following parameters to be important: μ_H, b_H, μ_A, k_h, K_X, η_h.

Table 3.2: Calibration based on input/output measurements at full-scale plants: selection of parameters and outputs reported in the literature (parameters tuned manually)

Parameters tuned from	Outputs	Reference
μ_H, k_h/K_X, K_S μ_A, K_{NHA} S_I	OUR profile effluent NH_4 and NO_3 effluent COD (0.9)	Siegrist and Tschui (1992) (Three plants)
μ_A, K_S and η_g	effluent NH_4 and NO_3	Pedersen and Sinkjær (1992)
μ_H, K_S, μ_A, S_S+X_S k_h	effluent NH_4 and NO_3 effluent NO_3	Pedersen and Sinkjær (1992)
Aerated volume, K_{OH}, K_{OA} COD fractions	effluent NH_4 and NO_3 influent COD and BOD	Weijers *et al*. (1994) (Two carrousels)
μ_H, K_S, μ_A	not described	Stokes *et al*. (1993)
K_S μ_A b_A η_g	not described batch test earlier experience not described	Dupont and Sinkjær (1994)

Between these lists, there is a discrepancy. One possible reason for this discrepancy is that for different plants and experiments different parameters are important. Another reason is that the model is not (well) identifiable, so that different combinations of parameter values give (almost) identical model behaviour. One solution might be to estimate all the parameters from these sets or even all the model parameters. The data must however contain enough information to make all the parameters identifiable, which is often not the case. As an alternative, a subset of parameters can be selected. The number of possible parameter subsets is huge however, which motivates application of systematic methods for the selection. In Sections 3.3 and 3.4, a procedure for such a selection is described.

An example of a study where a subset of parameters was fitted, with a parameter estimation procedure, is Kabouris and Georgakakos (1996a, b), who developed an extended Kalman filter for parameter and state estimation of ASM1. No denitrification was considered in this study. Moreover, a small sampling time (of 5 minutes) and availability of relatively many on-line measurements were supposed (total and soluble COD, total and soluble N_{KJ}, ammonia and nitrate and OUR). In a case study, it was tried to estimate nine of the ASM1 parameters, assuming constant influent flowrate. This was unsuccessful because of identifiability problems, especially of hydrolysis parameters k_h and K_X and of nitrification parameters μ_a and K_{NH}. To circumvent these problems, it was suggested to apply a sequential estimation procedure, by first estimating a subset of only seven parameters (fixing K_X and K_{NH}) and then estimating only two parameters K_X and K_{NH}, while fixing the other parameters. While such a sequential estimation approach circumvents convergence problems in the parameter estimation, it does of course not solve the identifiability problems that result from poor identifiability and consequently will likely yield biased parameter values. This study again motivates the need for methods to select

subsets of identifiable paramters. Parameters that are not estimated from full-scale data can be determined from additional experiments, such as respirometry, which is discussed below.

Respirometry and other dedicated experiments

Measurements on full-scale plants are relatively time-consuming and expensive, and do not provide sufficient information to estimate all relevant parameters due to insufficient excitation. As an alternative, special experiments can be used in addition to full-scale measurements. Very valuable in this respect is respirometry. In respirometry, the oxygen uptake rate (OUR) is measured, often as a function of time, in a sludge-wastewater mixture. Experimental conditions can be chosen such that measured OUR profiles are informative for determination of specific parameters. The measured OUR can be used directly or fitted by parameter estimation to (reduced models of) ASM1. The last approach is to be preferred because parameter values thus obtained have a direct significance for use in the model. When estimating parameters from measured respirograms, however, identifiability problems become manifest as will be discussed in Section 3.2.3.

Several respirometric batch experiments for determination of COD fractions and some of the biological parameters were proposed by Kappeler and Gujer (1992), one with wastewater sludge in a ratio of approximately 2:1 (test A), one with wastewater alone (test B). At present, automated respirometers are available (Vanrolleghem, 1994; Spanjers, 1993). These have been employed to identify ASM1 COD fractions and/or biological parameters using several experiments (e.g. Spanjers and Vanrolleghem, 1995; Witteborg *et al.*, 1996). A concise overview by Vanrolleghem *et al*. (1999a) is referred to for more details on respirometry in ASM1 calibration.

Batch experiments based on the ammonia uptake rate have been used to determine autotrophic growth and decay rate (Kristensen *et al*., 1992).

Besides respiration experiments, batch experiments based on determination of filtered and degradable COD fractions by COD balances have been proposed (Lesouef *et al.*, 1992). This kind of tests has a less direct relationship with the model, however (Spanjers and Vanrolleghem, 1995) and was found to be sensitive to measurement errors and insufficiently reproducible (Weijers *et al*., 1994).

While application of lab-scale experiments is invaluable, the transfer of lab-scale experiments to a model for a full-scale plant must be done with care. Two main reasons for possible problems are differences in experimental conditions between lab-scale and full-scale on one hand and differences in the models used on the other hand (Vanrolleghem *et al*, 1999a).

A list of possibly disturbing factors in experimental conditions in respirometry is the following: addition of ATU, transport limitation in the flocs, DO probe dynamics, difference in feed patterns and concentration profiles, difference in sludge history and differences in environmental conditions such as pH, temperature and mixing (Vanrolleghem *et al*., 1999a). Some of these are now briefly discussed.

Addition of allylthiourea (ATU) to inhibit nitrification is reported to disturb heterotrophic growth. However, Spanjers and Vanrolleghem (1995) demonstrated that avoidance of ATU addition through a model-based elimination of nitrification led to similar results, so the effect is probably limited.

Vanrolleghem *et al*. (1998) studied the cause of observed lags in respirograms. The observed lag could not be explained by poor mixing, diffusion limitation of dissolved oxygen or substrate in the floc or sensor dynamics. The sludge history seemed to be the cause of the lag, which disappeared after several acetate pulses. These pulses thus seemed to induce acetate

metabolism, which had decreased after a period of endogenous respiration. In addition, a long-term batch experiment was carried out. This showed that sludge characteristics change if the conditions in the test differ from normal full-scale operation.

One of the most important factors in the design of lab-scale batch tests is the ratio of initial substrate and initial biomass, S/X. At too low S/X, the response may be too short or too low; at too high S/X, the experiment may take too long. More importantly, the ratio may affect the sludge characteristics (Vanrolleghem *et al*, 1999a).

Another cause of possible errors in interpretation of batch tests is that the biomass in the test is not (necessarily) the same as the sludge from the plant. Therefore, one has to be careful to transfer model parameters based on wastewater only to the plant. An example is given by the tests proposed by Kappeler and Gujer (1992), that are discussed in Section 3.2.3.

Differences in model between full-scale and lab-scale occur if simple models are used for direct interpretation of respirograms. Here, the obtained parameter values must be carefully translated to the correct ASM1 parameters value. Another cause of possibly erroneous results, reported by van Niekerk *et al*. (1987), is if first order kinetics is used to describe a sum of zero order decays. Translation of a first order decay rate to full-scale then leads to overdesign. This is not likely to occur in ASM1 calibration, as this utilises Monod-kinetics with relatively low affinity constants, and thus corresponds mostly to zero order kinetics.

Concluding, translation of parameters obtained from lab-scale experiments has to be done with care. Differences are especially due to the complexity of sludge behaviour. Research and development of adequate lab-scale experiments is therefore highly desirable.

Influent characterisation: STOWA guidelines and biodegradable COD

In The Netherlands, a provisional procedure for influent characterisation has been suggested to cope with the lack of standard procedures (STOWA 96-08). This procedure is described in Section 3.5. It consists of physical-chemical characterisation in combination with BOD tests, the latter for determination of biodegradable COD that was indicated as the most important quantity for characterisation. Section 3.5 focuses on these BOD tests for determination of biodegradable COD.

Initial conditions

When calibrating (or validating) with dynamic simulation, initial conditions have to be known or estimated. Most important are the initial conditions of suspended components, because the dynamics of these states are the slowest. Therefore, wrong estimates have a pronounced effect on the simulation results and consequently cause bias in estimates of biological parameters. The solute components are less problematic as most of these components can be measured directly and exhibit much faster dynamics so that wrong estimates have a minor effect on parameter estimates. For the suspended components, only the total sludge concentration can be measured. In many cases, initial conditions are determined through prolonged simulations applying diurnal influent patterns and measured influent COD fractionation. Alternatively, Vanrolleghem *et al*. (1999) described methods to determine X_{BH}, X_{BA} and X_P based on steady-state mass balances. These methods require the yield and decay parameters for heterotrophic and autotrophic biomass to determine X_{BH} and X_{BA} respectively and the heterotrophic decay parameter and fraction inert products to determine X_P. Yet another approach is to estimate the initial state, but this increases possible identifiability problems. The problem of initial conditions is not discussed further here. This issue nevertheless will need further attention in ASM1 calibration.

Estimation algorithms

A comparison of parameter estimation methods for activated sludge parameter identification has been carried out by Vanrolleghem and Keesman (1996) (see also Fehnker, 1996) and is not discussed in this thesis.

Transport models

In calibration, development of adequate mixing models has received relatively little attention. No standard procedures are applied. Typically, for predenitrification reactors each compartment is modelled as a (series of) CSTR(s). Plug-flow type and carrousels are usually modelled by CSTRs in series, where the number is determined by trial-and–error or, less frequently, by empirical relationships. In some cases, additional information is used, for example the DO profile (Weijers *et al*., 1994).

A more systematic way to develop mixing models is by measuring Residence Time Distributions (RTDs, analogous to impulse responses) with tracer experiments. Parameters in combined models can then be determined with nonlinear estimation techniques. This approach has been applied by e.g. Siegrist and Tschui (1992), Coen *et al*. (1998) and De Clercq *et al*. (1999) to determine the number of CSTRs in the tanks-in-series model. In this model, radial gradients are neglected and more complicated flow patterns such as backflow are not considered. More complicated flow models than tanks-in-series were required to fit the RTD of a full-scale plant by Ottengraf (1971); here, the tanks-in-series model was extended with backflow. Newell *et al*. (1998) made a fit with bypass and dead zone to a pilot-plant reactor.

Especially in plants with surface aeration, vertical gradients in the DO concentration have been observed (Maier and Krauth, 1988; Barnard and Meiring, 1988). Recently, Alex *et al*. (1999b) were not able to calibrate a carrousel type plant with a tank-in-series model. Using flow patterns from a 3D numerical hydraulic model, a mixing model with 2-layers of tanks-in-series was derived. Parameters of this mixing model were used for tuning instead of biological parameters.

The examples indicate that calibration of mixing models is relevant for activated sludge calibration. Adequate mixing models will possibly become more complicated than those typically used now. It was decided however to first obtain a better understanding of ASM1 calibration. Calibration of mixing models will not be studied further in this thesis.

3.2.3 Identifiability of activated sludge plant models

Introduction

The overview of calibration strategies in Section 3.2.2 shows that, while considerable efforts have been put into calibration of ASM1 parameters, calibration needs further development.

As a starting point for development of strategies for calibration of full-scale plants, a useful question is whether input/output measurements of the process under normal operation provide sufficient information to uniquely estimate all parameters of the model. If this is the case, then the model can be calibrated from input/output data under normal operation alone.

If this is not the case, the next question could be if only a limited set of parameters is important for calibration and if this limited set can be uniquely estimated. If this is the case, then again the model can be calibrated from input/output data alone.

If this is not the case, then as an alternative, a subset can be selected of parameters that are estimated from the plant input/output data. For the (important) parameters that are not

estimated from input/output data, additional experiments should be developed. The number of possible parameter subsets is huge however, which motivates application of systematic methods for the selection.

This line of reasoning underlies the research described in this and the next sections. Model identifiability is used to investigate the questions stated above. Identifiability is the ability to determine a unique set of parameters when tuning the model to a given set of (output) data. In a correct calibration, the parameters have a unique value that has a physical interpretation. This is only possible if the model is identifiable.

A distinction can be made between structural and practical identifiability. Structural identifiability, also called deterministic, theoretic or a priori identifiability, is a property of the model structure. It relates to the question whether it is at all possible to obtain unique parameter values for a given model structure from selected outputs, in the case of perfect, noisefree measurements (Bellman and Åström, 1970). Structural identifiability is a minimum requirement.

For determining structural identifiability, several methods exist for linear models. The situation is more difficult for non-linear systems. In principle, Taylor expansion can be used, but the size and complexity of the resulting expressions renders the method suited only for relatively simple models. Linearization is another method, but gives only sufficient conditions; while the non-linear system may be identifiable, the linearized system may be not (Godfrey and DiStefano, 1985). Several other methods exist, but they are beyond the scope of this thesis.

Practical or *a posteriori* identifiability refers to the ability to obtain accurate parameter estimates from data, which are always imperfect. A structurally identifiable model may be practically unidentifiable if the measurements are insufficiently informative. Practical identifiability depends upon experimental conditions, including experimental design as well as quality and quantity of measurements. Practical identifiability will be used in the studies in Section 3.3 and 3.4. A definition and the methodology employed to study practical identifiability are given in Section 3.2.4. First, however, identifiability studies in the literature are reviewed.

Biokinetics: ASM1 identifiability

Biokinetic parameters from full-scale input/output data

From the structure and applied kinetic equations in ASM1, it is known that identifiability problems are to be expected. This is discussed in more detail in Appendix C. Therefore, for model identification, identifiability measures are needed to reveal how many and which parameters can be obtained from a particular experiment.

Sensitivity functions were proposed as an indication for identifiability problems in parameter estimation by Reichert *et al*. (1995), who used visual inspection of linear dependence of sensitivity functions to investigate identifiability for a denitrification model. A steady-state sensitivity analysis was used by Yuan *et al*. (1993) to investigate identifiability in a reduced version of the IAWQ Model for a high purity oxygen process. The DO concentrations in two reactors, oxygen purity and sludge concentration were chosen as outputs. It was concluded that heterotrophic yield and growth rate can be estimated from these outputs whereas nitrogen fractions i_{XP} and i_{XB} cannot.

While parametric sensitivity and sensitivity functions can provide a first indication of importance of parameters, for models with many parameters and many outputs it is difficult to

reveal possible dependencies amongst the parameters. Therefore, other identifiability measures such as the observability matrix and the Fisher information matrix (Section 3.2.4) are required.

The condition number of the observability matrix was proposed as a measure for (practical) state observability and parameter identifiability[18] and investigated for well-designed pilot plant experiments with intensive measurements (Ayesa *et al*., 1991, Larrea *et al*., 1992), which make these studies less representative for full-scale plants under normal operation. This measure was also used to compare alternative sensor locations (Ayesa *et al*., 1994, 1995); here a reduced model was applied, however. Moreover, the condition number alone is misleading as an indicator of practical identifiability. Julien *et al*. (1998) investigated theoretical identifiability from input/output measurements of an alternating plant. Here also a reduced model was applied, however.

Identifiability in respirometric experiments

Respirometric experiments are the most important class of experiments to yield additional information. Therefore, identifiability properties of these tests are discussed in some detail here. Structural identifiability in short respiration experiments was investigated by Dochain *et al*. (1995). This revealed that it is possible to estimate several parameter groups but not all the individual parameters. The study included nitrification. A slightly modified ASM1 was used however. More recently, Petersen *et al*. (2000) studied theoretical identifiability of a two-step nitrification model when using combined respirometric–titrimetric measurements. Combination with titrimetric measurements improved theoretic identifiability.

Vanrolleghem *et al*. (1995) optimised practical identifiability and experimental design of respiration experiments for a Monod model using the Fisher information matrix (see Section 3.2.4), resulting in significant improvement of parameter accuracy. Vanrolleghem and Spanjers (1995) studied structural and practical identifiability in the tests they suggested, but also employed a modified ASM1 model.

Table 3.3: Identifiable parameter groups from batch tests A and B (See text)

Wastewater characteristics	Sludge characteristics (biokinetics)
$(1-Y_{HA})\ S_{SA}$ (A)	$\mu_{HA}\ X_{BHA}\ (1-Y_{HA})/Y_{HA}$ (A)
$\mu_{HB}\ X_{BHB}\ (1-Y_{HB})/Y_{HB}$ (B)	$(1-Y_{HA})\ K_{SA}$ (A)
	$(1-Y_{HA})\ k_{hA}\ X_{BHA}$ (A)
	$\mu_{HB} - b_{HB}$ (B)
	k (See Chapter 4, Eq. 4.5.11) (B)

Note: Parameter subscripts A and B refer to batch tests A and B respectively.

Parameter estimation from measurements of two batch tests (A and B, wastewater with and without sludge, see Section 3.2.2 under respirometry) suggested by Kappeler and Gujer (1992) indeed suffered from identifiability problems (Linssen, 1994). Sijbers (1996) investigated theoretical identifiability of ASM1 in these batch tests with a reduced model with the original ASM1 kinetics. This led to the 7 identifiable groups in Table 3.3. In this study, nitrification was not considered. If the heterotrophic yield, Y_H, is known, then from these groups, at least in theory, S_S and X_{BH} in the influent can be determined, and X_{BH} of the sludge, μ_H, K_S, k_h and b_h, if the parameters in both tests are equal. Whether this is possible from actual respirograms is still an open question, which might be investigated by practical identifiability studies.

[18] The approach adopted was to estimate the unknown parameters and initial states with an extended Kalman filter. The observability matrix has close connections to the Fisher information matrix.

Witteborg *et al*. (1996) suggested a respirometric test to determine S_S in wastewater (see also STOWA 97-23). The value for Y_H is required and was determined with acetate respiration. The values for the yield thus determined however were significantly higher than otherwise reported values (0.80-0.82 vs. 0.65-0.67). This leads to erroneous values for S_S with errors up to 50% if acetate is not representative for influent S_S, which is doubtful indeed.

Summarising, respirometric experiments can yield additional information, but at least some of the stoichiometric and/or kinetic parameters, especially the heterotrophic yield, have to be known to compute individual model parameters from identifiable groups. As these are typically determined from other experiments, a complicating factor in interpretation of respirometric experiments is that the respective parameters values must be the same. For example, in tests A and B above, the parameters in test B apply to wastewater, while in test A they apply to sludge from the plant. The parameter values are not necessarily equal however, which has to be kept in mind when selecting and designing respirometric experiments for ASM1 calibration, as was discussed in the previous section.

Transport models identifiability

With respect to transport models, it is noted that RTDs are external descriptions, which contain no information on internal mixing. This is analogous to transfer functions, which correspond to an infinite number of state-space realisations. For first order kinetics, it is not relevant for the reactor performance how the internal mixing takes place and the external description provides sufficient information. With Monod kinetics, however, conversion based on RTDs may be overestimated. Consequently, additional information may be required for calibration of combined mixing models, for example from mechanistic flow models or from more detailed measurements. For identifiability analysis of composite models, many results from the study of identifiability of compartmental models can be applied (e.g. Delforge, 1981; Godfrey and DiStefano, III, 1985; van den Hof, 1995).

3.2.4 Methodology, overview of studies and description of test plant

Identifiability can be used to answer the question if (typical) input/output measurements of the process under normal operation provide sufficient information to uniquely estimate all parameters of the model. While in the literature several studies have been reported on identifiability of ASM1 or reduced models, they do not provide the answer to this question. Therefore, in Sections 3,3 and 3.4, identifiability of biological parameters from full-scale plant data is studied further to answer this question.

These identifiability studies reveal that not all ASM1 parameters are identifiable from input/output measurements (under normal operation). Identifiability is therefore also used as a systematic way to select identifiable subsets of parameters in a systematic way.

The focus will be on identifiability of the biokinetics (ASM1 parameters), rather than transport model parameters. This was done because it was considered important to first understand identifiability of the ASM1 parameters. Moreover, the focus is on continuously operated plants, especially carrousels, in contrast to alternating or intermittently operated plants. Data from continuously operated plants are less informative.

A well-known measure for practical identifiability is the Fisher information matrix (Mehra, 1974). This matrix is employed in the studies below. Let the criterion function be defined as the weighted sum of squared errors between model output vector $y(k,\theta)$ and measured output vector $y_p(k)$ with weights R_k:

$$J = \sum_{k=1}^{N} (y(k,\theta) - y_p(k))^T R_k (y(k,\theta) - y_p(k)). \quad (3.3)$$

The output is linearized in the neighbourhood of the optimal parameter vector θ_o as

$$y(t,\theta_o + \delta\theta) = y(t,\theta_o) + \left[\frac{\partial y(t,\theta)}{\partial \theta^T}\right]_{\theta_o} \delta\theta = y(t,\theta_o) + Y_\theta^T(t)\delta\theta, \quad (3.4)$$

with $Y_\theta(t)$ being the output sensitivity functions. Let Q_k be the covariance matrix of the measurement noise. Then the Fisher information matrix M can be written as

$$M = \sum_{k=1}^{N} Y_\theta(k) Q_k^{-1} Y_\theta^T. \quad (3.5)$$

For any unbiased estimator, the inverse of this matrix provides the Cramér-Rao lower bound on the covariance matrix of the parameter estimates. If M is singular, the experiment is said to be non-informative. If M has full rank, the model is locally identifiable. The rank and condition number of M are tests on identifiability, because M is an approximation of the Hessian of the objective function (Söderström and Stoica, 1989).

The Fisher information matrix, and thus the practical identifiability, depends on the model structure, the outputs selected, the number and distribution of data points, the measurement noise and on the model input signals as these affect the model output. Therefore, the practical identifiability of a model is determined by how these factors are chosen in a particular experiment.

Several functions of *M* can be defined as a measure of the uncertainty on the estimate of θ (Walter and Pronzato, 1990). These can be used as criteria to select or design experimental conditions with an optimal information content (in some respect). This is applied for example in design of respirometric experiments (see the previous section). The most important criteria are listed in Table 3.4 together with an interpretation.

Table 3.4: Experimental design optimality criteria (Munack and Posten, 1989)

Optimality	Objective	Interpretation
A	min tr(M^{-1})	Minimise mean variance
simplified A	max tr(M)	Minimise mean variance
C	min tr(H M^{-1}), H=diag(θ_i^{-1}, i=1,...,p)	Minimise relative (mean) variance
D	min det(M^{-1} (≡max det(M))	Minimise volume of ellipsoids
E	max λ_{min} (M)	Minimise largest error (maximal axis)
modified E	min cond(M) = $\frac{\lambda_{max} M}{\lambda_{min} M}$	Optimise condition number (achieve as spherical shape of the confidence region as possible)

In this thesis, these criteria are not used to optimise experimental conditions by manipulating

process inputs. Instead, the criteria are used as measures of practical identifiability to test how many and which parameters can be (sufficiently) accurately estimated from full-scale input-output data, under normal operation. The experimental conditions are assumed given. The model (structure) is (partly) determined by the selection of ASM1 to describe the biokinetics (besides selection of a transport-physical model). As outputs, those outputs are selected that are typically measured at full-scale plants. The noise is determined by the measurement method. Especially, the process input is assumed as given, namely as the naturally occurring influent variations. This was done, as it was the aim to reveal if normal operation is sufficiently informative to obtain all (important) parameters[19].

Of course, the criteria can also be applied to select for example optimal sensor locations, or the types of outputs. This was not done in this study. It is noted here that the practical identifiability criteria are also very suited as a straightforward, systematic tool to subsequently select additional experiments to input/output data. These can be selected (or designed) in such a way that the joint identifiability of full-scale data and additional experiments is optimised.

The D as well as the modified E criterion are selected to study identifiability in Sections 3.3 and 3.4. The following considerations motivate this choice. The simplified A criterion was rejected, because it can lead to uninformative designs, as it does not guarantee full rank of the Fisher information matrix (Munack and Posten, 1989). This matrix has to be full rank if the model is to be (locally) identifiable. The A and C criteria were rejected, because for these criteria it is necessary to compute the inverse of the Fisher information matrix, which can give numerical problems. The condition number is a good indication of identifiability, so this was chosen. It was observed however, that parameter subsets with low condition number often were associated with low traces (Weijers *et al.*, 1996a) and low determinants (Weijers *et al.*, 1996b). This means that, although parameter estimates may be independent, they may be (very) inaccurate. For this reason, a combined criterion that considers both the condition number and the determinant was applied.

Section 3.3 investigates local identifiability of the model's biological parameters. For local identifiability analysis, an *a priori* assumption on the parameter values must be made. This assumed value might be incorrect; moreover, the results of a local analysis may depend upon the particular parameter point chosen. Therefore, the sensitivity of the local analysis to the parameter values was studied in Section 3.4, by applying a randomised approach as a kind of global identifiability analysis. Section 3.3 has overlap with Section 3.4 in that partly the same results are given. Section 3.3 is included however as it contains results with selection of parameters based on the determinant alone as well as results based on the combined criterion.

Because the analysis reveals that not all parameters can be estimated and therefore additional experiments are required, one such experiment is investigated. In Section 3.5, a test for determination of biodegradable COD is developed and analysed. A reduced model that describes this test in ASM1 parameters is derived in Chapter 4.

In Sections 3.3 and 3.4, the identifiability properties of ASM1 are tested against field data from full-scale wastewater treatment plants. A wastewater treatment plant of the carrousel type (18.750 m^3) was used for this study. A layout of the plant is given in Figure 3.2.a.

[19] Moreover, it would be difficult to excite the biological part of a full-scale plant significantly. It would be interesting though to study if significant excitation is possible. For transport models, excitation is well possible by measuring pulse responses after addition of specific salt solutions.

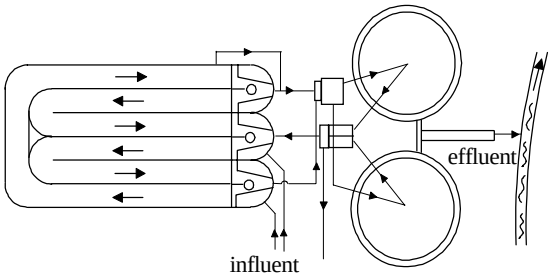


Figure 3.2.a: Plant lay-out

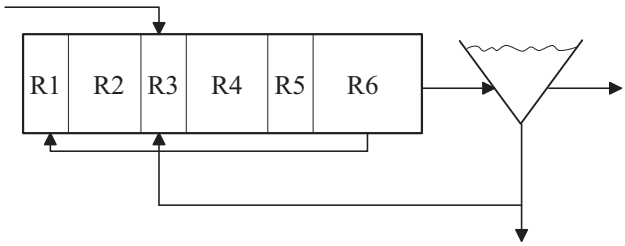


Figure 3.2.b: Model flowsheet

A special monitoring exercise was performed. Dynamic data were collected during 2 days for calibration and two days for validation with grab samples every two hours. The following outputs were measured:

- oxidation circuit: DO profile, MLSS, actual OUR (oxygen uptake rate), maximal OUR, sludge production;
- effluent: COD, N_{kj}, NH_4, NO_3, suspended solids.

The carrousels have been modelled by alternating aerated and non-aerated compartments. The aerated and aerobic parts in the circuit were modelled as aerated compartments R1, R3 and R5 in Figure 3.2.b. The other compartments R2, R4 and R6 represent the anoxic parts in the circuit. The aerobic volumes were determined by means of the measured DO profiles. The two final clarifiers were modelled as an ideal, static splitter.

3.3 Parameter estimation of ASM1 from full scale plant input/output data

Abstract[†]

The Activated Sludge Model No. 1 developed by the International Association on Water Quality is well accepted for dynamic simulation of removal of carbonaceous and nitrous compounds from wastewater in activated sludge plants. In several important applications of the model, it is essential to obtain meaningful parameters to describe full scale plant behaviour accurately, which is referred to as model calibration. Several procedures for model calibration have been proposed and applied in the literature, ranging from obtaining parameters directly from observed input/output behaviour of plants to using - sometimes many - additional, dedicated experiments. We investigated the possibilities and limitations of using only typical input/output data of plants by establishing how many and which parameters can be estimated from these data, in order to determine which additional experiments are really needed. For this aim, important and identifiable parameter subsets were selected by sensitivity and identifiability analyses. Two different identifiability criteria were used, the determinant of the Fisher Information matrix and a combined criterion including both determinant and condition number. These criteria led to almost identical sets of parameters. The results of the analyses were tested by parameter estimation using simulated data without and with noise, as well as measured data from a full scale carrousel type treatment system. The simulated data allowed more parameters to be estimated accurately from the output set used than the measured data, which is most probably caused by model mismatch with the plant. With both simulated and real data, the parameter sets selected could be uniquely estimated from the data, indicating the usefulness of selecting identifiable parameter subsets.

3.3.1 Introduction

As more strict demands are being put onto wastewater treatment, many activated sludge plants originally designed for removal of carbonaceous compounds (expressed as COD) have to be upgraded to include nitrogen removal as well. Enhanced nitrogen removal plants are sensitive towards disturbances in load and temperature that inevitably occur, and therefore dynamic simulation has become an indispensable aid in plant design and operation. The Activated Sludge Model No. 1 (ASM1) developed by the International Association on Water Quality (IAWQ) is considered state of the art and is now becoming routinely applied in many western countries. This model defines the biological processes taking place and their stoichiometry and kinetics. In some important applications of the IAWQ Model No. 1 (as a tool for upgrading existing plants, or as an aid in operation, e.g. for process analysis or model-based control), the model parameters must be fit to the plant and the conditions in the plant, because some of the parameters show a strong dependency upon plant operation and wastewater composition. This is referred to as model calibration, which usually consists of a combination of input/output measurements on the full-scale plant and additional, lab- or pilot-scale experiments, dedicated to specific parameters.

In the model, several components are distinguished such as readily and slowly biodegradable COD. These COD fractions and stoichiometric and kinetic parameters cannot be measured directly, however, and therefore have to be obtained indirectly. In this study the focus will be on the COD fractions and kinetic and stoichiometric parameters, as these are generally

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considered most problematic. Other parameters, such as parameters defining the plant flowsheet, and initial conditions are not considered and are assumed to be either directly measurable or obtainable from separate measurements or experiments.

Despite research efforts spent by several research groups during the past years, still no established procedure is agreed upon for this task. As a result, several approaches are being used, which differ in selection of outputs measured and parameters. Also in the procedure used for parameter estimation choices are made by the user (simultaneous or sequential estimation, sequence of estimation). This may result in difficulties in comparing results of different calibration exercises. The parameter values obtained from a calibration exercise may be biased and depend upon the procedure adopted as a consequence of identifiability properties of the model, and thus not have the physical meaning they are intended to have. Besides complicating comparisons of calibration results, application of the calibrated model may also be affected if the parameters obtained are not carefully interpreted. Consequently, we believe it is important to understand the identifiability properties of the model and to develop calibration procedures which reckon with these properties as much as possible.

The focus of this section is on calibration on the basis of full scale input/output plant data. It is important to know what information is contained in typical output measurements, in order to decide whether and which additional, dedicated experiments are really needed. Earlier research efforts did not address this question for the full model with data obtained during normal operation, although efforts have been put into obtaining parameters from well designed pilot tests [1] and from full scale plants [2]; in this last study a reduced order model was applied, however.

The theory section presents two criteria for selecting identifiable parameter subsets. Then it is described how these criteria and parameter estimation were used to establish how many and which parameters can be estimated from an assumed, typical set of input/output data. After this, the selected identifiable parameter subsets thus obtained are shown, followed by estimation results with these parameter subsets. These estimations were done by estimating parameters simultaneously from the total set of outputs available, using simulated data without and with noise as well as measured data.

3.3.2 Identifiability theory

Criteria for selecting identifiable parameter subsets from data available are described in this section. If least squares parameter estimation is used, the weighted sum J (Eq. 1) of squared errors between model outputs $y(k,\theta)$ and measured outputs $y_p(k)$ with weights R_k is minimized:

$$J = \sum_{k=1}^{N} (y(k,\theta) - y_p(k))^T R_k (y(k,\theta) - y_p(k)). \qquad (1)$$

Output sensitivity functions are obtained by linearization of this functional in the optimal parameter vector θ_o:

$$y(t,\theta_o + \delta\theta) = y(t,\theta_o) + \left[\frac{\partial y(t,\theta)}{\partial \theta^T}\right]_{\theta_o} \delta\theta = y(t,\theta_o) + Y_\theta^T(t)\delta\theta \qquad (2)$$

with $Y_\theta(t)$ being the output sensitivity functions. Sensitivity functions can be used as an indication for selecting parameters [5], as they indicate the importance of parameters. For models with many parameters and many outputs however, it is difficult to reveal all possible

dependencies amongst the parameters. This information is contained in the Fisher information matrix [4], which can be written as Eq. (3),

$$M = \sum_{k=1}^{N} Y_\theta(k) Q_k^{-1} Y_\theta^T(k), \tag{3}$$

with Q_k the covariance matrix of the measurement noise. Under certain assumptions, the inverse of the Fisher matrix provides the lower bound of the parameter covariance matrix [6] From (3) it can be seen that the Fisher matrix relates measurement accuracy, contained in Q_k, and model output parametric sensitivities $Y_\theta(t)$ to parameter estimate accuracy. Several functions of M can be defined as a measure of the uncertainty on the estimate of θ [8], of which two criteria have been applied here. The D criterion maximizes the determinant of M, thus minimizing the volume of confidence regions (which, by linearization, are assumed to be ellipsoids). The modified E criterion minimizes the condition number, defined as the ratio of the largest to the smallest eigenvalue of M, and thus achieves an as spherical shape as possible.

An important limitation of applying the Fisher matrix is the fact that it is a local property, computed in one, optimal point, of parameter space. As the optimum is not known a priori, an a priori assumption has to be made, which may not well represent the properties in the optimum. Therefore, additional testing was done by parameter estimation, as explained in the next section.

3.3.3 Method and case description

For the study, a wastewater treatment plant of the carrousel type in the Netherlands (18.750 m^3) was selected. At this plant, a monitoring campaign has been performed earlier (Weijers *et al.* 1994). The carrousel was modelled by alternating aerated and non-aerated compartments. The two final clarifiers of the plant were modelled as one ideal, static splitter.

For the analysis of identifiability, firstly a representative set of measured outputs was chosen, A set consisting of COD, Kjeldahl-N, NH_4 and NO_3 in the effluent and the sludge production was considered representative for typical, classical measurements. The sludge concentration was not included, as the model applied did not include a clarifier model and therefore could not describe observed dynamics in the sludge concentration.

For this output set, identifiable parameter subsets were selected by a procedure which consisted of the following steps (described in more detail in [10]). Firstly, an *a priori* parameter set was chosen for the analysis. This set consisted of default values for most of the parameters, and fS_S, fS_I,, fX_S, fX_I, K_{OA},and K_{OH} from an earlier, manual calibration on the same dataset [9].

Then a reduced set of most sensitive parameters was selected from the set of ASM1 kinetic and stoichiometric parameters and COD fractions, on the basis of this *a priori* assumption on the parameter values. Output parametric sensitivities were computed, and the parameters showing an average sensitivity larger than 0.2 (scaled by the highest sensitivity obtained for that paarticular output) were selected. The set thus found included Y_H, μ_H, b_H, Y_A, μ_A, K_S, K_{OA}, η_g, S_I, X_I and X_{BH}. In this particular case, the aerated volume fraction also appeared to be very important, which is a result of the flowsheet used. However, in the sequel this parameter will not be considered for estimation. With this reduced set, the following steps were carried out:

1. Select parameter subsets from the reduced set which show best identifiability.

For all parameter subset combinations containing 2 up to 8 parameters, the Fisher matrix was computed and the subsets were ranked according to the determinant (D criterion) and condition

number (Modified E criterion). The subsets yielding the highest determinant, respectively the lowest condition number was selected.

2. Test with estimation on simulated data

The thus selected subsets were estimated from simulated data without and with measurement noise added to the outputs. These estimations aimed at 1) discriminating between the influence of structural properties and measurement noise and 2) testing whether the identifiability properties from the locally computed Fisher information matrix are sufficiently representative to serve as a base for selecting identifiable parameter subsets.

3. Test with estimation on measured data

Finally, the subsets were estimated from measured data, which enables one to appreciate difficulties encountered in practice, as these data are not as ideal as simulated data, because model mismatch can occur.

3.3.4 Results and discussion

1. Identifiable parameter subsets selection

For the reduced parameter set, the Fisher information matrix was computed for increasing subset size. Parameters were scaled by typical parameter values to obtain equal relative weighting for the parameters. (If this scaling is not applied, high parameters are weighted more heavily than low parameters which leads to different relative parameter accuracy.) Then parameter subsets were ranked according to the determinant (Table 1) and the condition number (results not shown).

Table 1: Highest determinants of Fisher matrix for increasing number of parameters

Subset size	Determinant	Cond. Number	Parameter subset
2	$8.79\ 10^4$	32.5	Y_H, $\mu_A 20$
3	$84.8\ 10^4$	262	Y_H, $\mu_A 20$, fX_I
4	$615\ 10^4$	290	Y_H, $\mu_A 20$, fS_I, fX_I
5	$1451\ 10^4$	932	Y_H, $\mu_A 20$, $b_H 20$, fS_I, fX_I
6	$1003\ 10^4$	3415	Y_H, $\mu_A 20$, $b_H 20$, fS_I, fX_{BH}, fX_I
7	$448\ 10^4$	5599	Y_H, $\mu_A 20$, $b_H 20$, fS_I, fX_{BH}, fX_I, $\mu_H 20$
8	$145.0\ 10^4$	9754	Y_H, $\mu_A 20$, $b_H 20$, fS_I, fX_{BH}, fX_I, $\mu_H 20$, Y_A

The determinants given in Table 1 are the highest found among the determinants for all parameter subsets of the corresponding subset size n. The corresponding condition number is given as well. Apparently, the maximally attainable determinant decreases for the larger parameter subsets.

In the results obtained with the condition number as a criterion (data not shown), it was observed that the determinants associated with the lowest conditions numbers were much lower than the highest determinants (typically a factor of 50-500 lower). This means that, although the model is identifiable for the parameter subset combinations as far as the condition number is concerned, the parameter accuracy is not the highest achievable.

Therefore, as an alternative to the condition number, a combined criterion was used instead. From the parameter subsets, ranked according to the condition number, those subsets were chosen which had a low condition number and at the same time, a significantly higher determinant than surrounding sets. Following this heuristic procedure, Table 2 was produced.

Table 2: Combined criterion

Subset size	Determinant	Cond. Number	Parameter subset
2	$1.44\ 10^4$	4.795	X_I, $\mu_A 20$
3	$11.0\ \ 10^4$	35.1	X_I, S_I, $\mu_A 20$
4	$50.2\ \ 10^4$	110	$b_H 20$, fX_I, fS_I, $\mu_A 20$
5	$104.1\ \ 10^4$	295	$b_H 20$, fX_I, fS_I, $\mu_A 20$, η_g
6	$61.5\ \ 10^4$	634	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, η_g
7	$24.8\ \ 10^4$	1356	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, $\mu_H 20$, η_g
8	$10.5\ \ 10^4$	2400	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, $\mu_H 20$,Y_A, η_g

Some remarks are to be made here. Firstly, it is noted that the analysis reveals that the COD fractions fX_I and fS_I, can be estimated from output measurements together with other parameters. This differs from many procedures applied, where often fS_I is estimated separately from effluent COD alone.

Secondly, comparison of Tables 1 and 2 shows that similar subsets are obtained, except for Y_H. This parameter causes high condition numbers and at the same time high determinants.

More careful analysis revealed that for almost all outputs of the output set used, the sensitivity for Y_H was high. This causes the main diagonal element of the Fisher matrix Y_H to be higher than for other parameters. This leads to a relatively large eigenvalue associated with this parameter, which in turn leads to high condition numbers and large determinants. Thus the high sensitivity towards Y_H leads to accurate estimates of this parameter. From this consideration it is concluded that it may be advisable to include Y_H in the set of parameters to be estimated, as even small errors introduced by assuming this parameter known might lead to large errors in other parameters. However, including this parameter into the set may lead to larger numerical problems during estimation, because of probably worse conditioning.

2. Simulated data

Subsequently, the parameter subsets in Tables 1 and 2 were estimated from simulated data without noise. Up to the set of seven parameters, the estimation was within the specified parameter accuracy of 0.1%. This was achieved both with the Simplex (or Nelder-Mead) method and Levenberg-Marquardt method and reliability was checked by initialising the algorithm with two different starting points. With the 8 parameter subset, small deviations started to occur.

Then parameters were estimated from simulated data with noise levels of 2.5% and 5% of the mean output values (Gaussian white noise). The results for different parameter subset sizes are shown in Table 3 and 4. Here, also different starting algorithms and starting points were used. For both tables, the relative accuracy of the estimates is within 2.5 resp. 5% for sizes up to 5 parameters. For larger size of 6 up to 8 parameters, deviations of approximately 10% started to occur in the least sensitive parameters.

For noise levels of 5%, the inaccuracy in the estimates was approximately twice the inaccuracy with noise levels of 2.5%, as was to be expected. It can also be observed that, with increasing noise level, more iterations were needed when the number of parameters increased above 5. With 6 parameters, the requested accuracy was not obtained within the maximum number of iterations. The reason of this is not clear.

3. Measured data

Finally, the parameter subsets were estimated from measured data. Results are shown in Table 5 for set sizes up to 5 parameter for the sets selected with the combined criterion. For each

parameter subset for set sizes up to 5 parameters, almost the same optimal parameter set was found with different starting points and estimation methods. The uniqueness of the parameter values obtained despite large variation in starting points for the estimation confirms that these subsets were indeed identifiable, as was also concluded from the criterion used. Moreover, this result is obtained despite the local validity of the Fisher information matrix.

Table 3: Results of estimation of parameter subsets selected with combined criterion, simulated data with noise

N	Starting point†	noise %‡	Parameters								iterations
			fX_I	$\mu_A 20$	fS_I	b_H	η_g	fX_{BH}	$\mu_H 20$	Y_A	
2	1, 2	2.5	0.399	0.999							34
	1, 2	5	0.399	0.998							34
3	1, 2	2.5	0.399	1.000	0.0596						56
	1, 2	5	4.000	0.999	0.0588						56
4	1, 2	2.5	0.400	1.0007	0.0596	0.622					64
	1, 2	5	0.402	1.0014	0.0587	0.625					57
5	1, 2	2.5	0.401	0.999	0.0598	0.620	0.808				46
	1, 2	5	0.405	0.998	0.0591	0.620	0.816				57
6	1, 2	2.5	0.394	0.992	0.0599	0.635	0.797	0.657			82
	2	5	0.393	0.986	0.0595	0.641	0.800	0.633			598
7	1, 2	2.5	0.390	0.994	0.0609	0.637	0.785	0.661	4.18		92
	1	5	0.385	0.987	0.0613	0.650	0.775	0.629	4.35		1037
	2	5	0.385	0.987	0.0612	0.649	0.776	0.629	4.33		359
8	1, 2	2.5	0.388	1.005	0.0610	0.635	0.782	0.661	4.20	0.244	113
	1	5	0.380	1.007	0.0615	0.647	0.768	0.628	4.39	0.248	369
True point			0.398	1.000	0.0604	0.620	0.800	0.700	4.00	0.240	
† Starting point 1			0.358	0.900	0.0544	0.558	0.720	0.630	3.60	0.216	
Starting point 2			0.239	0.600	0.0400	0.372	0.600	0.700	2.40	0.144	

Table 4: Results of estimation of parameter subsets selected with determinant, simulated data with noise

N	Starting point†	noise %‡	Parameters								iterations
			Y_H	fX_I	$\mu_A 20$	fS_I	b_H	fX_{BH}	$\mu_H 20$	Y_A	
2	1, 2	2.5	0.6702		0.999						29
	1, 2	5	0.6704		0.998						29
3	1, 2	2.5	0.669	0.400	1.0016						50
	1, 2	5	0.668	0.402	1.0033						50
4	1, 2	2.5	0.670	0.400	1.0005	0.0596					72
	1, 2	5	0.669	0.401	1.001	0.0589					72
5	1, 2	2.5	0.670	0.400	1.001	0.0596	0.622				91
	1, 2	5	0.670	0.402	1.001	0.0587	0.624				100
6	1, 2	2.5	0.670	0.394	0.991	0.0599	0.635	0.658			100
	1	5	0.671	0.393	0.986	0.0593	0.646	0.633			1216
	2		0.671	0.392	0.985	0.0594	0.643	0.633			1208
7	1, 2	2.5	0.673	0.393	0.989	0.0609	0.637	0.666	4.16		122
	1, 2	5	0.675	0.389	0.977	0.0614	0.653	0.631	4.35		121
8	1, 2	2.5	0.674	0.391	1.005	0.0697	0.634	0.668	4.18	0.247	145
	2	5	0.679	0.383	1.010	0.0616	0.647	0.636	4.40	0.253	156
True point			0.670	0.398	1.000	0.0604	0.620	0.700	4.00	0.240	
† Starting point 1			0.603	0.358	0.900	0.0544	0.558	0.630	3.60	0.216	
Starting point 2			0.600	0.239	0.600	0.0400	0.372	0.420	2.40	0.144	

What can also be observed, is the fact that the values obtained for a particular parameter is dependent on the total number of estimated parameters. This can be explained as follows. When

estimating a set of parameters, the other, non-estimated parameter values have to be assumed. If such parameters are also estimated by increasing the subset size, not only the value of these extra parameter changes, but also of the other parameters estimated. This is a result of the identifiability properties of the model, and clearly shows that parameter values are not mutually independent and errors in assumed parameters are compensated for by errors in estimated parameters. This shows that one has to be careful in assigning a physical meaning to parameter values obtained.

Table 5: Results of estimation of parameter subsets selected with combined criterion, measured data

N	Starting point†	Method‡	Parameters				
			fX_I	$\mu_A 20$	fS_I	b_H	η_g
2	1, 2	S, LM	0.450	1.195			
3	1, 2	S, LM	0.440	1.192	0.0746		
4	1	S, LM	0.274	0.878	0.0841	0.173	
	2	LM	0.274	0.878	0.0841	0.173	
5	1	S, LM	0.351	0.863	0.0871	0.155	1.158
	2	LM	0.351	0.863	0.0871	0.156	1.152
† Starting point 1			0.398	1.000	0.0604	0.620	0.600
Starting point 2			0.239	0.600	0.0400	0.372	0.600

‡ S: Simplex, LM: Levenberg-Marquardt

If 6 or more parameters were estimated, non-realistic parameter values were obtained. This was not expected from estimation results with simulated data and is most probably caused by model mismatch, which was significant here due to the simplicity of the flowsheet used, neglect of clarifier dynamics and uncertainty in the influent due to grab sampling. Results of estimation of subsets selected with the determinant are given in Table 6.

Table 6: Results of estimation of parameter subsets selected with determinant, measured data

N	Starting point†	Method‡	Parameters					
			Yh	fX_I	$\mu_A 20$	fS_I	b_H	X_{BH}
2	1,2	LM	0.709		1.105			
3	1,2	LM	0.700	0.412	1.126			
4	1,2	LM	0.689	0.417	1.148	0.0736		
5	1	LM	0.103	0.450	1.350	0.0964	-0.0288	
6	1	LM	0.307	0.756	1.925	0.0923	-0.266	3.82
	2	LM	0.168	0.336	1.081	0.0966	-0.0375	0.445
† Starting point 1			0.67	0.398	1.000	0,0604	0.620	0.630
Starting point 2			0.60	0.239	0.600	0.0400	0.372	0.420

‡ S: Simplex, LM: Levenberg-Marquardt

Here, only up to 4 parameters could be estimated from the output set chosen. This was to be expected, because the condition numbers are worse and hence the identifiability is less good. In some cases, no convergence was achieved within the required number of iterations, which was set at 200 times the number of parameters to be estimated. For set sizes of 5 and 6 parameters, meaningless values were found (fractions larger than 1 or negative parameters). This could have been avoided by using constrained estimation, which was not done in this study in order to find limitations of identifiability. Also, problems with high condition numbers were observed during estimation, probably indicating occurrence of local minima.

Comparison of Table 5 and Table 6 indicates that the influence of estimating Y_H is smaller than was expected from the results obtained by identifiability criteria and estimation from

simulated data. It will be interesting to find out whether estimating Y_H will decrease bias of estimates of other parameters, which was expected from the preceding analysis.

3.3.5 Conclusions

Using identifiability analysis and parameter estimation series, we tried to establish how many and which parameters can be obtained from typical input/output data. For a carrousel system, sludge production and effluent COD, ammonia, Kjeldahl nitrogen and nitrate were chosen as a representative output set. Identifiability analysis with the Fisher matrix indicated that up to 8 parameters can be estimated from this set. This was confirmed by estimation with simulated data. This set included Y_H, μ_A20, b_H20, fS_I, fX_{BH}, fX_I, μ_H20 and Y_A, parameters that are generally considered important for calibration. From the results with simulated data, it is concluded that, in order to obtain more than 7 to 8 parameters, additional experiments are required. From the measured data used in this study, only up to 5 parameters could be estimated. This is very probably due to model mismatch, which was considerable. To be more conclusive for estimating with measured data, more elaborate flowsheet models will have to be applied to the same dataset, including modelling the final clarifier.

3.3.6 List of symbols

Stoichiometric parameters:

Y_H ::	Heterotrophic yield	(-)
Y_A ::	Autotrophic yield	(-)
f_p ::	Fraction biomass yielding inert products	(-)
i_{xb} ::	Fraction N in biomass	(kg N/kg COD)
i_{xp} ::	Fraction N in inert products	(kg N/kg COD)

Kinetic parameters:

μ_H ::	Heterotrophic growth rate constant	(s^{-1})
b_H ::	Heterotrophic decay rate constant	(s^{-1})
K_S ::	Affinity constant for S_S	(kg m^{-3})
K_{OH} ::	Heterotrophic affinity constant for S_O	(kg m^{-3})
K_{NHH} ::	Heterotrophic affinity constant for S_{NH}	(kg m^{-3})
K_{ALKH} ::	Heterotrophic affinity constant for S_{ALK}	(Mol m^{-3})
η_g ::	Correction factor for anoxic growth	(-)
μ_A ::	Autotrophic growth rate constant	(s^{-1})
b_A ::	Autotrophic decay rate constant	(s^{-1})
K_{OA} ::	Autotrophic affinity constant for S_O	(kg m^{-3})
K_{NHA} ::	Autotrophic affinity constant for S_{NH}	(kg m^{-3})
K_{NO} ::	Affinity constant for S_{NO}	(kg m^{-3})
K_{ALKA} ::	Autotrophic affinity constant for S_{ALK}	(Mol m^{-3})
k_h ::	Hydrolysis rate	(s^{-1})
K_x ::	Hydrolysis affinity constant	(kg m^{-3})
k_a ::	Ammonification rate	(s^{-1})
η_h ::	Correction factor for anoxic hydrolysis	(-)

Components:

S_S ::	Readily biodegradable COD	(kg m^{-3})
S_I ::	Soluble inert COD	(kg m^{-3})

S_{NH} ::	Ammonia and ammonium	(kg N m^{-3})
S_{NO} ::	Nitrite and nitrate	(kg N m^{-3})
S_{ND} ::	Soluble biodegradable organic N	(kg N m^{-3})
S_{ALK} ::	Alkalinity	(Mol m^{-3})
S_O ::	Dissoved oxygen	(kg m^{-3})
X_{BH} ::	Active heterotrophic biomass	(kg m^{-3})
X_{BA} ::	Active autotrophic biomass	(kg m^{-3})
X_S ::	Readily biodegradable COD	(kg m^{-3})
X_I ::	Particulate inert COD	(kg m^{-3})
X_{ND} ::	Particulate biodegradable org. N	(kg N m^{-3})
X_P ::	Particulate COD from decay	(kg m^{-3})
fS_I ::	fraction S_I in influent	(-)
fX_{BH} ::	fraction X_{BH} in influent	(-)
fX_S ::	fraction X_s in influent	(-)
fX_I ::	fraction X_I in influent	(-)
Other:		
DO ::	Dissolved Oxygen	(kg m^{-3})
COD ::	Chemical Oxygen Demand	(kg O_2 m^{-3})
BOD ::	Biological Oxygen Demand	(kg O_2 m^{-3})
Kjehldahl-N::	Kjeldal nitrogen concentration	(kg N m^{-3})
Q_k ::	measurement error covariance matrix	
R_k ::	weighting matrix	
y ::	output (column vector)	
θ ::	parameter vector	
p20 ::	value of parameter *p* at 20 °C	

3.3.7 References

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3.4 A procedure for selecting best identifiable ASM1 parameters

Abstract[†]

A systematic procedure for selecting identifiable parameter subsets for a given set of measured outputs is proposed. The aim is to only select those parameters that can be estimated uniquely from the dataset used. The proposed procedure consists of first selecting a reduced set of most sensitive parameters by sensitivity analysis and subsequently selecting identifiable parameter subsets using the Fisher information matrix.

For a particular set of outputs obtained from a typical calibration exercise at a carrousel type nitrogen removal plant, parameter subsets ranging from two to eight parameters were selected by this procedure. The procedure proved successful as the parameter subsets thus selected could be estimated accurately from simulated data without and with noise as well as from real data. However, the procedure is based on a property which is local in parameter space. Consequently, as an *a priori* assumption on the parameter vales has to be made at the start of the procedure, the selection results might be different from the results which would have been obtained by using the *a posteriori* parameter values. Hence, the sensitivity towards this *a priori* assumption was tested explicitly. For this purpose, the parameter space was sampled according to a Latin hypercube sampling scheme and the selection procedure was applied in all sampling points as if these were *a priori* estimates. From this extensive study it could be concluded that the results of the procedure were not too severely influenced by the *a priori* assumption on the parameter values. Therefore, the proposed procedure appears a powerful and practical tool for efficient and reliable model calibration.

Keywords

Activated Sludge, Identifiability, Mathematical Modelling, Optimal Experimental Design, Parameter Estimation

3.4.1 Introduction

In some important applications of the IAWQ Activated Sludge Model No. 1 (as a tool for upgrading existing plants, or as an aid in operation, e.g. for process analysis or model-based control), the model parameters, influent and sludge characteristics must be fit to the plant and the conditions in the plant, because some of these show a strong dependency upon plant operation and wastewater composition. This task is referred to as model calibration and it usually requires to perform a combination of input/output measurements on the full-scale plant and additional, lab-scale or pilot-scale experiments, dedicated to assess specific parameters.

In ASM1, several components are distinguished which cannot be measured directly, e.g. readily and slowly biodegradable COD, biomass fractions, etc. The same holds true for the stoichiometric and kinetic parameters. Consequently, these have to be obtained indirectly. In this study the focus will be on the COD fractions and kinetic and stoichiometric parameters, as these are generally considered most problematic. Other parameters, such as parameters defining

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the plant flowsheet, and initial conditions for the state variables are not considered in this study and are assumed to be either directly measurable or obtainable from separate measurements or experiments.

Despite research efforts spent by several research groups during the past years, still no established procedure is agreed upon for this model calibration task. As a result, several approaches are being used, which differ in selection of outputs measured and parameters selected for calibration (Weijers *et al.*, 1996). Also in the procedure used for parameter estimation, choices are made by the user (simultaneous or sequential estimation, sequence of estimation). The parameter values obtained may be biased and depend upon the procedure adopted, and thus not have the physical meaning they are thought to have. Besides complicating comparisons of calibration results, application of the calibrated model may also be affected if the parameters obtained are not carefully interpreted. Consequently, it is important to understand the identifiability properties of the model and to develop calibration procedures which reckon with these properties as much as possible.

The focus of this section is on calibration on the basis of full scale input/output plant data. It must be known what information is contained in typical output measurements, in order to decide whether and which additional, dedicated experiments are really needed. While efforts have been put into obtaining parameters from well designed pilot tests (Ayesa *et al.*, 1994) this question was not addressed for data obtained during normal operation in full scale plants, except for Ayesa *et al.* (1995) who applied a reduced order model, however.

The theory section presents two criteria for selecting identifiable parameter subsets and describes the Latin hypercube sampling (LHS) procedure. Then, the proposed procedure for selecting parameter subsets based on this identifiability theory is described, as well as the steps that were taken for testing this procedure by parameter estimations and the LHS-approach. To make this testing realistic, it was performed with a full-scale case study, for which a typical set of output data was available. The results section shows the identifiable parameter subsets obtained by applying the procedure, followed by the estimation results for these selected parameter subsets. These estimations were done by simultaneous estimation of the selected parameters, first using noise-free and noise-corrupted simulated data and then using real data, all for the same set of outputs available. Then the dependency of the parameter subset composition on the *a priori* parameter values is shown on the basis of a Latin hypercube sampling test. Finally, conclusions are drawn.

3.4.2 Identifiability theory and Latin hypercube sampling

Criteria for selecting identifiable parameter subsets from data available are described in this section. If least squares parameter estimation is used, the weighted sum J (Eq. 1) of squared errors between model outputs $y(k,\theta)$ and measured outputs $y_p(k)$ with weights R_k is minimised:

$$J = \sum_{k=1}^{N} (y(k,\theta) - y_p(k))^T R_k (y(k,\theta) - y_p(k)) . \qquad (1)$$

Output sensitivity functions are obtained by linearisation of this functional in the optimal parameter point θ_o:

$$y(t,\theta_o+\delta\theta)=y(t,\theta_o)+\left[\frac{\partial y(t,\theta)}{\partial\theta^T}\right]_{\theta_o}\delta\theta=y(t,\theta_o)+Y_\theta^T(t)\delta\theta \tag{2}$$

with $Y_\theta(t)$ being the output sensitivity functions. Sensitivity functions can be used for selecting parameters (Reichert *et al.*, 1995), as they indicate the relative importance of parameters. For models with many parameters and many outputs however, it is difficult to reveal all possible dependencies amongst the parameters. This information is summarised in the Fisher information matrix (Mehra, 1974), which can be written as

$$M=\sum_{k=1}^{N}Y_\theta(k)Q_k^{-1}Y_\theta^T(k), \tag{3}$$

with Q_k the covariance matrix of the measurement noise. Under certain assumptions (no model mismatch, white measurement noise), the inverse of the Fisher matrix provides the lower bound of the parameter error covariance matrix (Söderström and Stoica, 1989):

$$cov(\theta_o)\geq M^{-1} \tag{4}$$

The above shows that the Fisher matrix relates measurement accuracy, contained in Q_k, and model output parametric sensitivities $Y_\theta(t)$ to parameter estimate accuracy.

Several functions of M can be defined as a measure of the uncertainty on the estimate of θ (Walter and Pronzato, 1990). Two criteria have been applied here, the modified E criterion and the D criterion. The modified E criterion is identical to the condition number, defined as the ratio of the largest to the smallest eigenvalue of M, and thus compares the confidence region's shape with that of a sphere. Although the condition number provides a good indication of identifiability, it was observed that parameter subsets with low condition number often were associated with low traces and determinants, which means that, although parameter estimates may be independent, they may be (very) inaccurate. For this reason, it was decided that the D criterion was to be considered as well. The D criterion is equal to the determinant of M, thus corresponding to the volume of confidence regions (which, by linearisation, become ellipsoids).

For given outputs with measurement error (Q_k) and given number of samples (N), it is the model parametric sensitivities $Y_\theta(t)$ which map the measurement errors onto the parameter error. $Y_\theta(t)$ depends upon the excitation in the input signal, model structure (which are known) and on the (optimal) parameter vector θ_o (which is not known *a priori* and which is determined by the real output data). Thus with known input signal, model structure, measurement error and number of samples, the identifiability properties depend upon the real output data via the optimal parameter point θ_o.

From the above it is clear that an important limitation of applying the Fisher matrix is that it is a local property, computed in one, optimal, point of parameter space. As the optimal parameter point θ_o is not known *a priori*, an assumption has to be made, which in general will not coincide with the optimum and thus not well represent the properties in the optimum. For this reason, the sensitivity towards the *a priori* assumption was investigated by sampling the

parameter space according to a Latin hypercube sampling scheme and apply the parameter selection in each of the resulting parameter points, as if these were the *a priori* estimates. Thus, also the sensitivity towards the real output data set is tested. This can be seen as follows. As the optimal parameter point depends upon the output data, a small sensitivity towards the *a priori* assumption implies a small sensitivity towards the real output data set measured.

Latin hypercube sampling includes a stratified sampling of the parameter space which is preferable over random sampling. The scheme is an extension of Latin square sampling and was originally developed by Iman and Conover (1980) to enable sensitivity analysis for time-consuming computer codes through a limited number of simulation runs. For uniform probability distributions on the parameters, the sampling proceeds as follows. A number of samples N_{LHS} is defined. Then the range for each parameter is divided into the same number of N_{LHS} (equally sized) intervals and one observation is made in each interval using random sampling. One observation for the first parameter is then randomly selected, matched with a randomly selected observation on the second parameter and so on for all the parameters. These constitute sample (parameter point) 1. This procedure is repeated for the remaining parameter observations which exhausts all of the observations and results in a Latin hypercube sample.

3.4.3 Proposed procedure for selecting identifiable parameters

The procedure summarised in Figure 1 is proposed for selecting parameter subsets. The steps of the procedure are described in more detail here.

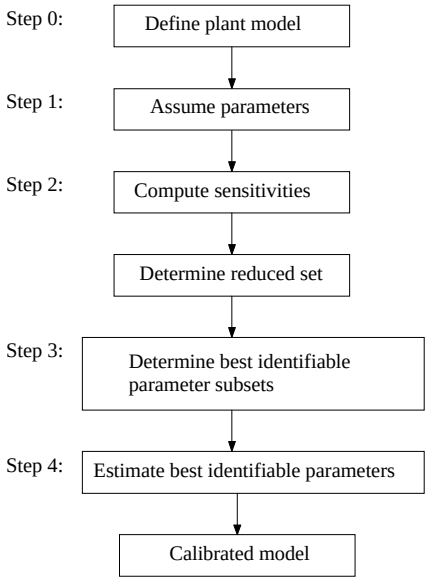

Figure 1: Procedure for selecting best identifiable parameter subsets

0. Define plant model, input data and initial conditions

It is assumed that other steps necessary in model calibration have already been taken. These include: (i) Obtaining design data such as plant layout and volumes; (ii) Obtaining plant input data and operational data as a function of time such as influent flow and concentrations of total COD and Kjeldahl-N, other (internal) flows and loads, temperature, aeration and control loops; also the fractions of soluble Kjeldahl-N and ammonia-N of the total Kjeldahl-N and the COD and Kjeldahl-N concentration of the sludge are assumed to be measured separately; (iii) Initial

conditions are assumed to be known and obtained either through measurements or through steady-state computation; (iv) A set of output measurements such as sludge production, effluent COD, effluent ammonia-N and nitrate-N is available; (v) The model and data are available in computer code. Thus, the next step to be taken is selection of parameters to be estimated and their estimation.

1. Define the set of outputs and an *a priori* parameter set

First, the set of outputs available for estimation is defined. For the analysis, an *a priori* assumption on parameter values has to be made. For example, default values taken from the literature can be applied.

2. Select a reduced set of most sensitive parameters.

This step is included to reduce the number of parameters with which the subsequent detailed analysis is done from approx. 25 to a number between 10 and 15 in order to reduce computation time in subsequent steps. Sensitivity coefficients $S_{\theta_i}^{y_j}$ were computed from the mean of the output sensitivity functions $Y_\theta(t)$:

$$S_{\theta_i}^{y_j} = \frac{\frac{1}{N}\sum_{k=1}^{N}\left|Y_{\theta_i}^{j}(k)\right|}{\frac{1}{N}\sum_{k=1}^{N} y^{j}(k,\theta_0)} \cdot \theta_{i0} \,. \tag{5}$$

The reduced set was selected according to either of the two following methods: (i) Scale the sensitivity coefficients for each output by the maximal sensitivity coefficient for that output. Select those parameters which show a scaled mean output sensitivity coefficient larger than 0.2 in at least one of the outputs. The idea behind this is to ascertain that at least one parameter will be selected for each output available. (ii) Rank the parameters according to averaged sensitivity coefficients, obtained by averaging over the outputs available:

$$\overline{S_{\theta\, i}^{y}} = \frac{1}{N_y}\sum_{j=1}^{N_y} S_{\theta_i}^{y_j} \,. \tag{6}$$

3. Select those parameter subsets from the reduced set which show highest identifiability.

In this step, the Fisher information matrix is computed for all possible subsets of the parameters selected on step 2. This is done for subsets of sizes increasing from 2 to n parameters, yielding the largest possible n (here, n was limited to 8 for reasons indicated at the results section). A ranking is then made of all parameter subsets according to the D as well as to the modified E criterion. For each subset size, the best subset is selected. The listing of best subsets for increasing n provides information on the maximum number of identifiable parameters from the output set. As the number of computations required in this step increases dramatically with the total number of parameters to be evaluated because of combinatorial explosion, the preceding step (obtaining a reduced set) is essential.

4. Estimate selected parameters from real data

If the procedure is successful, then for the parameter subset thus selected unique parameter values are obtained from the real dataset by nonlinear parameter estimation. Other, non-estimated parameters are maintained at their initially assumed values.

3.4.4 Testing the suggested procedure

To evaluate whether the procedure actually leads to identifiable parameter subsets, the following tests were performed:

1. Estimation from simulated data (i.e. with known 'true' parameter values)
The subsets selected with the above procedure were estimated from simulated data without and with measurement noise added to the outputs. These estimations aimed at i) discriminating between the influence of structural properties and measurement noise and ii) testing whether the identifiability properties from a locally computed Fisher information matrix are sufficiently representative to serve as a basis for selecting identifiable parameter subsets.

2. Estimation from real data
After this, the subsets were estimated from real data, which enables one to i) check whether unique parameter values are obtained despite possibly erroneous *a priori* parameter values and ii) appreciate difficulties encountered in practice, as these data are not as ideal as simulated data, because model mismatch can occur.

3. Assess sensitivity to a priori assumption on the parameter values
Finally, the Latin hypercube sampling was applied as an explicit test for the range of validity of the conclusions with respect to identifiability drawn on the basis of the *a priori* assumed parameter values.

3.4.5 Case description

For the study, a wastewater treatment plant of the carrousel type (18.750 m^3) was selected. At this plant, a monitoring campaign has been performed earlier (Weijers *et al*., 1994). The carrousel was modelled by alternating aerated and non-aerated compartments to achieve nitrogen removal. The two final clarifiers of the plant were modelled as one static splitter with ideal solids separation. In a measurement campaign of two days the influent and effluent were sampled every two hours.

3.4.6 Results and discussion

Procedure results

1. Definition of the set of outputs and *a priori* parameter set.
For the analysis of identifiability, a representative set of measured outputs was chosen first. A set consisting of COD, Kjeldahl-N, NH_4 and NO_3 in the effluent and the sludge production was considered representative for typical, standard measurements. Then an *a priori* parameter set was chosen for the analysis. This set consisted of default values for most of the parameters from Henze *et al.* (1987), and the influent COD fractions fS_S, fS_I,, fX_S, fX_I and affinity constants K_{OA}, and K_{OH} from an earlier, manual calibration on the same dataset (Weijers *et al*., 1994). The N fractions were also determined by manual calibration.

2. Selection of a reduced set of most sensitive parameters.
A reduced set of most sensitive parameters among the ASM1 kinetic and stoichiometric parameters and COD fractions was selected on the basis of the *a priori* assumption on the parameter values. Output parametric sensitivities were computed, and the selection was done by

method (i) described in the procedure section, that is by selecting those parameters which show a time-averaged, scaled sensitivity coefficient larger than 0.2 in at least one of the outputs. The set thus found included Y_H, μ_H, b_H, Y_A, μ_A, K_S, K_{OA}, η_g, fS_I, fX_I and fX_{BH}. In this particular case, the aerated volume fraction also appeared to be very important, which is an artefact introduced by the flowsheet used. For this reason in the sequel this parameter will not be considered for estimation. With this reduced set, the following step could be carried out.

3. Identifiable parameter subsets selection

For the reduced parameter set, for all parameter subset combinations containing 2 up to 8 parameters, the Fisher matrix was computed. For this computation, the output error covariance matrix Q_k was assumed diagonal and constant over the samples, and for each output the error was assumed to be proportional with the mean value over the samples for that output. An additional scaling of the sensitivity functions by the *a priori* parameter values was applied. The subsets were subsequently ranked according to the determinant (D criterion) and condition number (Modified E criterion) (results not shown). The subsets yielding the highest determinant, respectively the lowest condition number were selected. These results indicated that it was best to use a combined criterion, and from the parameter subsets with the best determinants that subset was chosen which had a significantly lower condition number than surrounding sets. Following this heuristic procedure, Table 1 was produced.

Table 1: Parameter subsets selected with combined criterion

Subset size	Determinant	Cond. Number	Parameter subset
2	$1.44\ 10^4$	4.795	fX_I, $\mu_A 20$
3	$11.0\ 10^4$	35.1	fX_I, fS_I, $\mu_A 20$
4	$50.2\ 10^4$	110	$b_H 20$, fX_I, fS_I, $\mu_A 20$
5	$104.1\ 10^4$	295	$b_H 20$, fX_I, fS_I, $\mu_A 20$, η_g
6	$61.5\ 10^4$	634	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, η_g
7	$24.8\ 10^4$	1356	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, $\mu_H 20$, η_g
8	$10.5\ 10^4$	2400	$b_H 20$, fX_{BH}, fX_I, fS_I, $\mu_A 20$, $\mu_H 20$,Y_A, η_g

Some remarks are to be made here. First, it is noted that the analysis reveals that the influent COD fractions fX_I and fS_I can be estimated from output measurements together with other parameters. This differs from many procedures applied, where often S_I is estimated separately from effluent COD alone, which may consequently introduce bias.

Second, with the determinant as sole criterion, very similar subsets are obtained, with the notable exception of Y_H. This parameter causes high condition numbers and at the same time high determinants. More careful analysis revealed that for almost all outputs of the output set used, the sensitivity for Y_H was high. This causes the main diagonal element of the Fisher matrix corresponding to Y_H to be higher than for other parameters. This leads to a relatively large eigenvalue, which in turn leads to high condition numbers and large determinants. Thus the high sensitivity towards Y_H leads to accurate estimates of this parameter. From this consideration it must be concluded that it is advisable to include Y_H in the set of parameters to be estimated, as even small errors introduced by assuming this parameter known might lead to large errors in other parameters. However, including this parameter into the set may lead to larger numerical problems during estimation, because of worse conditioning.

Results of testing the selection procedure

1. Test by estimating from simulated data with known 'true' parameter values

The parameter subsets of Table 1 were estimated from simulated data without noise. In the

estimation, a parameter scaling was applied, in order to improve numerical properties and reduce differences in relative accuracy for the parameters. The values assumed in the starting point were used for scaling. Up to the set containing seven parameters, the estimation was within the specified relative accuracy of 0.1%. Reliability was checked by using different search algorithms and initialising them with different starting points. With the 8 parameter subset, small deviations started to occur, in the order of magnitude of 1% (results not shown).

Subsequently, parameters were estimated from simulated data with noise levels of 5% of the mean output values (Gaussian white noise). The results for different parameter subset sizes are shown in Table 2, expressed as relative deviation from the known 'true' values in percents which is possible because the true values are known. Here also two different starting points were used for most set sizes. For both tables, the relative accuracy of the estimates is within 5% for sizes up to 5 parameters. For larger size of 6 up to 8 parameters, deviations of approximately 10% started to occur in the least sensitive parameters. From this result and from the result without noise, it was decided to set the maximum subset size at 8 parameters.

Table 2: Results of estimation of parameter subsets selected with combined criterion from simulated data with noise, presented as relative deviation (%) from known 'true' value

N	Starting point[†]	Parameters							
		fX_I	$\mu_A 20$	fS_I	b_H	η_g	fX_{BH}	$\mu_H 20$	Y_A
2	1, 2	0.30	-0.18						
3	1, 2	0.53	-0.10	2.64					
4	1, 2	0.91	-0.14	2.79	0.73				
5	1, 2	1.89	-0.24	-2.10	-0.15	1.96			
6	2	-1.33	-1.42	-1.48	3.40	0.025	-9.60		
7	1	-3.34	-1.27	1.50	4.82	-3.19	-10.11	8.70	
	2	-3.29	-1.27	1.33	4.74	-3.02	-10.09	8.20	
8	1	-4.50	0.70	1.81	4.34	-4.04	-10.36	9.63	3.29
'True' point		0.398	1.000	0.0604	0.620	0.800	0.700	4.00	0.240
[†] Starting point 1		0.358	0.900	0.0544	0.558	0.720	0.630	3.60	0.216
Starting point 2		0.239	0.600	0.0400	0.372	0.600	0.700	2.40	0.144

2. Test by estimating from real data

The selected parameter subsets for set sizes up to 5 parameters were estimated from real data (Table 3). The results are given as estimated parameter values, because no relative deviations can be computed as the true values are not known. From the results per subset size, it can be seen that almost the same optimal parameter set was found with different starting points and estimation methods. As unique parameter values were obtained, this confirms that these subsets were indeed identifiable, as was concluded from the selection criterion used. Remarkable is that this result is obtained despite the fact that the Fisher information matrix has only local validity and differences up to 100% of the *a priori* assumed values occur.

Table 3: Results of estimation of parameter subsets selected with combined criterion from real data

N	Starting point[†]	Method[‡]	Parameters				
			fX_I	$\mu_A 20$	fS_I	b_H	η_g
2	1, 2	S, LM	0.450	1.195			
3	1, 2	S, LM	0.440	1.192	0.0746		
4	1	S, LM	0.274	0.878	0.0841	0.173	
	2	LM	0.274	0.878	0.0841	0.173	
5	1	S, LM	0.351	0.863	0.0871	0.155	1.158
	2	LM	0.351	0.863	0.0871	0.156	1.152
[†] Starting point 1			0.398	1.000	0.0604	0.620	0.600
Starting point 2			0.239	0.600	0.0400	0.372	0.600

[‡] S: Simplex, LM: Levenberg-Marquardt

On the other hand, the results of Table 3 also show that the values obtained for a particular parameter are dependent on the total number of estimated parameters. This can be explained as follows. When estimating a set of parameters, the other, non-estimated parameter values have to be assumed. Errors in the assumed parameters are compensated for by the errors in the estimated parameters. If the parameter subset increases in size, less parameter values are assumed and the distribution of the errors over the parameters changes, resulting in a change of all parameter estimates.

This shows that estimated parameter values are not mutually independent even though by the selection criterion used they were selected on minimal interdependency, so one has to be careful in assigning a physical meaning to parameter values obtained. Increasing the subset size to 6 or more parameters resulted in non-realistic parameter estimates. This was not predicted by the test results with the simulated data and is most probably caused by model mismatch, which was significant in this case due to different causes. This model mismatch may lead to unrealistic parameter values, as wrong model structure is (partly) compensated for by erroneous parameter estimates. For more definite conclusions on the number of practically identifiable parameters, more detailed study is required in this case.

Another exercise reported in more detail in Weijers *et al.* (1996) consisted of evaluating subsets selected with the determinant as ranking criterion. With this ranking only up to 4 parameters could be estimated from the output set chosen. This was to be expected, because the condition numbers are worse and hence the identifiability properties are less good. It is too early however to conclude that the combined criterion is to be preferred as it is advisable to estimate Y_H for reasons indicated above.

3. Test sensitivity to a priori assumption by applying Latin hypercube sampling
The selection of reduced parameter sets and of best identifiable parameter subset, step 2 and 3 in the procedure given above, were repeated with the 23 parameters considered relevant. From the literature and experience, ranges considered realistic were defined for all of these parameters. The ranges defined are given between square brackets: Y_h[0.55 - 0.67], f_p[0.08 - 0.2], Y_a[0.1 - 0.25], μ_{h20}[2 - 10], K_s[2.5 - 20], K_{oh}[0.1 - 1], K_{nhh}[0.02 - 0.2], b_{h20}[0.1 - 1.5], η_g[0.6 - 1.0], η_h[0.35 - 0.4], K_{no}[0.1 - 0.5], k_{h20}[2 - 4], K_{x20}[0.03 - 0.15], k_{a20}[0.016 - 0.8], μ_{a20}[0.2 - 1.2], K_{nha20}[0.8 - 10], K_{oa}[0.1 - 1]; b_{a20}[0.04 - 0.15], fS_i[0.04 - 0.2], fS_s[0.05 - 0.25], fX_s[0.4 - 0.6], fX_i[0.05 - 0.4], fX_{bh}[0.01 - 0.2], f_{Xba}[0.001 - 0.01].

115 Parameter points were sampled, each of these representing a particular point in 23-dimensional parameter space and thanks to the LHS sampling design guaranteed to cover the whole space. For all 115 parameter points, sensitivity functions of the five outputs with respect to all 23 parameters were computed. Then reduced sets were determined by applying method (i) described in the procedure section (compute time-averaged output sensitivities, scale by the maximum output sensitivity, select reduced sets consisting of all parameters with at least one scaled output sensitivity value larger than 0.2). The occurrences within the reduced sets thus obtained for the 115 different LHS parameter sets were as follows (ranked according to the number of occurrences): fS_i 115, μ_{a20} 115, Y_a 115, Y_h 115, η_g 111, K_{nha20} 95, K_{oa} 88, b_{h20} 85, k_{h20} 79, K_{oh} 62, fX_i 39, μ_{h20} 29, K_{x20} 18, K_{no} 16, K_s 16, η_h 10, fS_s 5, k_{a20} 1, fX_{ba} 0, fX_{bh} 0, b_{a20} 0, K_{nhh} 0, f_p 0. Although these results indicate an order of importance, it was observed that with the selection criterion used (value > 0.2), the size of the reduced set varied too severely, namely from 4 to 15 parameters depending on the LHS parameter set considered. It thus appears that this criterion is not effective for reducing the set to a consistent set of important parameters that

would hold independent of the *a priori* assumption of the parameter values. To accommodate for this, method (ii) for step 2 of the procedure was chosen, which also agrees better with the behaviour of the least squares criterion used within estimation as it does not artificially change the sensitivity of an output by scaling with the maximal sensitivity of that output. This alternative consists of omitting the scaling by the maximal sensitivity for each output and instead, ranking the parameters according to the sensitivity coefficients, averaged over the 5 outputs. In Figure 2, the rankings thus obtained within the individual LHS samples are plotted as a function of the sampling number for the 6 most sensitive parameters.

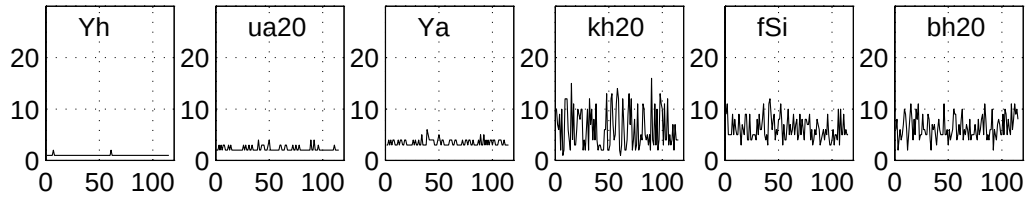

Figure 2: Parameter ranking over the LHS sample if ranked according to mean sensitivity over the outputs

These plots have been organised from left to right ordered by a second ranking, which consists of averaging the output-averaged sensitivity coefficients over the 115 LHS samples and rank the parameters and corresponding plots in descending order of this LHS-sample-averaged sensitivity.

In Figure 3, the results are summarised as histograms of the rankings for all of the parameters. Also these histograms have been organised from top left to bottom right in descending order of LHS-sample-averaged sensitivity. It can be observed that if about 14 parameters are selected, the most important are consistently present. This means that the set can indeed be reduced, and a size of 14 appears adequate. What can also be observed is that some parameters show a much larger variation in their relative sensitivity than other parameters. This especially holds true for k_h, K_{nha}, fX_i and to a lesser extent for K_{x20} and μ_{h20}. Hence, with respect to the latter parameters the composition of the reduced set seems to depend on the *a priori* assumed values. Some of the other parameters such as f_p, η_h, fX_{bh} and fX_{ba} show a large variation in sensitivity, but are always in the range of least sensitive parameters and consequently can be omitted consistently.

Finally, parameter subset compositions were determined over the LHS sample, after first reducing the set to 14 parameters. A subset size of 8 parameters was chosen, and the determinant of the Fisher information matrix was used as the selection criterion. This choice was made, because the heuristic procedure used with the combined criterion considering both the condition number and the determinant does not lend itself for straightforward ranking, which was required to analyse the large sample used. The occurrences of parameters in the subsets obtained was as follows: Y_h 115, k_{h20} 115, fS_i 115, μ_{a20} 114, b_{h20} 100, K_{no} 88, η_g 82, fX_i 61, Y_a 38, K_{oh} 37, K_{x20} 32, K_{nha20} 23, K_{oa} 0, η_h 0. This shows that the same 5 parameters Y_h, k_{h20}, fS_i, μ_{a20} and b_{h20} in the subsets obtained in almost all of the samples, and K_{no}, η_g and *fXi* in most of the subsets, indicating that the subset size composition does not change severely by the *a priori* assumption on the parameter values.

The results obtained with LHS sampling indicate that the procedure can be applied to obtain identifiable parameter subsets. The number of identifiable parameters was limited (to 8), however, which means that not all important parameters can be estimated with the output set

defined. Errors in non-estimated, fixed parameters may then lead to errors in estimated parameters, especially because non-selected parameters can have a strong interaction with selected parameters; in fact, this is the reason they are rejected in the identifiable subset selection step. To get around this problem, more outputs and/or dedicated experiments yielding information on these parameters have to be looked for. The selection procedure proposed can be utilised for this task as well.

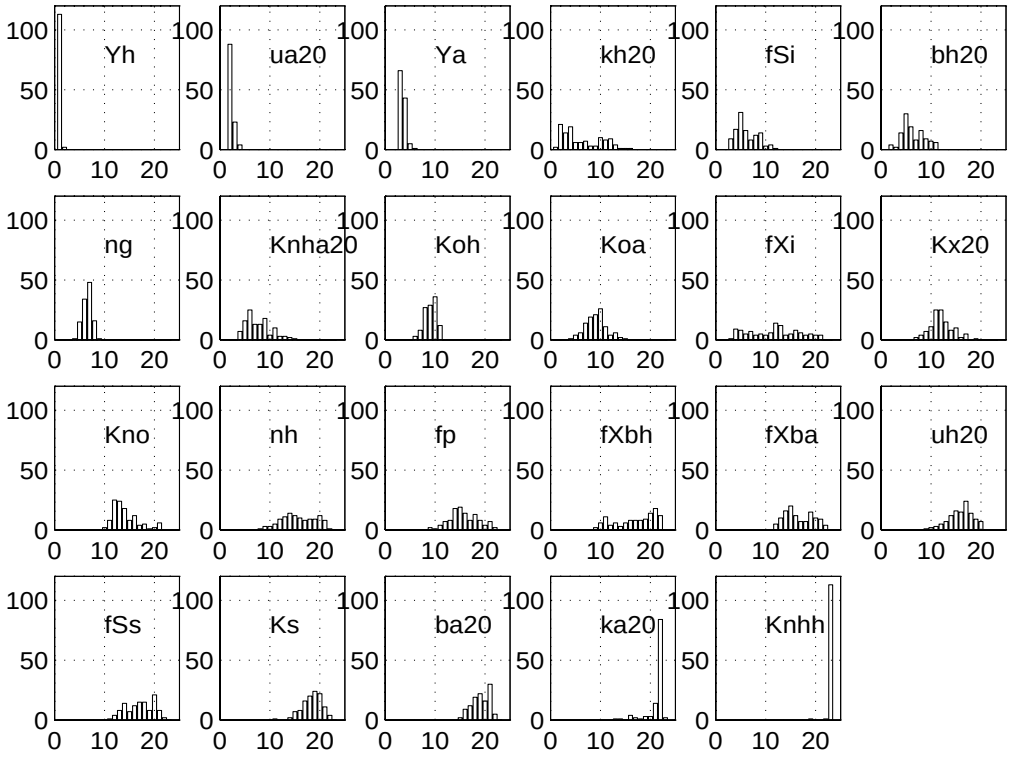

Figure 3: Histograms of occurrences of ranking positions of parameters

3.4.7 Conclusions

A procedure was suggested for selecting important and identifiable parameter subsets for calibrating ASM1. This procedure utilises sensitivity functions and the Fisher information matrix. However, these are local properties in parameter space and consequently may depend upon an *a priori* assumption on parameter values which has to be made. Therefore, the procedure was tested by estimation on simulated as well as measured data, which indicated that the procedure was successful in selecting identifiable subsets. In addition, a Latin hypercube sampling procedure covering the whole parameter space showed that the results obtained by the procedure are not too severely influenced by the *a priori* assumption. This means that a tool has been developed which is helpful in selecting parameters that can be uniquely estimated from the data available. The next challenge is now to use this approach to find optimal experimental designs which optimally combine full scale plant input/output data with dedicated experiments, especially respirometry, in order to obtain all relevant parameters.

3.4.8 Acknowledgement

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3.5 BOD tests to determine biodegradable COD

Abstract[†]

Application of Activated Sludge Model No. 1 requires an influent characterisation of COD over the different model COD components. Total biodegradable COD (COD_{BD}) is the most important quantity in this characterisation. The use and interpretation of BOD tests for the determination of biodegradable COD were investigated. Of four grab samples, the BOD evolution in time was measured up to fifteen days, with addition of nitrification inhibitor. From the BOD curves, total BOD (BOD_∞, or BOD infinite) was estimated with first and second-order models. Parameters were fitted with one (or two, for the second-order models) kinetic parameter per individual sample as well as one (two) for all samples together. The BOD curves were adequately described by first-order kinetics. The estimated kinetic parameters showed considerable variation over the samples from the same wastewater. As a consequence, the ratio BOD_∞/BOD_5 was not constant for a given wastewater. The ratio BOD_∞/COD_{tot} on the contrary proved much more constant. Therefore, the total COD instead of BOD_5 is suggested as a basis for determination of biodegradable COD. The BOD_∞ estimated has to be converted to COD_{BD}. The conversion factor was computed by simulating the BOD tests using ASM1, reduced for aerobic conditions. This approach provides a quantitative basis for this conversion factor. The sensitivity of this conversion factor to model parameter values and COD fractionation was determined, which showed that the conversion has to be adjusted for non-default values of the heterotrophic yield.

Keywords

Modelling; model calibration; influent characterisation; total BOD; activated sludge; wastewater treatment.

3.5.1 Introduction

Development of easy-to-use methods for influent characterisation suitable for practical application is very important in the modelling of activated sludge processes, and has therefore received considerable attention over the last years. The Activated Sludge Model No. 1 (ASM1, Henze *et al.*, 1987) has become a standard model to describe the dynamics of wastewater treatment plants. An influent characterisation is required for most applications of the model. Examples of such applications are: checking of design under dynamic operating conditions (in designing new or upgrading existing plants), process analysis, design of control systems for process optimisation or as an aid in operation. Different approaches for the COD characterisation task have been proposed, ranging from physical/chemical methods (e.g. Lesouef *et al.*, 1992) via respirometric experiments (e.g. Spanjers and Vanrolleghem, 1995) to dedicated pilot plant tests (e.g. Dold *et al.* 1986; Henze *et al.*, 1987). Recently, a project has been carried out on influent characterisation (STOWA, 1996), consisting of a literature review, an inventory of methods applied in practice by the waterboards and universities and a sensitivity analysis. It was concluded that, still, no method is available which is standard, reliable, reproducible, and easy-to-use.

[†] This section has been published as: *On BOD tests for the determination of biodegradable COD for calibrating Activated Sludge Model No. 1* by S.R. Weijers (1999) Wat. Sci. Tech. **39** (4) pp.177-184.

In the same report, biodegradable COD was indicated as the most important quantity for characterisation. Guidelines for influent characterisation are given, which consists of physical-chemical characterisation in combination with BOD tests, where the BOD tests are used to determine total biodegradable COD. Two conversion factors are required, one to convert BOD_5 to BOD_∞, based on a first-order assumption on BOD kinetics (Eq. 1), and one to convert BOD_∞ to COD_{BD} (Eq. 2):

$$BOD_\infty = BOD_5/(1-e^{-5\,k}) \quad (1)$$

$$COD_{BD} = BOD_\infty/(1-Y_{H,BOD}) \quad (2)$$

With suggested values of k = 0.23 and $Y_{H,BOD}$ = 0.2, this would give COD_{BD}/BOD_5 =1.463 · 1.25 = 1.83. With this approach, however, two problems exist: 1) k varies with the wastewater; values between 0.1 and 0.7 have been reported (Metcalf & Eddy, 1979), which give BOD_∞/BOD_5 conversion factors of 1.03 up to 2.54; Henze *et al.* (1995) report values for BOD_∞/BOD_5 approximately between 1.43 and 1.67; 2) The value of $Y_{H,BOD}$ is not quantitatively motivated. As a result, there is uncertainty in the conversion of BOD_5 to COD_{BD}. A suggested approach to solve the first problem is to measure BOD_{20} and use this as BOD_∞; however, the BOD_{20} test is not reproducible (Kuipers, 1996). Therefore, as an alternative to BOD_{20} tests, it has been suggested to estimate BOD_∞ by fitting first-order models to BOD curves. As another approach to circumvent these problems, van Loosdrecht (1996) suggested a COD_{BD}/BOD5 conversion factor of 2 instead of 1.83, based on typical yields that are observed in microbiological studies. However, this approach also lacks quantitative foundation and would therefore introduce considerable uncertainty.

The importance of developing methods for determining biodegradable COD, the lack of experience with BOD tests for this purpose and problems with its interpretation indicated above motivated the work described in this section. One particularly interesting question is whether it is possible to have one conversion factor for a specific wastewater to convert BOD_5 to COD_{BD} or whether conversion factors based on other quantities must be used.. The set-up of BOD tests, estimation of BOD_∞ from the measured data, the precision of the estimation results and determination of BOD_∞/BOD_5 and COD_{BD}/BOD_∞ conversion factors are successively studied below.

3.5.2 Methods and theory

In two measurement campaigns, series of BOD tests lasting up to 15 days were carried out in the framework of a modelling campaign of the Venlo WWTP. In the first campaign, duplo BOD tests were taken for 4 grab samples and one composite sample. BOD was measured at t=2 or 3, 5 and 9 or 10 days, without nitrification inhibitor. Results from the first measurement campaign were used to improve the set-up of the BOD test series. In the second campaign, for each of four grab samples, two triplo BOD tests were carried out, one with and one without nitrification inhibitor, measuring BOD at t=2,5,7,9,12 and 14 days (or 1,4,6,8,11 and 13 days). At the first and last time instant, an additional triplo test was done. From the curves with nitrification inhibitor thus obtained the BOD_∞ was estimated in four ways: 1) one rate constant per individual sample (separate estimation); 2) one rate constant over all samples (joint estimation); 3) two rate constants per individual sample (separate estimation); 4) two rate constants over all samples (joint estimation). First-order kinetics are normally used to describe BOD curves. Here, also second-order kinetics were applied to investigate whether this would

better describe BOD curves, thus checking for sluggish start-up due to possibly low initial biomass concentration. First-order kinetics are decribed by Eq. 3:

$$BOD_p(t) = BOD_\infty (1 - e^{-k\,t}) \tag{3}$$

and second-order kinetics by Eq. 4:

$$BOD_p(t) = BOD_\infty \left(1 - \frac{k_2}{k_2 - k_1} e^{-k_1 t} + \frac{k_1}{k_2 - k_1} e^{-k_2 t}\right), \quad k_1 \neq k_2; \tag{4a}$$

$$= BOD_\infty \left(1 - e^{-k_1 t} - k_1 t e^{-k_1 t}\right), \quad k_1 = k_2. \tag{4b}$$

The Nelder-Mead (or Simplex) method was used for parameter estimation. Least squares parameter estimation minimises the weighted sum *J* (Eq. 1) of squared errors between model outputs $y(k,\theta)$ and measured plant outputs $y_m(k)$ with weights R_k:

$$J = \sum_{k=1}^{N} (y(k,\theta) - y_m(k))^T R_k (y(k,\theta) - y_m(k)). \tag{5}$$

Output sensitivity functions were obtained by linearisation of this functional in the optimal parameter point $\hat{\theta}$:

$$y(k,\hat{\theta} + \delta\theta) = y(k,\hat{\theta}) + \left[\frac{\partial y(k,\theta)}{\partial \theta^T}\right]_{\hat{\theta}} \delta\theta = y(k,\hat{\theta}) + Y^T(k,\hat{\theta})\delta\theta \tag{6}$$

with $Y(k,\hat{\theta})$ being the output sensitivity functions. From the output sensitivities and the variance of the measurement noise σ_k^2 the Fisher information matrix was computed (Walter, 1997):

$$F(\hat{\theta}) = \sum_{k=1}^{N} \frac{1}{\sigma_k^2} Y_\theta(k,\hat{\theta}) Y_\theta^T(k,\hat{\theta}). \tag{7}$$

where the noise variance was estimated from the reduced sum of squares, applying unweighted least squares:

$$\sigma_k^2 = \hat{\sigma}^2 = s^2 = \frac{1}{N-p} \sum_{k=1}^{N} (y(k,\hat{\theta}) - y_m(k))^2 = J(\hat{\theta})/(N-p), \tag{8}$$

with p being the number of estimated parameters. Under certain assumptions (no model mismatch, white measurement noise and some more, see Walter 1997), the inverse of the Fisher matrix provides the lower bound of the parameter error covariance matrix:

$$\mathrm{cov}(\hat{\theta}) \geq F^{-1}(\hat{\theta}). \tag{9}$$

The above shows that the Fisher matrix relates measurement accuracy, contained in σ_k^2, via model output parametric sensitivities $Y(\hat{\theta},t)$ with parameter estimate accuracy. The standard deviation of the *i*th estimated parameter $\hat{\theta}_i$ was obtained from the square root ρ_i of the *i*th diagonal element of the inverse Fisher matrix. Under the normality assumption, an approximate

95% confidence interval is then given by [$\hat{\theta}_i$ - 1.96ρ_i , $\hat{\theta}_i$ - 1.96ρ_i] (Rosenbrock and Storey, 1966, Walter, 1997). Also under the normality assumption, an approximate, ellipsoidal 95% confidence contour was computed from:

$$(\theta - \hat{\theta})^T F(\theta - \hat{\theta}) = 1.96. \tag{10}$$

Exact confidence contours were computed with the according $F_\alpha(p,N-p)$ levels as approximate confidence levels (Draper and Smith, 1981):

$$J(\theta) = J(\hat{\theta})\left\{1 + \frac{p}{N-p} F_\alpha(p, N-p)\right\} \tag{11}$$

As an additional judgement on the quality of fit, the condition number of the Fisher matrix F was computed, the condition number being defined as the ratio of the largest and smallest eigenvalue, CN = $\overline{\sigma}(F)/\underline{\sigma}(F)$.

The BOD_∞ to COD_{BD} conversion factor was computed by simulating the BOD tests using ASM1, reduced for aerobic conditions. This reduction consisted of: 1) setting all Monod terms with dissolved oxygen (DO) limitation to 1; 2) setting all terms with DO inhibition to 0, thus neglecting denitrification and anoxic hydrolysis; 3) not considering inert components originally present in the wastewater (ASM1 component X_I), however including loss of biodegradable COD in the death-regeneration cycle due to inert product formation from biomass decay (X_P); 4) omitting alkalinity; 5) omitting nitrification (by setting X_{BA}=0). The experimentally determined BOD_∞ was used to compute initial conditions on COD fractions in the simulation following the STOWA guidelines. Default ASM1 model parameters were used in the simulation. The STOWA guidelines for influent characterisation are briefly summarised below.

Measure: Influent: Total COD_{tot}, membrane filtrated (0.45 μ) COD_{mf}, BOD_5, NH_4-N
Effluent: $COD_{eff,mf}$

Compute: $S_I = 0.9\ COD_{eff,mf}$; $S_S = COD_{mf} - S_I$; $X_{BH} = 0$; $X_S = COD_{BD} - S_S$;
$COD_{susp} = COD_{tot} - COD_{mf}$; $X_I = COD_{susp} - X_S$.
$S_{NH} = NH_4$-N ; $S_{ND} = 0.03\ COD_{mf}$; $X_{ND} = 0.04\ COD_{susp}$.

The conversion factor COD_{BD}/BOD_∞ was then computed from the ratio of the initially present COD_{BD} ($Ss(0)+X_S(0)+X_{BH}(0)$) and the BOD at infinite time (computed from integration of simulated OUR), $COD_{BD}(t=0)/BOD(t_e)$ (here, t_e was chosen 40 days, guaranteeing a relative precision of less than 0.001). In addition, the sensitivity of the conversion factor to model parameter values as well as to COD fractionation was computed.

3.5.3 Results and discussion

In the first series, 4 of the tests did not follow a first-order response. The BOD at t=9 or 10 was higher than expected from the points at t=2 or 3 and t=5 (results not shown). It was suspected that this effect was due to nitrification. Simulation of the BOD test with (a reduced) ASM1 without and with nitrification using default model parameters and a preliminary influent characterisation supported this idea. Therefore, it was concluded that in this series only data up

to t=5 days could be used. Because too little data points were available to estimate rate constants for individual samples, in this series kinetic rate constant(s) could only be estimated for all samples together. In the second series, more points were measured to allow estimation of kinetic constants for each individual sample. In the second series, the influence of nitrification was confirmed: BOD without nitrification inhibitor was approximately 50% higher at the end than BOD with inhibitor. In Figure 1, the estimation results are shown for the tests with nitrification inhibitor added.

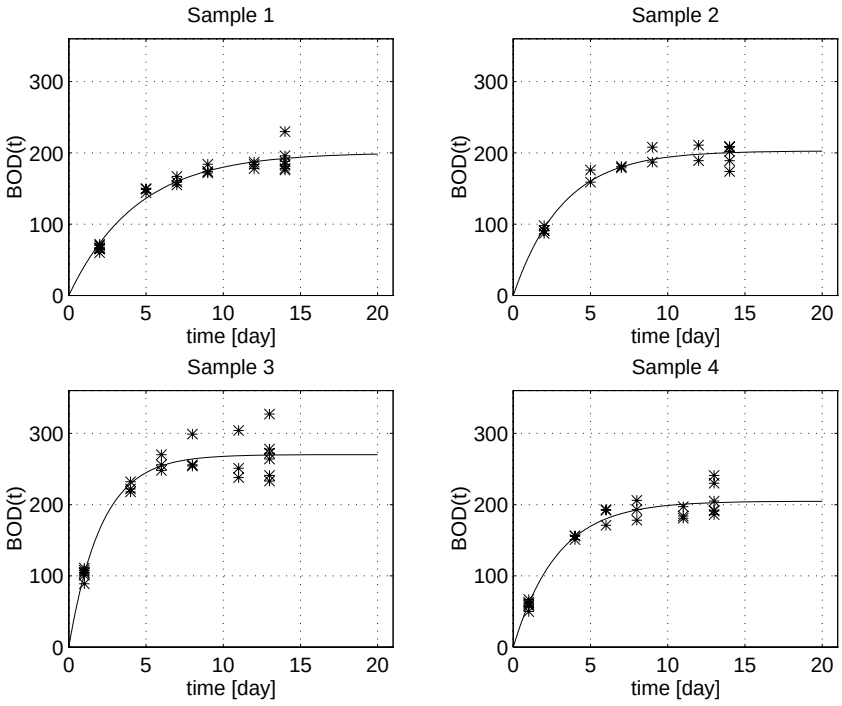

Figure 1: Estimated BOD curves, separate estimation

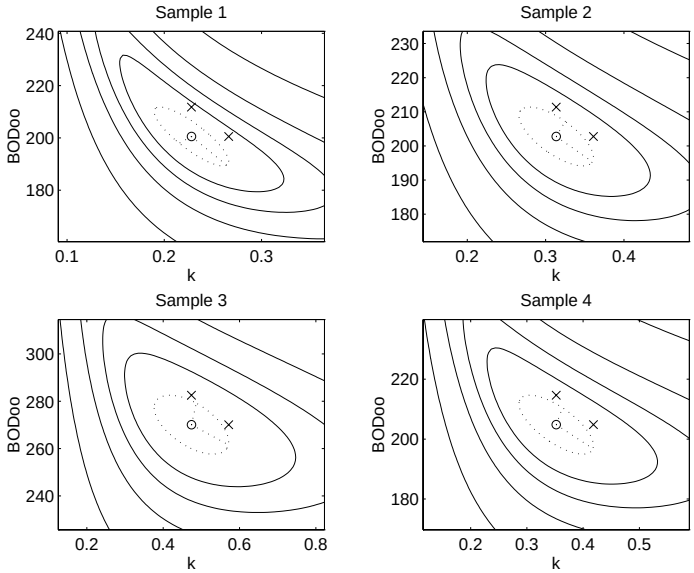

Figure 2: Estimated parameters (o), 1.96·standard deviation (x), approximate confidence contours (ellipse) with eigenvectors (…) and exact contours with approximate confidence levels (—) (90%, 95%, 97.5% and 99%)

Confidence contours are shown in Figure 2 and in Table 1, the results are summarised. The estimated rate constants and BOD_∞ values are given together with their standard deviations.

It can be observed that different k values are found for the samples, which would result in different BOD_∞/BOD_5 conversion factors. The ratio BOD_∞/COD_{tot} is fairly constant, however. The ratio of BOD_5 (computed from estimated parameters) to COD_{tot} shows a much larger spread. Using one rate constant for all samples, indicated as joint estimation, results in an expected decrease in the spread of BOD_5/COD_{tot}, at the expense of an associated increase in the spread in BOD_∞/COD_{tot}.

Table 1: Estimated rate constants and BOD_∞ for first-order fits, separate and joint estimation

	Sample 1	Sample 2	Sample 3	Sample 4	Average (sd)	sd (%)
Separate k (sd)	0.228 (0.020)	0.313 (0.024)	0.474 (0.050)	0.352 (0.034)	0.342 (0.102)	
BOD_∞ (sd)	201 (6)	203 (4)	270 (6)	205 (5)		
BOD_∞/COD_{tot}	0.400	0.394	0.438	0.424	0.414 (0.021)	5
BOD_5/COD_{tot}	0.2704	0.311	0.397	0.352	0.333 (0.054)	16
CN(*F*)	12	6.8	7.1	8.3		
J (N)	3,028 (24)	1,911 (24)	10,232 (18)	4,390 (24)		
Joint k		0.353 (0.021)				
BOD_∞	181 (5)	198 (5)	282 (5)	205 (5)		
BOD_∞/COD_{tot}	0.360	0.385	0.457	0.424	0.406 (0.043)	11
BOD_5/COD_{tot}	0.298	0.318	0.379	0.352	0.337 (0.036)	11
CN(*F*)			6.1			
J (N)			27,610 (90)			

The results of simultaneous estimation are given in Figure 3. In Sample 1, it can be seen that the early BOD values are overestimated (too high k), while in Sample 3 they are underestimated (too low k). Also an F-test on the parameter estimates was carried out, which failed for a 95% confidence level. (The F-test did not fail however with higher confidence levels). From the results, it appears that the k value may vary over different samples of the same wastewater, which is most probably due to differences in the amount and the kinetics of the influent (heterotrophic) biomass. Influent characterisation based on separate estimation therefore shows more consistent results, as will become clear in the sequel (see also Table 5). It is concluded that 1) it may be dangerous to base COD_{BD}/BOD_5 conversion factors on only one tested BOD sample; and 2) that it may be dangerous to use BOD_5 as a basis of biodegradable COD estimation from k values identified in earlier experiments, even if obtained from several, different samples.

Estimation of two rate constants was not useful, and led to over-parameterisation in all cases as judged from the high condition numbers of the Fisher Information matrix. All values of the condition number were higher than 5000, and in some cases much higher. It is consequently concluded that the BOD curves can be adequately described by first-order kinetics.

Subsequently, the BOD tests were simulated using the reduced ASM1 (Figure 4). A COD characterisation was carried out following the STOWA guidelines, from the measurements listed in Table 4 and using the estimated BOD_∞. Also measurement results without nitrification inhibitor are shown. In the simulation also X_{BH} is required. Here, X_{BH} was assumed to 25% of biodegradable suspended COD, X_{BD}. It is emphasised that the plotted BOD curve is not an estimated curve, but a curve obtained using ASM1 default parameters. The simulated BOD

overestimates the BOD, especially at the beginning of the curve. Adjustment of some of the ASM1 parameters and influent characterisation, especially the amount of biomass, might be used to fit the curve to the measurements, but this was not the subject of this study.

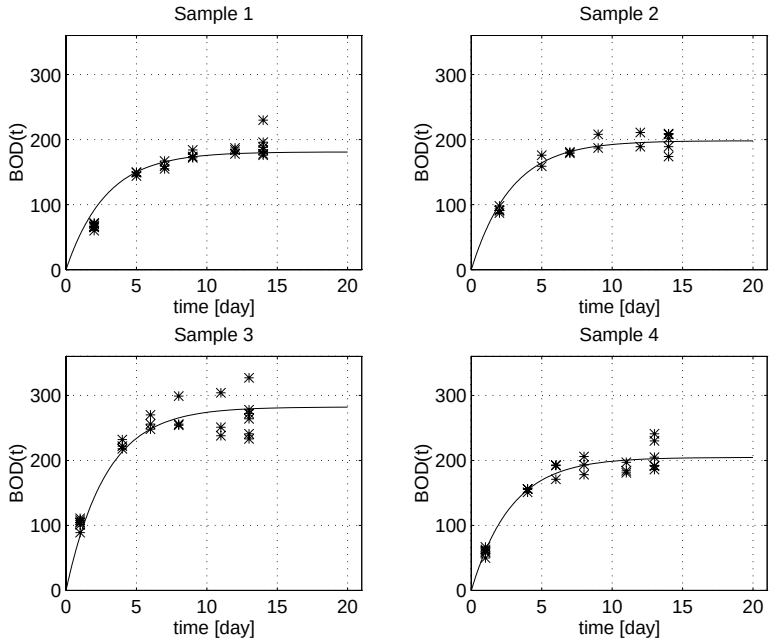

Figure 3: Estimated BOD curves, joint estimation

The simulated BOD curve can be typically divided into 3 areas: 1) High respiration rate determined by μ_H at high S_S; 2) lower respiration rate determined by k_h due to hydrolysis of X_S, both during day 1; and 3) lower respiration rate determined by decay of X_{BH} (most of the time). The initial steep increase in BOD in Figure 4 (t<1d.) corresponds to area 1 and 2. The period thereafter (t>1d.) corresponds to area 3.

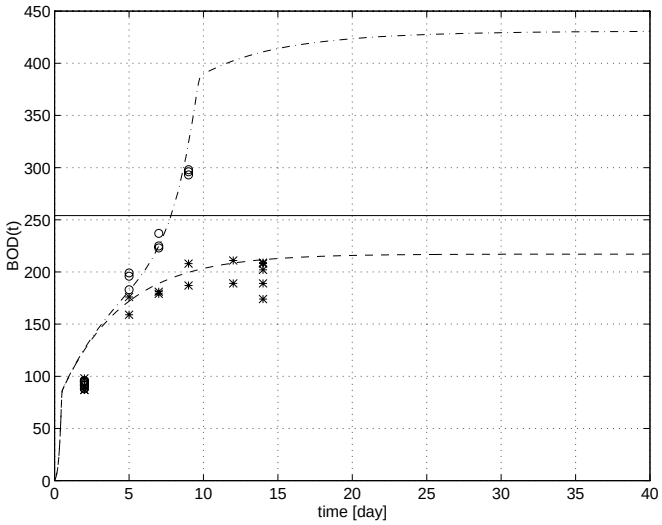

Figure 4: Measured and simulated batch test (Sample 2) without (*, --) and with (o, -.-.) nitrification

The conversion factor was computed for different influent characterisations. For X_{BH} fraction smaller than 25% of COD_{BD}, the conversion factor was between 1.17 and 1.19. The ratio of S_S/X_S had negligible influence. For practical situations, the uncertainty in the conversion factor

due to uncertainty in COD characterization will thus be limited to approximately 1%. The larger conversion factor at higher X_{BH} values in ASM1 can be understood as follows. If $X_{BH}(0)$ is low and the sum of $S_S(0)$ and $X_S(0)$ are high, respiration of $S_S(0)$ and $X_S(0)$ causes a significant contribution BOD, without associated inert product formation.

Table 2: Conversion factor COD_{BD}/BOD_∞ with different COD characterisations

$S_S(0)$	$X_S(0)$	$X_{BH}(0)$	COD_{BD}/BOD_∞
224	22.5	7.5	1.172
0	246.5	7.5	1.172
224	29	1	1.169
224	22.5	7.5	1.172
224	5	25	1.178
224	1	29	1.180
164	30	60	1.191
100	30	124	1.217
0	30	224	1.258

Sensitivity coefficients of the factor to model parameters are given in Table 3. Only the stoichiometric coefficients Y_H and f_P have a significant influence on the conversion factor. It is concluded that for practical situations, only Y_H is of relevance.

Table 3: Sensitivity coefficients of conversion factor COD_{BD}/BOD_∞ to parameter variations

Y_H	f_p	μ_H	K_S	b_H	k_h	K_X
0.431	0.156	-0.007	0.00656	0.00651	-0.00003	0.00002

Finally, the effect of the value of Y_H was determined by calculating the conversion factor for different values of this parameter. The result is plotted in Figure 5. This figure can be used to determine the conversion factor for calibrated values of Y_H. Influent characterisation results (Y_H=0.67) are given in Table 5.

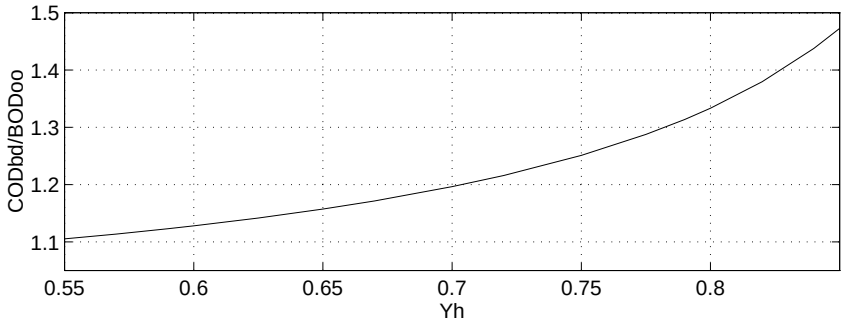

Figure 5: Conversion factor COD_{BD}/BOD_∞ as a function of Y_H.

Table 4: Measured and computed quantities for influent characterisation

	COD_{tot}	COD_{mf}	$COD_{eff,mf}$	NH_4-N	COD_{susp}
Sample 1	503	241	26	40	262
Sample 2	515	248	30	33	267
Sample 3	617	282	31	39	335
Sample 4	483	227	35	35	256

The spread of the influent characterisation obtained when using results from separate estimation is much smaller than when using results from joint estimation. For this particular influent, with joint estimation even invalid results were obtained for the amount of suspended biodegradable COD (X_S+X_{BH}). It can also be seen that the fraction of biodegradable COD is fairly constant for

the different samples of the same wastewater. It is concluded that total COD is a better basis for determining the biodegradable COD fraction than BOD_5. A COD_{BD}/COD_{tot} ratio can be used to obtain COD_{BD} for samples of which COD_{tot} has been measured, this ratio being determined through separate estimation from preferably several, different samples.

Table 5: COD fractionations with separate and joint estimation (COD_{BD}/BOD_∞=1.18)

			Separate			Joint		
	fS_I	fS_S	$fCOD_{BD}$	fX_{BD}	fX_I	$fCOD_{BD}$	fX_{BD}	fX_I
Sample 1	0.04	0.43	0.47	0.04	0.48	0.42	-0.01	0.53
Sample 2	0.05	0.43	0.47	0.03	0.49	0.45	0.02	0.50
Sample 3	0.04	0.41	0.52	0.10	0.44	0.52	0.10	0.44
Sample 4	0.06	0.41	0.50	0.09	0.44	0.50	0.09	0.44
Mean			0.49	0.07	0.46	0.47	0.05	0.48
sd			0.02	0.04	0.03	0.04	0.06	0.05

Note: $fX_{BD} = fX_{BH} + fX_S$; sd : standard deviation

3.5.4 Conclusions

Total BOD (BOD_∞) for a given wastewater can be obtained through estimation from measured BOD curves, preferably from different samples. Addition of nitrification inhibitor is required. Separate estimation of a rate constant for each individual sample is advised, as the BOD kinetics may vary from sample to sample. For the same reason, the BOD_5 is not a good basis for determination of biodegradable COD using an (one) identified rate constant, even if this is obtained from several samples. The estimated total BOD can be converted to biodegradable COD using a COD_{BD}/BOD_∞ conversion factor, which can be computed on the basis of ASM1. This approach provides a quantitative motivation for this conversion factor, interpreting BOD tests in correspondence with the intended use in ASM1. With default ASM1 parameters, the COD_{BD}/BOD_∞ conversion factor can be assumed 1.18 ± 0.01. For non-default values of Y_H, the conversion factor must be adjusted. Total COD is suggested as a basis for computation of biodegradable COD for other (e.g. historical) samples instead of BOD_5, because the ratio of biodegradable COD and total COD is much more constant for a given wastewater than the ratio of COD_{BD} and BOD_5.

3.5.5 Acknowledgements

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3.6 Discussion and conclusions

In this chapter, modelling of activated sludge plants was studied, focusing on the bioreactor. Both biokinetics and transport physics are important in reactor modelling. Biokinetics are typically modelled with ASM1, while transport in the reactor is usually modelled with combined models from ideal model reactors. For accurate prediction of real activated sludge plant behaviour therefore, both ASM1 parameters and transport models need to be calibrated.

Most emphasis has been put on calibration of ASM1 model parameters. An assessment of calibration strategies in the literature shows that no clear procedures for ASM1 calibration exist. This is partly due to the identifiability properties of the model, which were therefore further studied.

First, an analysis of local identifiability of biological parameters from full-scale wastewater treatment plants was carried out (Section 3.3). The results of this analysis indicated that from realistic input/output measurements approximately eight parameters could be estimated. This was confirmed by additional tests estimating parameters from artificial data. Using real plant data, only five to six parameters could be uniquely estimated. This lower number obtained when using real data was most probably due to model mismatch of the transport model.

Subsequently, a procedure was suggested for global analysis of practical identifiability in Section 3.4, to investigate the dependency of the results of the local analysis towards the parameters values that must be assumed *a priori*. This procedure includes an efficient randomised approach employing Latin Hypercube Sampling. A parameter identifiability ranking was made to reveal dependency of results on the a priori selection of the parameter values in the local analysis. This ranking showed that approximately twelve to fourteen parameters can be considered important and should be considered in calibration. Other parameters may be fixed and taken from the literature. While the exact results obtained may differ from plant to plant, we expect the same trends will be observed for other continuously operated systems.

The results of this global analysis further led to conclude that additional experiments are required, because not all parameters can be estimated from full-scale input/output data. Respirometric tests are promising to provide additional information. Especially, they can be applied for separate influent characterisation. For this purpose, a BOD test for determination of biodegradable COD was studied. Analysis of the results showed that instead of the suggested use of BOD_5 as a basis to determine biodegradable COD, total COD should be used. This is because different kinetics may occur in BOD tests for a given wastewater. Interpretation of results of respirometry however is complicated by the fact that biologic parameters may differ from those in the plant.

A special note is made with respect to the heterotrophic yield, Y_H. This parameter is required for interpretation of respirometric experiments. It appears to be the best identifiable parameter from full-scale input/output data. While several authors have suggested using default values for this parameter, it thus seems preferable to estimate this parameter from full-scale data.

Practical identifiability analysis based on the FIM, especially using the determinant or a combined criterion based on the determinant and the condition number, proved a very powerful tool for design of experiments in ASM1 calibration. This tool can be used in a second step after

selection of identifiable parameters, namely for selection of additional experiments. For example, using the condition number, one might select to determine those parameters that have the strongest interaction with the parameters identified from full-scale plants.

While the identifiability results obtained and procedures proposed in this chapter provide important insight and tools for improved ASM1 calibration, the state-of-art assessment also indicated that the role of mixing in ASM1 calibration needs further attention.

Chapter 4 Model reduction

Sitting back, he yawned. The optimisation took so long. He knew the system was stiff, and to accelerate the simulations he had already selected the special solvers for stiff differential equations. Moreover, he had used several options for speeding up the computations like employing the sparse structure of the system and analytic computation of the Jacobian matrix. Indeed, the simulations were now much faster. However, he realised that for the optimisation he had in mind, this was not sufficient. He had to look for a more fundamental solution. Would it be possible to break down the problem into smaller pieces? He suddenly realised there might be a connection with a related problem he once read about and he immediately set out to look for it.

This chapter treats model reduction and consists of two parts. The first part, Sections 4.1 - 4.4, develops a method for model reduction to obtain (nonlinear) reduced models for controller design or as internal model in model based control[†]. Section 4.1 motivates the need for model reduction and gives an overview of reduction approaches in the literature. Section 4.2 reviews model reduction of activated sludge models, especially ASM1. Activated sludge models are stiff, which means that the processes have timescales that differ over one or more orders of magnitude. Therefore, separation into models for different timescales is a logical approach for reduction. The review shows that such reduction is often performed quite heuristically and more insight in the timescale properties of ASM1 is desired. Singular perturbation is a systematic technique for such reduction with some nice properties and is studied into more depth in Sections 4.3 and 4.4. Section 4.3 reviews application of singular perturbation to bioprocess systems to reveal if methods exist to obtain or detect the so-called standard form, which is the difficult part of reduction by singular perturbation. The model is in standard form if it can be separated into slow and fast states, which is required for order reduction with singular perturbation. Because existing methods appear insufficiently straightforward, Section 4.4 develops a method for this task. Three procedures are proposed, namely a direct scaling procedure, a procedure based on timescale estimation and an analytic scaling procedure. The procedures are tested on a simple continuous general bioprocess model. The timescale estimation procedure is successful in all cases studied and appears a helpful tool in model reduction through timescale separation. Application of the technique to reduce ASM1 is beyond the scope of this thesis, however. The analytical scaling leads to the standard form in some cases and provides valuable insight into conditions for model reduction in bioprocess systems. However, the procedure is not successful in all the cases studied. The direct scaling procedure is not suited as a general method.
The second part[‡], Section 4.5, focuses on model reduction of ASM1 in a batch test for a specific purpose, namely for interpretation of the BOD test to determine biodegradable COD that was studied in Section 3.5. A quasi-steady-state assumption is applied to obtain a reduced first-order model of ASM1. This reduced model is useful to support quantitative interpretation of batch tests for the important task to determine biodegradable COD in ASM1 calibration.

[†] This part has been submitted for publication in Focus in Biotechnology.
[‡] This part has been published as *Model reduction of ASM1 for interpretation of BOD tests for determination of biodegradable COD* by S.R. Weijers (1999) Proc. ECB9 (9th European Conference on Biotechnology).

4.1 Introduction

4.1.1 Need for reduction of rigorous, mechanistic models

Dynamic simulation based on rigorous, physics-based mechanistic modelling has become a standard tool in many engineering fields. Examples are finite element models in structural dynamics, computational fluid dynamics, the SPICE program for circuit analysis in electrical engineering and dynamic flowsheeting in chemical engineering. In biotechnology, process modelling is well established (Roels, 1983).

Rigorous models are applied for a variety of tasks. They are useful in system design, especially to check system behaviour under extreme dynamic loading conditions. They are very helpful in understanding system behaviour in science and engineering. As they typically contain much prior knowledge from the relevant application domain, their prediction accuracy and range of validity can be high in principle, if the model building and model tuning tasks are designed to achieve this accuracy. However, the costs of rigorous models are generally high because of the effort required to construct them.

For engineering tasks described above, typically high-dimensional models result. Despite the usefulness of rigorous, large models for the tasks described above, for the following important tasks simple models are better suited:
Process control: Many control theory concepts are only applicable to low-order models. The high dimensionality of large models result in enormous computational requirements, ill-conditioned problems and often stiff numerical problems due to interaction of slow and fast dynamics (Kokotovic *et al.*, 1986). Relatively low-order reduced models are therefore required for controller design and as internal models in model-based control,.
Model identification: Rigorous mechanistic models typically require high investments in model tuning and validation. Moreover, problems that are more fundamental exist because large models typically exhibit lack of parameter identifiability. In addition, mechanistic models contain internal states whose behaviour is difficult to verify (or falsify), which is referred to as verifiability (Jeppsson, 1996). The need for simple, well-identifiable models holds true for off-line identification and even stronger for on-line identification for process monitoring and adaptive control.
Understanding of model behaviour: Although rigorous models may be helpful in system understanding, at the same time this understanding is hampered by their complexity. Much understanding can be acquired from reduced models describing only the most important phenomena.
System design through rigorous optimisation: many design problems might be solved more straightforwardly by applying an analytic design procedure, using (mathematical) multi-criteria optimisation, as discussed in Chapter 2. Due to their size, however, rigorous models are not suited for direct system design using optimisation; rather, they are most often used to check designs. Straightforward, systematic system design employing rigorous multi-objective optimisation would be facilitated if simple models containing the most important phenomena would be available.
Concluding, one may state that model reduction is required for several important tasks.

In wastewater engineering, rigorous modelling and dynamic simulation have become well accepted during the past decade since the publication of Activated Sludge Model No.1 (ASM1, Henze *et al.*, 1987). This model is now becoming routinely used in wastewater engineering. Model tuning of ASM1 has become an important task for process analysis, process optimisation

and process control and was studied in Chapter 3. Furthermore, advanced, model based control of wastewater treatment plants is expected to be important in meeting more stringent treatment requirements in an economical way. The mechanistic models based on ASM1 studied in Chapter 3 are not directly suited for control. If these mechanistic models accurately describe the process dynamics, however, reduced models can be extracted for controller design thus re-using the knowledge in the mechanistic models. Consequently, model reduction of ASM1 has received considerable attention in the literature.

In bioprocess engineering, reduced models may be fruitfully applied in process optimisation and process control, for example for dynamic optimisation of individual (fed-)batch processes, batch process scheduling and model based process monitoring.

4.1.2 Problem statement and methodology

This chapter wants to contribute to advancing the field of model reduction of ASM1 and bioprocess models, with emphasis on application in (model based) control and identification. The ultimate goal is to provide a methodology to derive nonlinear reduced models for different time-scales in a straightforward, systematic manner. In this chapter, the goal is to develop a method that can provide the starting point for such a straightforward nonlinear reduction procedure. This section outlines the methodology that is followed in Sections 4.1 - 4.4 to develope such a method.

To select a suitable reduction method, it is useful to first list desired properties of a candidate reduction method. The following properties are considered as desired in this thesis.

Nonlinear reduction methods are preferred, because nonlinear models can have a larger validity range than linear models.

The stiffness of activated sludge process argues to develop models that are suited for different timescales. For example, control of dissolved oxygen (DO) requires a different timescale than control of ammonia (and nitrate) or control of sludge. Models on these different timescales are therefore required for each of these control tasks, either for controller design or as internal model. Moreover, this fits well in a hierarchical control approach. Therefore, especially model reduction based on timescale separation is a logical approach.

Moreover, it is desired that the reduction method is systematic and straightforward to avoid time-consuming trial-and-error and iterations, and to be independent of (too much) application-domain dependent knowledge. Ideally, the reduction method would also supply an estimate of the error induced by the reduction.

Another desired property of reduction methods is that the states of the model retain their physical interpretation after reduction. This will enable a more direct interpretation of the controller design results and control actions. Moreover, if adaptive control is applied, identified parameters have a direct physical interpretation.

Finally, as this thesis focuses on the pre-denitrification plants and carrousels, the method should be applicable to derive reduced methods for these systems. Several reduced models have been derived for pre-denitrification plants, or, more exactly, for aerobic and anoxic conditions. However, reduced models for systems where simultaneous denitrification takes place, such as typically is the case in carrousels, are lacking. Methods that are helpful in reduction for these systems are therefore desired.

The need for reduced models in wastewater engineering has resulted in a variety of reduction approaches and reduced order models of ASM1. Section 4.1.3 discusses the most important reduction approaches in the literature. Section 4.2 gives a state-of-art overview of ASM1 model

reductions that are classified along the discussed reduction approaches. Aim of this overview is to obtain clarity into the limitations and possibilities of different reduced models and reduction methods. This should support selection of a suitable reduced model or reduction method.

The review in Section 4.2 shows that reduction through timescale separation is applied by several authors, but often in a heuristic fashion. Moreover, the timescale properties of ASM1 are not very well understood.

The technique of singular perturbation is therefore studied into more depth to better understand the timescale properties of ASM1 and thus provide a basis for developing a reduction methodology. The technique has the desirable properties of a candidate reduction technique listed above. It provides the mathematical basis for reduction by timescale separation, provides an error estimate, it is a systematic technique, and may therefore lead to a more straightforward reduction procedure. Moreover, it is applicable to nonlinear systems and, under certain conditions, the physical interpretation of states is retained.

In Section 4.3.1, the theory of singular perturbations (as used by Kokotovic *et al*., 1986) is summarised. For application of the singular perturbation technique for order reduction, the model must be in the so-called standard form. This means that the states of the model can be partitioned into ‘fast’ and ‘slow’ scales. (Also partitioning into more timescales is possible, e.g., fast, medium and slow). In that case, the reduction boils down to either eliminating the fast states to obtain the slow model or to eliminating the slow states to obtain the fast model. Upon reduction, the physical interpretation of states is then preserved.

If the model is not in standard form, a state transformation may be applied to bring it into standard form. In that case, the physical interpretation of the states is not retained. In fact, the fast and slow modes cannot be assigned to disjunct sets of states. This is not studied here.

It also happens that the model can be partitioned into slow and fast states, but that it is not easy to recognise this from the model equations. In that case, writing the model equations in a different way, e.g. by scaling, may show immediately from the scaled equations that the partitioning is possible indeed. Finding such a scaling is difficult however. In fact, recognising whether the model is in standard form and detection of the fast and slow timescales is the difficult part of the reduction technique.

Therefore, the study in this chapter focuses on recognising the state partitioning into fast and slow states and on recognising or obtaining the standard form.

One application of singular perturbation theory to an activated sludge plant model has been reported, which is discussed in Section 4.2.3. The authors applied a method that is based on eigenvalues for the state partitioning. The reduction was only partly successful. Section 4.3.2 reviews application of singular perturbation to reduction of – more general and closely related - bioprocess systems into more detail to obtain a more fundamental insight into timescale properties of bioprocess models in general and of ASM1 in particular. The review shows that singular perturbation of bioprocess models is not sufficiently well understood and it does not yield a method or rule for the state partitioning. Therefore, a method for this task is developed. A scaling procedure summarised in Section 4.3.3 provides the starting point for this method.

Three procedures are proposed in Section 4.4 as candidates for the state-partitioning task. They are tested on a simple bioprocess model in different operating conditions.

4.1.3 Reduction approaches for process engineering systems

Starting point in model reduction is the definition of the goal for which the model is intended. It can be argued that, for biological systems even stronger than in other basic sciences, the goal of the model determines its formulation (Vansteenkiste and Spriet, 1982). The goal determines selection of model inputs, including possible reference trajectories and disturbances, selection of model outputs and determines which model accuracy is required over which time horizon.

For the actual model reduction in this review, several approaches are distinguished and briefly explained below. The models obtained with these approaches differ in their degree of 'greyness'. Models that are obtained via systematic reduction of a white model whilst preserving the physical interpretation of the system states can be considered light grey. Simple, mechanistic input-output models are considered grey (Carstensen *et al*., 1995). The last category are black box models, such as polynomial models or artificial neural networks. It is noted that also mixed forms can be applied, e.g. models contain a mechanistic part and an artificial neural network (e.g. van Can, 1997). Alternatively, artificial neural networks can be configured to contain prior knowledge, e.g. of model structure.

The models are expected to allow further extrapolation beyond the experimental domain with increasing 'lightness'.

1. New model building from 'scratch'

One way to construct simple models is to disregard existing rigorous models and to build simple models from scratch. Of course, strictly speaking this is no model reduction. Nevertheless, the prior knowledge contained in rigorous models is often either implicitly or explicitly used in this approach.

2. Simplifying assumptions

Application of simplifying assumptions is a very frequently applied approach in model reduction. Here, we distinguish simplifying assumptions with respect to:

- Components; e.g. aggregation of variables (for example COD and BOD as total measures of pollutant concentrations);
- Processes; e.g. aggregation of reactions (for example modelling nitrification as a one-step process whilst it is a two step process);
- Lumping of space distribution: neglect or simplification of gradients in one or more directions;
- Kinetics, e.g. simplification of complicated kinetic schemes;
- Dynamics; these are treated in the next paragraph.

Often, simplifying assumptions are applied in a rather heuristic fashion, especially with respect to components. Several systematic methods can be applied for reduction of distributed systems, which are outside the scope of this chapter.

3. Neglect of dynamics by quasi-steady-state assumptions and singular perturbation

The neglect of dynamics that are fast or slow compared to the time scale of interest is discussed in its own right here as it is a central reduction approach. For example, it provides the basis for application of hierarchical control. In hierarchical control, a layered control approach is applied to control large, composite systems, for example in plant wide control. The control problem is decomposed into a hierarchical set of several levels of smaller sub-problems. On each level, dynamics of lower levels are assumed very fast and considered to be in (pseudo)-steady-state and dynamics of higher levels are assumed very slow and considered as constant.

In many cases, neglect of dynamics is performed heuristically. From field specific, physical understanding and process knowledge, fast states are omitted or slow states considered constant, without firm motivation. Although heuristically reduced models may (seem to) perform satisfactory, there is a need for a more thorough understanding of criteria for performing this reduction, preferably supported by formal proof or error analysis.

A well-known heuristic reduction approach is the quasi-steady-state approximation (QSSA) for reactive intermediate species. This approach, first introduced by Bodenstein and Lutkemeyer (1924) (Bowen *et al.*, 1962), has been extensively used in kinetic modelling. Criteria for its application were originally that concentration and time scale of the intermediate species are small. Later, the nature and consequence of the QSSA have been studied more thoroughly.

Singular perturbation is a mathematical technique to analyse timescale multiplicity and to perform a systematic order reduction and error analysis. It is the appropriate tool to provide the mathematical basis for quasi-steady-state assumptions. Its application to the QSSA in Michaelis-Menten kinetics is well studied, as will be summarised in Section 4.3.3.

4. Order reduction methods
In modern control engineering, order reduction of linear models is a very important task in control system design. Models for control are often obtained from linearization of high-dimensional rigorous models, resulting in very high dimensional models. Modern controller design methods, especially robust control design methods, yield even higher dimensional controllers. Order reduction of model or controller has become a necessity if they are to be implemented, as high-order controllers are usually not accepted in industry. Moreover, they may exhibit extremely poor robustness against controller parameter errors.

Consequently, order reduction has rapidly progressed and since the milestone publication by Moore (1981), a variety of reduction methods have been developed and are relatively well understood. Examples of reduction methods are Hankel norm reduction, balanced reduction and modal reduction. More recently, closed loop model reduction has received attention; see for example Wortelboer (1994), who also gives a thorough discussion on linear reduction methods.

For nonlinear system, balanced reduction methods have been developed (see Scherpen, 1994). With these methods, however, it may be more difficult to preserve the physical interpretation of states, as a state transformation is typically involved. Moreover, these methods do not provide a time-scale separation. Instead, they eliminate states that are poorly jointly observable and controllable and thus contribute least to input-output behaviour. Because we want to preserve the physical interpretation of states and focus on timescale separation, these methods are not considered further.

5. Black–box identification
Reduction through black box identification is an approach that requires little prior knowledge. Linear black box identification can be applied for weakly nonlinear systems within a limited domain. To construct reduced models of nonlinear systems with validity over a larger domain, nonlinear black box modelling techniques may be applied, especially artificial neural networks (ann's). The design of test signals in reduction through identification is very important. By selecting appropriate frequency ranges for the excitation signals, black box models may be obtained for different time scales.

4.2 Reduction approaches for ASM1

This section reviews approaches applied to reduce ASM1[20]. The emphasis is put on systems with enhanced nitrogen removal. In most of the cases presented, the purpose of model reduction is application for identification or control. The subsections follow the arrangement of reduction approaches as presented in Section 4.1.2. For each case discussed, the treatment system, goal for model reduction, motivation for selected approach will be indicated together with the reduced models. The ASM1 model has been described in Chapter 3 and Appendix A. For more information is referred to Henze *et al*. (1987) and other sources (e.g. Dold and Marais, 1986).

4.2.1 New model building from 'scratch'

Marsili-Libelli (1989) developed a low-order model for conventional activated sludge systems with BOD removal and nitrification. Motivation was that literature models are not suited for control, due to their complexity and poor identifiability. The model was developed to describe a) biodegradation carbonaceous COD b) nitrification c) DO utilisation d) sludge sedimentation. As a growth model a predator/prey modified Volterra-Leslie logistic equation was used instead of the usually applied, poorly identifiable Monod model. Theoretical and practical identifiability of the model were investigated and an observer was constructed based on this model.

Isaacs (1996) formulated several simple models for control of the Biodenipho system, which is an alternating, sequential semi-batch type system with nitrogen (and phosphorus) removal. Four (or six) phases are applied in each cycle. The control and model horizon is one phase, with a time scale in the order of several minutes. Three model-based control strategies were tested, external carbon addition control (ECAC), dissolved oxygen setpoint control (DOSPC) and cycle length control (CLC). All controllers employ a relational model and a predictive model. The predictive model is used to compute required denitrification rate, nitrification rate or cycle length during one phase. The predictive model was roughly the same in all control strategies, assuming zero-order kinetics both in nitrification and denitrification phase. Changes in biomass amount and composition need not be predicted, as actually measured denitrification and denitrification rates from the last preceding cycle are used. Different relational models were applied in the different strategies, as explained below. The relational model in CLC is trivial.

In ECAC, the prediction model computed the required denitrification rate r_d; the required external carbon addition rate q_{COD} to achieve this r_d is computed from the following relational model with the constants $r_{d,\,b}$ and $r_{d,\,max}$:

$$r_d = r_{d,b} + r_{d,max} \cdot \frac{q_{COD}}{K_{COD} + q_{COD}} \qquad (4.2.1)$$

In the model, the half-rate constant K_{COD} was fixed, thus the model is linear in parameters. The model parameters were estimated on-line from measured carbon addition and denitrification rates in preceding cycles using recursive least squares.

In DOSPC, the required nitrification rate r_n is computed with the prediction model. The required DO setpoint to achieve this nitrification rate is computed from the relational model and is held constant during one phase (using DO control).

[20] With 'model reduction', we will also denote 'model order reduction'.

$$r_n = r_{n0} + r_{n,max} \cdot \frac{S_O}{K_O + S_O} \qquad (4.2.2)$$

This relational model is estimated from measured DO and nitrification rates in preceding cycles using recursive least squares.

4.2.2 Simplifying assumptions

Several simplifying assumptions are applied in ASM1 reduction, which can be classified as follows (for an explanation of the symbols, see Chapter 3, Appendix A or the symbols list):

Simplification with respect to components
COD components:
1. No hydrolysis, no distinction between soluble and suspended biodegradable COD
2. Do not consider inert products as a separate component (X_I includes X_P)
3. Do not consider inert components at all (no S_I,X_I, X_P)

N components:
4. No suspended organic bound entrapped N (No X_{ND})
5. No ammonia production from organic bound nitrogen (No S_{ND})

Alkalinity:
6. Do not consider alkalinity

Simplification due to separation of aerobic and anoxic conditions
7. No denitrification under aerobic conditions
8. No nitrification under anoxic conditions

Simplifying assumptions with respect to kinetics
9. Replace terms with Monod kinetics by first-order or zero-order kinetics (the last corresponds to neglect of dependency on one or more limiting substrates)

Simplification with respect to dynamics
10. Neglect DO dynamics
11. Neglect dynamics of solute components
12. Neglect dynamics of suspended components

If one considers the huge number of possible combinations of simplifying assumptions, it is clear that a large number of reduced order models can be formulated. Up till now, a limited number of reduced order models have been published, which are presented in this section.

van Impe *et al*. (1991) and Vanrolleghem (1994) formulated a reduced and modified ASM1 model to be used in adaptive control. This is not discussed further, as it was developed for conventional activated sludge systems.

Carstensen *et al*. (1995) formulated grey models to have operational dynamic models capable of giving on-line information on the present state of the wastewater treatment plant. The system was the Biodenipho process, which has an alternating, sequential semi-batch type of operation, where nitrification and denitrification are separated in time. Different models are applied for both conditions. No biomass growth is modelled.

Nitrification: 1) The rate equation for ammonia removal contains both the maximal autotrophic growth rate and yield, which are not identifiable if the rate equation is not coupled to growth model for autotrophic biomass. Therefore, one overall maximal nitrification rate parameter is

used 2) No method for measuring the concentration of the autotrophic biomass exists, so the measured total solids concentration is used. This gives the following rate expressions during one batch phase.

$$\frac{dS_{NH}}{dt} = -r_{nit,max} \cdot \frac{S_{NH}}{K_{NH} + S_{NH}} \cdot \frac{S_O}{K_O + S_O} X_{SS} \tag{4.2.3}$$

$$\frac{dS_{NO}}{dt} = r_{nit,max} \cdot \frac{S_{NH}}{K_{NH} + S_{NH}} \cdot \frac{S_O}{K_O + S_O} X_{SS} \tag{4.2.4}$$

Denitrification: 1) One overall maximal denitrification rate is used. 2) No method for measuring the concentration of heterotrophic biomass exists, so the measured total solids concentration is used. 3) The ammonium load to the plant is used as this proved a correlated measure of the readily biodegradable substrate concentration, similar to Isaacs (1996) (eq. 4.2.1).

$$\frac{dS_{NO}}{dt} = -r_{denit,max} \cdot \frac{S_{NO}}{K_{NO} + S_{NO}} \cdot \frac{r_{load}}{K_{load} + r_{load}} X_{SS}\,. \tag{4.2.5}$$

Lukasse *et al*. (1997a,b, 1998a,b, 1999) developed reduced models for control of nitrogen removal in an activated sludge process consisting of one CSTR; clarifier dynamics were neglected. Two levels of model reduction were applied:

1) For nonlinear (open-loop) optimisation (optimisation horizon 1 day, Lukasse *et al*., 1998a).
To investigate optimal aeration strategies, a nonlinear model was developed. Dynamics of all suspended components, including biomass, were neglected. With respect to solute components, inert COD and alkalinity were not considered; DO dynamics were neglected by considering DO as an input instead of a state variable (assuming tight control). Ammonia production due to hydrolysis and ammonification was simplified by using a (constant) influent ammonia correction factor (in fact, this last simplification implies a quasi-steady-state assumption on hydrolysis and ammonification). These assumptions result in a reduction of ASM1 to a reduced third-order nonlinear model with the state variables S_S, S_{NH}, S_{NO}.

2) In receding horizon optimal control (Lukasse *et al*., 1997a,b, 1998a,b,1999).
To circumvent the disadvantages associated with the open-loop strategy, especially associated with uncertainty, feedback was introduced by applying RHOC (Receding Horizon Optimal Control), a Model Predictive Control law. Here, the requirement was to obtain an identifiable model, suited for on-line optimisation of an alternating process, with a timescale interest of hours. Assumptions were stated in Lukasse *et al*. (1997a and 1998a,b) (slightly different models were used, however): the system was forced to be either aerobic or anoxic by restricting $S_O \in \{0, 3\}$, transients between aerobic and anoxic phase were neglected, Monod kinetics was simplified to Blackman kinetics, arguing that the corresponding affinity constants were small and the substrate dependency only serves as a switching function. Additional assumptions were 1) If S_{NH}=0 and the system is aerobic, then the nitrification rate is such that all ammonia entering the reactor is nitrified. 2) ammonia and nitrate concentrations in the sludge recycle are equal to the concentrations in the reactor. This leads to the following equations:

$$\frac{d}{dt}\begin{pmatrix} S_{NH} \\ S_{NO} \end{pmatrix} = \begin{pmatrix} -r_{NH} \\ r_{NH} + r_{NO} \end{pmatrix} u + \begin{pmatrix} D_{in} S_{NH,in} \\ -r_{NO} \end{pmatrix} \tag{4.2.6}$$

$$r_{NH} = \begin{cases} r_{NH,max} & S_{NH} > 0 \\ D_{in} S_{NH,in} & S_{NH} = 0 \end{cases} \tag{4.2.7a}$$

$$r_{NO} = \begin{cases} r_{NO,max} & S_{NH} > 0 \\ 0 & S_{NH} = 0 \end{cases} \tag{4.2.7b}$$

with $u \in \{0,1\}$. (1 for aerobic, 0 for anoxic). For use in adaptive RHOC, $S_{NH,in}$, $r_{NH,max}$ and $r_{NO,max}$ were estimated based on measurement of S_{NH}, S_{NO} and S_O.

Jeppsson (1996) developed a reduced model for ASM 1 for application in control including adaptive control and requiring identifiability and 'verifiability' of the parameters and states. This last property expresses the specification that the states of the model are verifiable with information obtained from measurements. Reactors are assumed to be either aerobic or anoxic (separated) and ideally mixed (pre-denitrification system). The model has been used in studies by other authors (Ayesa *et al*, 1995) and is presented here into more detail.

The following assumptions and simplifications were made:
1. Do not consider alkalinity
2. Do not consider inert components (biologically not relevant, X_I is slow)
3. No ammonia production from organic bound nitrogen (No X_{ND}, S_{ND})
4. No hydrolysis, no distinction between soluble and suspended biodegradable COD (hydrolysis is not well understood; difficult to measure S_S and X_S; neglect fast dynamics of S_S).
5. Neglect DO dynamics: assumed to be controlled
6. Approximate Monod expressions by Blackman kinetics (it is assumed that substrate concentration is low).

Under these assumptions, five model components remain, namely X_{BH}, X_{BA}, S_{NH}, S_{NO} and X_{COD}. Two models were derived, one for anoxic and one for aerobic conditions.

Under anoxic conditions, there is no nitrification. Three processes take place: growth of heterotrophs, decay of heterotrophs and decay of autotrophs. The resulting model contains four parameters: r_H, Y_H, b_H and b_A.

$$r_{X_{BH}} = r_H \cdot X_{COD} X_{BH} - b_H X_{BH} \tag{4.2.8}$$

$$r_{X_{BA}} = -b_A X_{BA} \tag{4.2.9}$$

$$r_{X_{COD}} = -\frac{1}{Y_H} r_H \cdot X_{COD} X_{BH} + b_H X_{BH} + b_A X_{BA} \tag{4.2.10}$$

$$r_{S_{NH}} = -i_{XB} \left(r_H \cdot X_{COD} X_{BH} - b_H X_{BH} - b_A X_{BA} \right) \tag{4.2.11}$$

$$r_{S_{NO}} = -\frac{1 - Y_H}{2.86 Y_H} r_H \cdot X_{COD} X_{BH} \tag{4.2.12}$$

Under aerobic conditions, there is no denitrification. Four processes take place: growth of heterotrophs, decay of heterotrophs, growth of autotrophs and decay of autotrophs. The model contains six parameters: r_H, Y_H, b_H, r_A, Y_A and b_A.

$$r_{X_{BH}} = r_H \cdot X_{COD} X_{BH} - b_H X_{BH} \tag{4.2.13}$$

$$r_{X_{BA}} = r_A S_{NH} X_{BA} - b_A X_{BA} \tag{4.2.14}$$

$$r_{X_{COD}} = -\frac{1}{Y_H} r_H \cdot X_{COD} X_{BH} + b_H X_{BH} + b_A X_{BA} \tag{4.2.15}$$

$$r_{S_{NH}} = -i_{XB}\left(r_H \cdot X_{COD} X_{BH} - b_H X_{BH} - b_A X_{BA}\right) - \left(i_{XB} + \frac{1}{Y_A}\right) r_A S_{NH} X_{BA} \tag{4.2.16}$$

$$r_{S_{NO}} = \frac{1}{Y_A} r_A \cdot S_{NH} X_{BA} \tag{4.2.17}$$

Further reduction can be achieved by assuming all decay constants equal. Motivations for this reduction are that mainly the net growth rate is important and that the decay parameter is difficult to estimate.

Julien *et al*. (1998) developed reduced-order models for identification and control for aerobic and anoxic conditions, with ammnnia, nitrate and DO as state variables.

DO dynamics are often decoupled from the other ASM 1 equations, for use in (adaptive) control of DO. An example is the following (Lindberg, 1997). The decoupled balance equation for DO over a CSTR by assuming quasi-steady-state for the other components is written as

$$\frac{dS_O}{dt} = D(S_{O,in} - S_O) + k_L a(S_O^* - S_O) - r_{S_O}. \tag{4.2.18}$$

The conversion term, r_{So}, (which is the Oxygen Uptake Rate, OUR), is a time-varying parameter into which other states and parameters are lumped. It is modelled with a simple, discrete-time black-box model[21]:

$$r_{S_O}(k) = OUR(k) = \frac{1}{(1 - fq^{-1})(1 - q^{-1})} e(k) \tag{4.2.19}$$

4.2.3 Dynamics of variables

It is generally known that activated sludge systems exhibit stiff dynamics, with time scales ranging from seconds to weeks. This also holds true for activated sludge models based on ASM1. This section first summarises published material on time scale properties of ASM1 and subsequently summarises reductions based on simplifying assumptions with respect to dynamics.

[21] There may however be a danger in doing so, as the OUR is also affected by S_O itself and by S_S, which can both vary relatively quickly.

IAWQ Report No. 1 (Henze *et al.*, 1987) distinguishes three groups of variables: dissolved oxygen S_O, dissolved components and particulate components. This was concluded from a timescale estimation employing only the output (no input) transport terms and consumption (no production) terms of the balance equations. This yielded a time constant for S_O in the order of 1 s., for S_S, S_{ND} S_{NH} S_{ALK} in the order of 1 min, for X_{BH}, X_{BA}, X_S, X_P, and X_{ND} in the order of 10 min. These were estimates for time steps in Euler integration, and then this poses no problems because the resulting estimate is rather conservative. This analysis however may give misleading results as it may grossly overestimate the rate.

Weijers *et al*. (1995) carried out an analysis based on the Jacobian matrix of a pre-denitrification system, consisting of one anoxic and one aerobic reactor. The time constants, computed in a steady-state under typical operating conditions, ranged form 30 s., associated to a very low DO concentration (0.0114 mg/l) in the anoxic reactor, up to 13 days, associated to inert particulate COD. It is noted that the fastest time constant of 30 s. is much larger than 1 s., reported in (Henze *et al.*, 1987). It was observed that at elevated DO concentrations, DO dynamics were much slower (approximately 10 times as slow) than at the very low concentration of 0.0014 mg/l. This was observed both in the aerobic reactor (S_O =1.2 mg/l) and in the anoxic reactor (if for computation of the Jacobian matrix S_O was artificially elevated to 2 mg/l to be in the same order of magnitude as the other solute components). These results indicate that stiffness of DO dynamics is introduced if the DO concentration is much lower than the concentrations of other components that are involved in the same reactions.

Based on qualitative reasoning, Olsson and Jeppsson (1994) classified cause-effect relationships between available manipulated variables and measurable variables into different time scales. The motivation for classification was to achieve decomposition based on time scales for plant-wide control. Jeppsson (1996) summarised these in an incidence matrix, distinguishing fast (minutes), medium (hours), and slow (> days) dynamic influence. The matrix displayed that most outputs are effected by several inputs, where different variables may act on different time scales, which is caused by the strong internal couplings in the system. Interactions occur also within a timescale. Consequently, the authors expect that control of the activated sludge process requires a multivariable approach.

In a quantitative study of dynamics of ASM 1, Steffens *et al.* (1997) used a procedure developed by Robertson and Cameron (1997; see Section 4.3.4), to make a state partitioning. This required association of states to eigenvalues. They classified as fast S_S, X_S, S_{NH}, S_{ND} and X_{ND}, as medium S_I, S_{ALK} and S_{NO} and as slow X_{BA}, X_{BH}, X_I and X_P.

Subsequently, they applied singular perturbation to obtain a systematic reduction of ASM1 by removing fast and slow states. In addition to the eigenvalues, to select reducible states, they applied additional criteria on the relative error introduced (Robertson and Cameron (1997), Section 4.3.4). For fast mode reduction, S_S, S_{NH}, S_{ND} and X_{ND} were obtained using a relative error of 5% and with a lower bound on the time scale of interest of 12 h. The fast mode reduced model without these state variables showed a large error (100%) in S_{NH} however as a result of nonlinearity. For slow mode reduction, only X_{BA} was obtained as reducible state using a (large) relative error of 10% and with an upper bound on the time scale of interest of 20 minutes. The slow mode reduced model (constant X_{BA}) however showed a large error of 40% in S_{NH} after one day. Consequently, slow mode reduction with X_{BA} in this case was possible only for relatively short time horizons of approximately 6 h.

It is remarkable that the error if assuming constant X_{BA} was so large, and this confirms the disadvantages of heuristic reductions and the need to better understand timescale properties.

4.2.4 Order reduction methods

Van Schagen *et al.* (1995) applied algebraic reduction techniques to reduce a linearized ASM1 model of a carrousel system for application in LQG control of ammonia and nitrate with aeration in a carrousel system. No details on the method applied are given however.

4.2.5 Black–box identification

Lindberg (1997) applied subspace state space identification to identify a fourth-order linear model from a nonlinear model including 5 reactors based on ASM 1 and a settler model. The linear model was used in multivariable setpoint control of ammonia and nitrate in a predenitrification plant, with external carbon dosage, internal recirculation flow rate and the DO setpoint as manipulated variables. The study was to illustrate application of black-box identification, the nonlinear model being used to generate artificial data, rather than to perform model reduction. Nevertheless, it also illustrates how identification may be used to reduce a calibrated ASM1 model when this is available.

Some case studies of neural network application to model activated sludge systems have been reported (Su *et al.*, 1992; Côte *et al.*, 1995). Neural networks may also be used to obtain nonlinear reduced models. By incorporating prior knowledge into the structure of neural net, a larger validity range may be obtained. Identification of ann's for modelling of a phosphorous removal activated sludge plant model was unsuccessful, even for interpolation only (Vanrolleghem, personal communication). No other cases for wastewater treatment plant modelling however are known to the author.

4.2.6 Discussion and conclusions

The literature review shows that several approaches are applied in ASM1 model reduction. In almost all reported cases, the reduction was applied to lumped systems without concentration gradients, assuming the system to be either aerobic or anoxic. Thus, the reduction concentrated on reduction of the reaction kinetics, rather than reduction of transport and mixing in the reactor.

Of the approaches applied to model reduction of ASM1, simplifying assumptions have been applied most frequently. These assumptions lead to a variety of reduced models, depending upon the goals and system for which the model is intended. Proposed models range from simple black-box zero-order kinetic models via grey-box models with different Monod terms both neglecting biomass dynamics, to the more complicated model of Jeppsson, which includes biomass growth and decay. The first category is only valid over a short time horizon and within the domain of experimental conditions. The latter category may be used for process optimisation over a longer time horizon, and might be to some extent valid beyond the domain of experimental conditions.

The selection of simplifying assumptions is generally guided by the type of the treatment system, the input/output relations to be modelled and the time horizon of the model prediction, in a heuristic fashion. In several cases, the accuracy of the reduced models is not tested. From the set of reduced models, no single best reduced model can be selected. A more systematic investigation of the validity and implications of the various simplifying assumptions under different conditions (system, goals, input/outputs) would facilitate a more straightforward selection of simplifying assumptions and resulting reduced models.

Assumptions with respect to dynamics are usually applied to dynamically decouple (some of) the system equations, especially for application in hierarchical control. A thorough understanding of the time scale properties of the model is required to value validity and implications of reduced models based on these assumptions. Still however, little systematic efforts have been done to analyse and understand these properties. The biokinetic model itself is complicated, describing several biological and chemical processes that are strongly coupled. Furthermore, it is used to describe relatively complicated process configurations. Consequently, the dynamics of the model are not fully understood.

A disadvantage of the order reduction techniques and linear identification is that the validity of the linear model thus obtained is limited.

It is concluded that there is a need for more systematic order reduction methodology for activated sludge models. Moreover, more insight in dynamics of ASM1 is desired. In Section 4.3, for these reasons, singular perturbation is studied into further detail.

4.3 Singular perturbation of bioprocess systems: theory and review

Singular perturbation application to bioprocess systems is reviewed in this section. This method is a promising candidate to be part of a systematic methodology to derive reduced nonlinear models for different time scales, e.g. for application in hierarchical control, as was discussed in Section 4.1.2.

In 4.3.1, that part of the theory is presented that is required to understand the material in Sections 4.3 and 4.4. Section 4.3.2 reviews application of singular perturbation to bioprocess models. Section 4.3.3 presents a procedure to obtain the standard form that is required for application of singular perturbation for timescale separation. This procedure provides the basis for developing two procedures for state partitioning in Section 4.4. Section 4.3.4 discusses some methods that can be considered complementary to scaling in detecting fast and slow states.

4.3.1 Singular perturbation theory

Let the system be described by n+m equations in state-space notation (Kokotovic *et al.*, 1986)

$$\dot{x} = f(x, z, u, t, \varepsilon),\ x(t_0) = x_0, x \in R^n,\ u \in R^p \tag{4.3.1}$$

$$\varepsilon\dot{z} = g(x, z, u, t, \varepsilon),\ z(t_0) = z_0, z \in R^m. \tag{4.3.2}$$

with $\varepsilon>0$ a small scalar. Then for $\varepsilon\rightarrow 0$ the order reduces to n, because substituting a root $\bar{z}_i = \phi_i(\bar{x}, \bar{u}, t)$ of the equation $0 = g(x, z, u, t, 0)$ in (4.3.2) yields a reduced model:

$$\dot{\bar{x}} = f(\bar{x}, \phi_i(\bar{x}, \bar{u}, t), \bar{u}, t, 0) \equiv \bar{f}(\bar{x}, \bar{u}, t),\ \bar{x}(t_0) = x_0, \tag{4.3.3}$$

which describes the slow dynamics of the system, also referred to as the outer system or outer layer, or quasi-steady-state ($\bar{x}$ refers to the quasi-steady-state). Model (4.3.1), (4.3.2) is said to be in the so-called standard form if and only if the following crucial condition is satisfied.

Condition 3.1:
In a domain of interest, the equation $0 = g(x, z, u, t, 0)$ has $k\geq 1$ distinct real roots $\bar{z}_i = \phi_i(\bar{x}, \bar{u}, t), i = 1,2,..,k.$

The quasi-steady-state $\bar{x}(t)$ can be prescribed to start from x_0 and thus be a uniform approximation of x(t), that is, $\bar{x}(t) = x(t) + O(\varepsilon)$ holds for all $t \in [t_0, t_e]$, including t_o. The quasi-steady-state $\bar{z}(t)$ however is not free to start from a prescribed initial condition, and the approximation $\bar{z}(t) = z(t) + O(\varepsilon)$ can be expected to hold only on an interval excluding t_o, that is, for $t \in [\delta, t_e]$, with $\delta > t_0$. During an initial interval $[t_0, \delta]$ (the so-called boundary layer), the original variable z approaches $\bar{z}$. The substitution $t_f = t/\varepsilon$ ("stretching" the initial time) converts (4.3.1), (4.3.2) to a set of equations describing the fast dynamics of the system, the so-called boundary layer or inner system or inner layer (4.3.4).

$$\frac{d\hat{z}}{dt_f} = g(x_0, \hat{z}(t_f + \bar{z}(t_0), 0, t_0)), \quad \hat{z}(0) = z_0 - \bar{z}(t_0) \tag{4.3.4}$$

The solution to this problem provides a boundary layer correction term $\hat{z} = \bar{z} - z$ which is used in a possible approximation $z = \bar{z}(t) + \hat{z}(t_f) + O(\varepsilon)$, valid for $t \in [t_0, t_e]$, The important Tikhonov's theorem with respect to the boundary layer system states that (4.3.3) is a valid approximation of (4.3.1), (4.3.2) for all $t \in [t_0, t_e]$ if the following two strong stability conditions on the boundary layer system are satisfied.

Condition 3.2:
The equilibrium $\hat{z}(t_f) = 0$ of the boundary system (4.3.4) is asymptotically stable uniformly in x_0 and t_0, and $\hat{z}(0) = z_0 - \bar{z}(t_0)$ belongs to its domain of attraction, so $\hat{z}(t_f)$ exists for $t_f \geq 0$.

Condition 3.3:
The eigenvalues of $\partial g / \partial z$ evaluated, for $\varepsilon = 0$, along $\bar{x}(t), \bar{z}(t)$, have strictly negative real parts, i.e. Re $\lambda\{\partial g/\partial z\} \leq c < 0$.

Thus, singular perturbation theory allows us to treat slow and fast dynamics separately. Equations (4.3.3), (4.3.4) provide a zero-order approximation of the system behaviour in the slow and fast time scales respectively, which is exact for $\varepsilon = 0$. Higher order approximations are required to perform a formal error analysis and to obtain more accurate reduced models as $\varepsilon > 0$. They are obtained through series expansion of the state variables in powers of the perturbation parameter. Two possible procedures are to apply the matching procedure (Kokotovic *et al.*, 1986) or the boundary function method (Vasil'eva *et al.*, 1995). A further treatment of approximations is beyond the scope of this chapter.

4.3.2 Review of model reduction of (bio)process systems by singular perturbation

In this section, first a rule proposed by Bastin and Dochain (1990) is discussed. It is shown that this rule is not generally valid. Other references are therefore investigated to find a general rule for reduction of bioprocess systems through singular perturbation.

Bastin and Dochain (1990) propose a simple, general rule for order reduction in their book on estimation and control of bioreactors. Given the balance for component ξ_i:

$$\frac{d\xi_i}{dt} = \sum_{j \neq i} (\pm) k_{ij} \varphi_j - D\xi_i - Q_i + F_i \,, \tag{4.3.5}$$

(with k_{ij} the stoichiometric coefficients, φ_j the reaction rates, D the dilution rate, F_i the inflow and Q_i the gaseous outflow (if applicable) of component i) for a continuous, ideally mixed bioreactor, the simplification is achieved by setting ξ_i and $d\xi_i/dt$ to zero which yields the algebraic equation:

$$\sum_{j\neq i}(\pm)k_{ij}\varphi_j = Q_i - F_i \ . \tag{4.3.6}$$

This rule is not general however for several reasons. Firstly, it is not indicated in a general sense in which cases the dynamics of a component can be neglected, that is, which component i can be assumed fast, and when and why ξ_i can be assumed zero. The general rule is motivated with two specific situations only, which are briefly discussed below, namely 1. neglect of product dynamics for volatile products with low solubility, and 2. neglect of substrate dynamics in a model with biomass and substrate. These examples do however not cover nor explain all possible situations where multiple timescales allow reduction.

1. Singular perturbation technique for products.

This case considers product formation in the following reaction scheme involving one substrate and one product:

$$S \longrightarrow P$$

When the product is volatile and has low solubility, its concentration remains relatively low. In this case, the saturation constant can be chosen as the perturbation parameter. Writing the product concentration P as ΠP_{sat}, $0\leq\Pi\leq1$, with P_{sat} the saturation constant, with $\varepsilon=P_{sat}$, gives the standard form:

$$\frac{dS}{dt} = \varphi - D\,S + D\,S_{in} \tag{4.3.7}$$

$$\varepsilon\frac{d\Pi}{dt} = k\varphi - \varepsilon D\,\Pi - Q \tag{4.3.8}$$

with Q the rate of mass removal in gaseous form. For $\varepsilon\rightarrow0$, a reduced model is obtained by substituting the resulting algebraic equation , $k\varphi=Q$ into (4.3.7):

$$\frac{dS}{dt} = k^{-1}Q - D\,S + D\,S_{in} \tag{4.3.9}$$

In this case, the rule holds (for P_{sat} sufficiently small).

2. Singular perturbation technique for substrate.

For the following simple microbial growth process (See also Section 4.4.2):

$$S \overset{\curvearrowright}{\longrightarrow} X$$

the component balance equations write:

$$\frac{dX}{dt} = \mu X - D\,X \tag{4.3.10}$$

$$\frac{dS}{dt} = -k_1 \mu X - D S + D S_{in} \tag{4.3.11}$$

Multiplying by V and using V as a perturbation parameter gives (with $VD\ S_{in} = F_{S_{in}}$ and $X_T = VX$):

$$\frac{dX_T}{dt} = \mu X_T - D X_T \tag{4.3.12}$$

$$\varepsilon \frac{dS}{dt} = -k_1 \mu X_T - \varepsilon D S + F_{S_{in}} \tag{4.3.13}$$

which, for $\varepsilon \to 0$, with $k_1 \mu X_T = F_{S_{in}}$, reduces to:

$$\frac{dX_T}{dt} = -D X_T + \frac{1}{k_1} F_{S_{in}} . \tag{4.3.14}$$

In this derivation, the authors state that it should be understood that the volume is not assumed to be zero, but small enough to neglect ε(dS/dt) and εDS. Therefore, it is considered legitimate to divide the reduced equation by V again to obtain:

$$\frac{dX}{dt} = -D X + \frac{1}{k_1} D S_{in} . \tag{4.3.15}$$

However, it can be argued the volume is not the adequate perturbation parameter in this case because. 1. It is not the volume that makes the term εDS go to zero; in fact, the dilution rate $D = F_v/V$ (with F_v the volumetric flow rate) becomes very large for small ε and the term reads $F_v S$. 2. Without any additional information, there is no reason to select the substrate as the fast state; in fact, the same argumentation can be applied to neglect the biomass dynamics. 3. The physical reasoning is not sound, as smallness of the volume is not the cause of multiple time scales. 4. Consequently, the derivation is mathematically not consistent. In Section 4.4, it will be shown that in some cases the ratio of the biomass and substrate concentration can be used as a perturbation parameter; procedures that are more systematic are developed there.

Secondly, the rule is defined for a single, isolated equation. In the more general case however, several equations are coupled, e.g. via the reaction network, in which case the proposed general rule cannot be applied in its simple form. In those cases, the reduction procedure is much more involved, as will be discussed after discussing the two specific examples mentioned.

Van Breusegem and Bastin (1991) investigated model reduction of reaction systems with more general reaction networks, in the case of one (ideally mixed) reactor. The reduction problem was addressed under the assumption that some reactions are faster than others. As a perturbation parameter, the average of the fast rate constants was used. In natural coordinates, the problem is not always in standard form however, as Condition 3.1, existence of distinct roots, is not guaranteed. A change of coordinates was suggested to bring the problem into standard form. As the state transformation is non-singular, the reduced model can be transformed back into natural coordinates. In natural coordinates, however, there is generally no

direct partition in fast and slow variables and the singular perturbation can not be applied to the original, untransformed system, which we however like to preserve the interpretation of states. The procedure was successfully tested on a two-step enzyme reaction (Van Breusegem and Bastin, 1991) and on a two-step model of a methanogenesis process (Van Breusegem and Bastin, 1992)

Vasil'eva *et al.* (1995) discern as the critical case that class of applied problems in which the condition of isolated, distinct roots of the reduced equation $0 = g(x, z, u, t, 0)$ is not satisfied. In fact, in many problems in chemical kinetics the condition is not satisfied. A procedure is presented using the boundary function method for constructing approximate solutions based on asymptotic expansions for the standard form. A modification of this procedure is presented to deal with this critical case and applied to chemical reaction networks (in batch reaction), where small and fast reactions are involved. As a perturbation parameter, the smallest of the large rate constants was selected. It is interesting to note that this modified procedure does not start from nor produces the standard form. It is noted that this case again shows that a separation in fast and slow reactions does not correspond to a clear partitioning in slow and fast variables. Instead, it leads to a set of simplified systems for the fast and slow timescales.

Weiss and Preisig (1997) studied simplifying assumptions in the process of modelling composite process systems. Very large transfer coefficients between subsystems or very small capacities of subsystems for example can lead to lumping of the transferred intensive variables in the concerning subsystems. The difficulties and accuracy in this type of simplifications were studied on a relatively simple yet generic example of *n* tanks with various levels and temperatures, assuming that some of the transfers are very quick. The modified procedure of Vasil'eva *et al.* was applied (in fact, the systems studied are very similar, with fast and slow transfers instead of fast and slow reactions) to reduce the system and estimate the resulting error. Reduction of heat balances to describe the temperatures in the tanks was much more involved and less accurate than reduction of total mass balances to describe the heights. The singular perturbation parameter in this case is the inverse magnitude of the fast transfers relative to the slow transfers.

The references reviewed above all apply to lumped systems. Dochain (1994) applied singular perturbation to reduce an (infinite-dimensional) distributed parameter bioprocess system model to a (finite-dimensional) lumped parameter model. The general distributed parameter system studied is a plug flow reactor with dispersion. For the reduction, the system was rewritten using dimensionless numbers, employing as perturbation parameter the mass Peclet number, which expresses the ratio of the residence time and characteristic time for dispersion. A first-order approximation using a series expansion of the solution and using matching to determine initial conditions of inner and outer solutions yielded a lumped reduced model.

To apply singular perturbation for order reduction into fast or slow states of a given model, the model must be in standard form and a state partitioning must be made.

A general rule for reduction of continuous bioprocess systems was given by Bastin and Dochain (1990). However, this rule is not generally valid, and is not helpful in general in deciding which parameters can be considered fast (only products with very low solubility).

Other procedures have been derived for reduction of models in non-standard form. For reduction of models in natural (original) coordinates, a procedure exists for the so-called critical case (no distinct roots of the quasi-steady-state). However, the discussed references do not help to recognise or obtain the standard form. A procedure that does this is summarised below.

4.3.3 Scaling in model reduction

4.3.3.1 A method for state partitioning based on scaling

Aim of this section is to illustrate the usefulness of a systematic scaling procedure for state partitioning, to recognise or obtain the standard form. Frequently, the model to be reduced using is in non-standard form and must be brought into the standard form. One way to do so is to select or find a suitable, small perturbation parameter. This is often nontrivial and requires considerable physical knowledge; smallness of a parameter alone is not a sufficient condition. Selection of a perturbation parameter is associated with the issue of scaling, as smallness is a relative notion, and scaling is helpful to bring the model in the standard form and to select a suitable perturbation parameter. Kokotovic *et al*. (1986) presents several approaches in scaling, including the use of dimensionless parameters, parameter scaling and state scaling. However, no systematic, straightforward procedure for scaling is given.

Heineken *et al.* (1967) applied singular perturbation theory to provide a mathematically sound analysis of the quasi-steady-state assumption (QSSA) in derivation of Michaelis-Menten enzyme kinetics. Segel and Slemrod (1989) used a systematic approach based on scaling to obtain nondimensionalised equations in which it is easier to reveal the relative magnitude of parameters. With the applied scaling procedure, they were able to refine the conditions for application of the QSSA. The procedure they applied is outlined as follows and how they applied it to Michaelis-Menten kinetics is summarised in Section 3.3.2:

1. Estimate slow and fast time scales τ_f and τ_s.
2. Test on the necessary condition for the QSSA on the time scales.
3. Test on the necessary condition on the smallness of the error in the slow state during the pre-steady-state.
4. For both timescales, choose state scaling and subsequently derive scaled equations; this step should yield the perturbation parameter.
5. Reduce the model
6. Test the reduced model, e.g. through numerical simulations

The tests on the necessary conditions may also provide perturbation parameter candidates. In their chapter, in addition to these steps a formal analysis was performed using approximate solutions of the scaled equations. Both the derivations of the approximate solutions and a formal error analysis are beyond the scope of this chapter.

4.3.3.2 Application of an analytic scaling procedure to Michaelis-Menten kinetics

In the reaction model employed in derivation of Michaelis-Menten kinetics, an enzyme E combines with substrate to form an ES complex, which dissociates to either E and S or to E and product P:

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} C \xrightarrow{k_2} E + P$$

With the initial conditions $E(0)=E_0$, $S(0)=S_0$, $C(0)=0$, $P(0)=0$, and using the fact that $E(t)+C(t)=E_0$, the following basic mathematical problem results:

$$\frac{dS}{dt} = -k_1(E_0 - C)S + k_{-1}C, \qquad S(0)=S_0, \tag{4.3.16}$$

$$\frac{dC}{dt} = k_1(E_0 - C)S - (k_{-1} + k_2)C \quad , \qquad C(0)=0. \tag{4.3.17}$$

Application of the QSSA to simplify this system is standard and can be found in any elementary textbook on biochemistry. The QSSA implies that after a short pre-steady-state, the complex concentration C is approximately constant and the decrease of the concentration S due to complex formation can be neglected as C_0 is small. The derivation is not repeated here. Only the main points are indicated.

We now focus on the procedure of Segel and Slemrod (1989). The steps for Michaelis-Menten kinetics were as follows.

1. Estimation of timescales:

The fast time scale is associated with the complex formation. To estimate the fast time scale τ_f, the approximate analytical solution of (4.3.17) for the fast timescale is used by supposing S is slow and can be approximated by S_0:

$$C(t) = \overline{C}[1 - \exp(-kt)], \tag{4.3.18}$$

with:

$$\overline{C} \equiv \frac{E_0 S_0}{K_m + S_0}, \quad k \equiv k_1(S_0 + K_m) \quad \text{and} \quad K_m \equiv \frac{(k_{-1} + k_2)}{k_1}. \tag{4.3.19}$$

and we obtain

$$\tau_f = k^{-1}. \tag{4.3.20}$$

The slow timescale is associated with the substrate after the pre-steady-state and is estimated using the following characterisation of a timescale (Here, Segel and Slemrod (1989) refer to Segel (1984), p.56):

$$\tau_s = (S_{max} - S_{min}) / \left|\frac{dS}{dt}\right|_{max}.$$

Here, the maximum and minimum concentration of S are $S_{max}=S_0$ and $S_{min}=0$. The maximum rate after the pre-steady-state is estimated by substituting $S=S_0$ and (4.3.19) into (4.3.16):

$$\tau_s = \frac{K_m + S_0}{k_2 E_0}. \tag{4.3.21}$$

2. Test on the necessary condition for the QSSA on the time scales.

The necessary condition for the QSSA to hold is that the duration of the pre-steady-state is much shorter than the characteristic time for substrate change, $\tau_f << \tau_s$, which gives:

$$\eta << (1 + \kappa)(1 + \sigma)^2, \tag{4.3.22}$$

with the dimensionless parameters

$$\sigma \equiv \frac{S_0}{K_m}, \ \eta \equiv \frac{E_0}{K_m}, \ \kappa \equiv \frac{k_{-1}}{k_2}. \tag{4.3.23}$$

3. Test on the necessary condition on the smallness of the error in the slow state during the pre-steady-state.

For the change in the substrate concentration to be negligible, the relative concentration change $\Delta S / S_0$ must be very small during the pre-steady-state, which is estimated by:

$$\left|\frac{\Delta S}{S_0}\right| \approx \frac{1}{S_0}\left|\frac{dS}{dt}\right|_{max} \cdot \tau_f \tag{4.3.24}$$

Using (4.3.16) with C=0 to determine $\left|dS/dt\right|_{max}$ yields the following additional condition in dimensional variables, which is stronger than (4.3.22):

$$\eta << (1+\sigma). \tag{4.3.25}$$

The result also indicates a perturbation parameter candidate, namely $\eta/(1+\sigma)$.

4. For both time scales, derive scaled equations.

In the pre-steady-state, the time is scaled by τ_f. The substrate concentration is scaled by S_0 and the complex concentration C by the maximal complex concentration $\overline{C}$. With the introduction of the following dimensionless variables into (4.3.16) and (4.3.17),

$$s \equiv \frac{S}{S_0}, \ c \equiv \frac{C}{\overline{C}}, t_f \equiv \frac{t}{\tau_f} \tag{4.3.26}$$

the scaled equations are obtained for the fast time scale:

$$\frac{ds}{dt_f} = \varepsilon\left[-s + \frac{\sigma}{\sigma+1}cs + \frac{\kappa(\kappa+1)^{-1}}{\sigma+1}c\right], \qquad s(0)=1, \tag{4.3.27}$$

$$\frac{dc}{dt_f} = s - \frac{\sigma}{\sigma+1}cs - \frac{1}{\sigma+1}c \quad , \qquad c(0)=0. \tag{4.3.28}$$

After the pre-steady-state, the time is scaled by τ_s. The same state scaling then yields:

$$\frac{ds}{dt_s} = (\kappa+1)(\sigma+1)\left[-s + \frac{\sigma}{\sigma+1}cs + \frac{\kappa(\kappa+1)^{-1}}{\sigma+1}c\right], \tag{4.3.29}$$

$$\varepsilon\frac{dc}{dt_s} = (\kappa+1)(\sigma+1)\left[s - \frac{\sigma}{\sigma+1}cs - \frac{1}{\sigma+1}c\right]. \tag{4.3.30}$$

Thus, we now have the problem in standard form, and have obtained a perturbation parameter:

$$\varepsilon \equiv \frac{\eta}{1+\sigma} \equiv \frac{E_0}{K_m + S_0} \tag{4.3.31}$$

This result is more accurate than the traditional perturbation parameter, E_0/Km. Segel and Slemrod (1989) obtained this more accurate result through applying this systematic physical scaling procedure. Besides physical scaling, Segel (1972) also applied mathematical scaling procedures with the aim to test whether this result can also be obtained with less prior knowledge. Through one such method, minimal simplification, the same results were obtained; it is not clear however whether this method will always work.

5. and 6. Reduce model and test the reduced model
From the standard form, the model was reduced. In numerical simulations, the conditions on the time scales and errors were verified and confirmed to be correct.

4.3.3.3 Relationship of scaling with regime analysis and dimensional analysis

In (bio)process engineering, regime-analysis is a tool to detect rate-limiting mechanisms by comparing the timescales for different transport and reaction processes. For example, Oosterhuis (1983) applied regime analysis to the scale-up of bioreactors. Evidently, there is a relationship with the detection of occurrence of multiple time scales as described above. An important difference is that regime analysis compares the relative size of the individual terms in the balance equations, while the timescale estimation, as applied by Segel and Slemrod above, considers the total rate expression of extensive variables. Both methods can be used in a complementary fashion. Dimensionless groups, obtained by the ratios of characteristic scales of different phenomena, also provide insight into the system. The insight obtained by using scaled equations is a strong argument for the use of scaling to convert the equations to dimensionless form, as advocated by Segel (1972), even if this scaling requires some physical reasoning.

4.3.4 Other methods for time-scale analysis

In Section 3.3, a procedure was described for detection of multiple time scales in models and transformation of the problem to the standard reducible form. Robertson and Cameron (1997) presented another approach to detect timescale multiplicity and for state partitioning for use with singular perturbation reduction. Their procedure might be suited for large systems if the scaling procedure described above is too laborious, or could be used as a complementary technique. The essential issues of the procedure are briefly summarised here.

Starting from the definition of a timescale of interest, slow and fast modes are detected using a linearized model. The timescale of interest is determined by the intended application, e.g. control of ammonia and nitrate in activated sludge plants or control of the sludge concentration, which require different timescales. The first require medium timescales, the latter slow timescales. Fast mode reduction is performed based on an eigenvalue-to-state association. This is done using a homotopy parameter. The procedure starts with a system in which the eigenvalue-to-state association is known (in their study, a matrix with only the diagonal of the Jacobian matrix was used). The eigenvalues are traced when going from this system to the system for which the eigenvalue-to-state association must be determined (the full Jacobian matrix). A so-called homotopy parameter as used to gradually change from the known system (homotopy parameter is zero) to the unknown system (homotopy parameter equal to one).

If a group of fast time constants exists, then the states associated with these time constants are candidates for reduction. Slow mode reduction proceeds via Taylor expansion of the free response. From linear systems, randomly generated by Monte-Carlo sampling, empirical relationships for the maximum relative error both for fast and slow mode reducibility were derived. After detection of slow and fast states, these are removed from the nonlinear model. The procedure provides no guarantee that the system is in the standard form and no formal error analysis is given. Tests on an evaporator system and compressor start-up yielded good results; results on ASM1 were less successful as discussed in Section 4.2.3.

We indicate two disadvantages of the slow mode detection method. Error estimation can be too optimistic if in reality a forced response is dominant, because only the free response is considered in the selection criterion. Furthermore, relatively small changes of a slow mode variable can be associated with relatively large changes in other variables, especially if these have small absolute value (such as dissolved oxygen or ammonia in the case of ASM1). Consequently, on the other hand, the method can be too conservative.

Wasynczuk and Decarlo (1981) suggested an approach for reduction of composite models. This method is useful for order reduction of large-scale systems such as in plant-wide control, and is therefore briefly described in here. The procedure indicates whether model reduction on a component level is possible or not. This must be checked, because interaction may introduce dynamics in the timescale of subsystem dynamics. It this is the case, then the model reduction can not be performed simply by reduction of the individual subsystems only.

In the analysis, the so-called component connection model is employed, which separately defines the subsystem equations and the interconnection matrix. The procedure consists of eigenvalue tracking applying a homotopy parameter, which is multiplied by the interconnection matrix, and is used to vary from completely decoupled subsystems to the fully interconnected system. This indicates if reduction on a subsystem level is sufficient to reduce the complete system.

4.3.5 Conclusions

Application of singular perturbation for reduction of (bio)process models was reviewed. Bastin and Dochain (1990) suggested a simple rule for order reduction, which is not generally applicable, however. In reduction of a system with biomass and substrate, the suggested selection of the perturbation parameter was not satisfactory. Segel and Slemrod (1989) applied a methodology based on scaling to formally derive Michaelis-Menten kinetics. The methodology can support detection of multiple timescales, which are necessary for applying quasi-steady-state assumptions and order reduction with singular perturbation. Furthermore, it may help to bring the model in the standard form and to select a suitable perturbation parameter that is required for application of the singular perturbation method. The methodology forms the basis to develop a method to recognise or obtain the standard form and for state partitioning. This is applied to a simple yet basic and important bioprocess with biomass and substrate, which is similar to the model studied by Bastin and Dochain (1990), in the next section.

4.4 Scaling for singular perturbation in a simple bioprocess system

4.4.1 Introduction and methodology

This section investigates application of singular perturbation to reduction of bioprocess models. The following observations motivate this further investigation. Section 4.2 made clear that

more insight into the timescale properties of ASM1 is required. Section 4.3 showed that only a few occasions have been described in which there is a clear perturbation parameter and associated timescale separation, namely the case of low solubility of volatile products and the occurrence of fast and slow reactions. In ASM1 however, these are not the predominating causes of multiple timescales, as no volatile products are applied in the model and the reaction rates, although different, do not differ orders of magnitude. Therefore, we want to find additional causes of multiple timescales and associated perturbation parameters. Moreover, these findings are also of relevance for bioprocess systems in general.

The following strategy is adopted. Three procedures for state partitioning are proposed. They are applied to a very simple but basic and important model system, closely resembling the system used by Bastin and Dochain (1990), Section 4.3.2). This should reveal to reveal time scale multiplicity and the physical conditions that cause multiple timescales. These conditions are related to a singular perturbation parameter, if possible, and it is checked whether the model can be brought into standard form.

The three procedures to obtain or recognise the standard form are evaluated with respect to straightforwardness and required prior knowledge. The following procedures are applied:

1. Direct scaling;
2. Timescale estimation for variables;
3. Analytical scaling procedure.

These procedures are now described and are applied to the model system described in Section 4.4.2.

4.4.1.1 Procedure 1: Direct scaling

This procedure attempts to bring the model into standard form directly, without a thorough scaling procedure and without introducing dimensionless parameters. The background to apply this procedure here is the conjecture that stiffness is associated with large concentration ratios. For example, in analysis of DO dynamics, it appeared that a fast timescale occurred only if the DO concentration was very low. Moreover, in wastewater treatment systems the suspended components are usually regarded as slow, and (most of) these variables have a much larger concentration than the suspended components. From these observations, it was hoped that a simple yet physically meaningful rule for order reduction could be derived.

4.4.1.2 Procedure 2: Time scale estimation for variables

Procedure 2 is a systematic procedure for detection of timescale multiplicity through estimation of timescales of variables. This procedure is proposed as an alternative and complementary procedure where procedure 3 fails.

In the example in Section 4.3.3, it was already known that multiple time scales occurred, and to which variables the fast respectively the slow time scales were associated. Generally, this is not the case; in fact, the eigenvalue-to-state association procedure presented in Section 4.3.4 was developed for this purpose.

Here we will propose a different procedure to estimate timescales of variables. This procedure is a modification and extension of the procedure of Segel and Slemrod (1989) in Section 4.3.3,

and does not require analytical timescale or error estimates. Instead, a mixed numerical / analytic approach is applied to detect timescale multiplicity and to estimate the error in slow states during the initial layer, thus checking whether the quasi-steady-state approximation applies.

We start with the system

$$\dot{C} = f(C,u,t,\varepsilon),\ C(t_0) = C_0, C \in R^{n+m},\ u \in R^p \tag{4.4.1}$$

and try to find a partitioning into fast and slow variables $C^T = [C_f^T\ C_s^T]$ so that we can write (4.4.1) in standard form as

$$\dot{C}_s = f_s(C_s,C_f,u,t,\varepsilon),\ C_s(t_0) = C_{s0}, C \in R^n,\ u \in R^p\ , \tag{4.4.2}$$

$$\varepsilon\dot{C}_f = f_f(C_s,C_f,u,t,\varepsilon),\ C_f(t_0) = C_{f0}, C \in R^m. \tag{4.4.3}$$

The procedure consists of the following steps that are subsequently discussed below:

Step 1. Estimate initial timescales of all variables and select the fast variables.
Step 2. Estimate timescales of slow variables in the outer layer (in quasi-steady-state).
Step 3. Check the multiplicity of time scales.
Step 4. Estimate the error of the slow variables.
Step 5. Reduce model if preceding steps indicate that the QSSA applies.

Step1: The initial timescale τ_{fi} for variable i in Step 1. is estimated with:

$$\tau_{fi} = \frac{\left|C_{i0} - \overline{C}_i^0\right|}{\left|\frac{dC_i}{dt}\right|_{max,in}} \tag{4.4.4}$$

with $\overline{C}_i^0$ the quasi-steady-state value of variable i with the other variables C_j, $j \neq i$ at their initial values C_{j0} and $|dC_i/dt|_{max,in}$ the maximal rate during the inner layer, which in this chapter is evaluated with all state variables at their initial conditions.

We would like to avoid the need to compute $\overline{C}_i^0$. Therefore, one can try to rewrite (4.4.3) to eliminate $|C_i(0) - \overline{C}_i^0|$ as follows. In the quasi-steady-state for $\overline{C}_i^0$ we have:

$$0 = f_i(C_{j0,j\neq i}, \overline{C}_i^0, u, t, \varepsilon)\ . \tag{4.4.5}$$

Subtracting equation (4.4.5) from the rate equation for C_i (this is allowed, because the quasi-steady-state equation is zero) gives (4.4.6) (Note: |.| denotes the absolute value).

$$\left|\frac{dC_i}{dt}\right|_{max,in} = \left|f_i(C_{j0,j\neq i}, C_{i0}, u, t, \varepsilon) - f_i(C_{j0,j\neq i}, \overline{C}_i^0, u, t, \varepsilon)\right| \tag{4.4.6}$$

We can try to write this as a product with a term $(C_{i0} - \overline{C}_i^0)$:

$$\left|\frac{dC_i}{dt}\right|_{max,in} = \left|g_i(C_{j0,j\neq i}, C_{i0}, \overline{C}_i^0, u, t, \varepsilon)\cdot(C_{i0} - \overline{C}_i^0)\right|$$

to obtain:

$$\tau_{fi} = \frac{\left|C_{i0} - \overline{C}_i^0\right|}{\left|g_i(C_{j0,j\neq i}, C_{i0}, \overline{C}_i^0, u, t, \varepsilon)\cdot(C_{i0} - \overline{C}_i^0)\right|}$$

$$= \quad |\, g_i(C_{j0,j\neq i}, C_{i0}, \overline{C}_i^0, u, t, \varepsilon)\,| \tag{4.4.7}$$

In some cases, it is thus possible to eliminate $\overline{C}_i^0$ completely and to obtain an expression for the time constant as a function of the parameters and initial conditions only.

The variables that have a (much) faster associated timescale than other variables are selected as the fast variables, and thus the partitioning is made.

Step 2. The slow timescale τ_{si} for the slow variables i can be estimated with:

$$\tau_{si} = \frac{\left|C_{i0} - \overline{C}_i\right|}{\left|\frac{dC_i}{dt}\right|_{max,out}} \tag{4.4.8}$$

with C_{i0} the initial value of variable i, $\overline{C}_i$ its steady-state value and $|dC_i/dt|_{max,out}$ the maximal rate during the outer layer. To avoid the necessity of computing $\overline{C}_i$, it is assumed that the difference between initial value and steady-state are in the same order of magnitude as the initial value and (4.4.8) can be approximated by (4.4.9).

$$\tau_{si} = \frac{\left|C_{i0}\right|}{\left|\frac{dC_i}{dt}\right|_{max,out}} \tag{4.4.9}$$

The maximal rate during the outer layer is evaluated with the slow state variables at their initial values C_{j0} and the fast states at their quasi-steady-state values.

Step 3. is straightforward, unless the difference between fast and slow timescales is not very large. Here, we will pragmatically consider a factor of about 10 between largest fast timescale and smallest slow timescale sufficient for timescale separation.

Step 4. The error in the slow variables during the initial, inner layer is estimated to check whether the error is small enough to qualify the slow variables as slow. If this is not the case, this does not mean that there are no multiple timescales, but rather that they cannot be assigned to disjunct fast and slow variables, i.e. the problem is not in standard form. A first, conservative approximation employs the maximal rate during the inner layer, with the advantage of computational simplicity as all required quantities are known already. The condition then is:

$$\left|\frac{\Delta C}{C_0}\right| \approx \frac{1}{C_0}\left|\frac{dC}{dt}\right|_{max,in} \cdot \tau_f \quad << 1 \tag{4.4.10}$$

with τ_f the largest of the small time constants and $|dC/dt|_{max,in}$ the maximal rate during the inner layer. The estimation is more accurate and less conservative if an average rate is applied:

$$\left|\frac{\Delta C}{C_0}\right| \approx \frac{1}{C_0}\left|\frac{dC}{dt}\right|_{av,in} \cdot \tau_f \tag{4.4.11}$$

In the sequel, the average rate computed as the mean of the initial rate and the rate after the inner layer at $t=\tau_f$ will be used to compute the error, unless stated otherwise.

Step 5. Reduce model if preceding steps indicate that the QSSA applies.
If the conditions checked in steps 3. and 4. are satisfied, then this indicates that the quasi-steady-state approximation applies and the model may be reduced. One can try to formulate scaled equations and select a perturbation parameter and thus bring the problem into standard form. If this is not successful, then we can proceed as follows. From the partitioning into slow and fast variables, it can be simply concluded that the rate for the fast variable is much higher than the rate for the slow variable and therefore can be written as:

$$f_f = \frac{1}{\varepsilon} h_f(C_s, C_f, u, t, \varepsilon),$$

where $h_f(C_s, C_f, u, t, \varepsilon)$ is in the same order of magnitude as $f_s(C_s, C_f, u, t, \varepsilon)$, because $f_f(C_s, C_f, u, t, \varepsilon)$ is much higher than $f_s(C_s, C_f, u, t, \varepsilon)$. Therefore, (4.4.1) can be written as (4.4.2), (4.4.12):

$$\dot{C}_s = f_s(C_s, C_f, u, t, \varepsilon),\ C_s(t_0) = C_{s0}, C \in R^n,\ u \in R^p\ , \tag{4.4.2}$$

$$\dot{C}_f = \frac{1}{\varepsilon} g_f(C_s, C_f, u, t, \varepsilon),\ C_f(t_0) = C_{f0}, C \in R^m, \tag{4.4.12}$$

and it is seen that the system is almost in standard form. Although we do not have ε in analytic form, we know it is small enough (through the preceding steps) and we may apply the QSSA to obtain the quasi-steady-state value for C_f by equation (4.4.5). An error estimate is also provided through step 4.

4.4.1.3 Procedure 3: Analytical scaling procedure

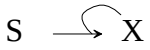
In procedure 3, the methodology proposed by Segel and Slemrod (1989) (Section 4.3.3) is applied. This procedure proceeds via scaling and selection of a perturbation parameter. For a complete scaling procedure, analytic timescale estimates are required for scaling the fast and slow timescale and analytic error estimates are derived.

4.4.2 Model system: chemostat with biomass and substrate

4.4.2.1 Model system definitions and analysis

A simple chemostat with one biomass and one substrate will be used to test the proposed procedure. In this subsection, the system is described, some analytical relationships are presented and the cases that are discussed in the next subsections are indicated.

In a completely stirred tank reactor, biomass X grows on a single substrate S (the arrow in the formula denotes an autocatalytic reaction). Motivation for choosing this system is that this is a very simple yet basic and important continuous biotechnological process that can exhibit multiple time scales. This simple system is well understood and is a good study object as better understanding its timescale behaviour is helpful to understand systems that are more complicated as well.



The reactor is schematically shown in Figure 4.1.

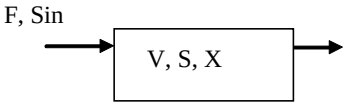


Figure 4.1: Chemostat with biomass growth on one substrate

For this system, assuming Monod kinetics, model equations (4.4.13), (4.4.14) can be written.

$$\dot{X} = \mu \frac{S}{K+S} X - D\ X \tag{4.4.13}$$

$$\dot{S} = -k_1\ \mu \frac{S}{K+S} X - D\ S + D\ S_{in} \tag{4.4.14}$$

The dimensionless parameters defined for this system are the dimensionless residence time and the Monod number:

$$\tau^* = \frac{\mu}{D} \quad (4.4.15)\ ;\ Mo = \frac{K}{S_{in}} \tag{4.4.16}$$

For the system to be viable, no washout must occur so there is a lower limit to the dimensionless residence time:

$$\tau^*_{min} = \frac{\mu}{D_{max}} = 1 + Mo \tag{4.4.17}$$

The steady-state concentrations are given by (4.4.18) and (4.4.19).

$$X_\infty = \frac{1}{k_1}\{S_{in} - \frac{DK}{(\mu - D)}\} = \frac{1}{k_1}\{S_{in} - \frac{K}{\tau^* - 1}\} \tag{4.4.18}$$

$$S_\infty = \frac{DK}{(\mu - D)} = \frac{K}{\tau^* - 1} \tag{4.4.19}$$

Upon linearization in a state x={X, S}with u=D, the following linearized system is obtained:

$$\dot{x} = \begin{bmatrix} \frac{\mu S}{K+S} - D & \frac{\mu K X}{(K+S)^2} \\ -k1\frac{\mu S}{K+S} & -k1\frac{\mu K X}{(K+S)^2} - D \end{bmatrix} x + \begin{bmatrix} 0 \\ S_{in} \end{bmatrix} u \tag{4.4.20}$$

from which the eigenvalues are computed:

$$\lambda_{1,2} = -D,\ -D + \mu\frac{S(S+K) - k_1 XK}{(S+K)^2} \tag{4.4.21}$$

Starting point in the subsequent timescale analysis is the conjecture that occurrence of multiple timescales is associated with a large concentration difference between the states. The ratio S/X in steady-state is written as a function of the dimensionless parameters τ^* and Mo:

$$\frac{S_\infty}{X_\infty} = \frac{1}{k_1}\{\frac{Mo}{\tau * -1 - Mo}\} \tag{4.4.22}$$

and six cases are distinguished as indicated in Table 4.1 and briefly explained below.

Table 4.1: Cases distinguished in timescale analysis; for explanation, see text

Case	Ratio S_∞/X_∞	Condition for τ^*	Other condition	Section
1	S << X	$\tau^* >> 1$	Mo << 1	4.4.2.2
2	S<< X	$\tau^* >> 1$	Mo ≈ 1	"
3	S << X	$\tau^* > O(2)^1$	Mo << 1	4.4.2.3
4	S ≈ X	$\tau^* > O(3)^1$	Mo ≈ 1	4.4.2.4
5	S ≈ X	$\tau^* = 1+Mo+\tau_\varepsilon$	$\tau_\varepsilon \approx$ Mo, Mo <<1	4.4.2.5
6	S >> X	$\tau^* = 1+Mo+\tau_\varepsilon$	τ_ε << Mo	4.4.2.6

[1]: Big O stands for "order of magnitude". The eigenvalues are computed in the steady-state.

From (4.4.22), we see that S/X is low when Mo is very small or τ^* very large.

Case 1 and 2: When τ^* is very large (high residence time), substrate conversion is almost complete and biomass produced is only slowly withdrawn. At high feed substrate concentration S_{in} (small Monod, Case 1), the concentration difference is larger at a given residence time than at lower S_{in} (Monod ≈ 1), because the biomass concentration is higher whilst the substrate concentration remains unchanged (Case 2). This is easily seen from (4.4.19).

Case 3: At moderate dilution rate, but far from washout, which is expressed by the condition $\tau^* > O(2)$, the ratio S/X can still be small when the feed concentration is very high (this is the case when the Monod number is very small).

Case 4: If S_{in} is moderate at moderate dilution rate, then the ratio S/X will be O(1).

Case 5: At high dilution rate, relatively close to washout, we write τ^* as $\tau^* = 1+Mo+\tau_\varepsilon$. This is an interesting situation, as biomass productivity is optimal close to washout, namely for $\tau_\varepsilon = \sqrt{Mo + Mo^2}$.

Case 6: At still higher dilution rates, when $\tau_\varepsilon << Mo$, the situation is so close to washout that substrate conversion is almost zero and high ratio S/X results.

For typical values representing the different cases, the ratio S_∞/X_∞ and the ratio of the eigenvalues are given in Table 4.2. Equations (4.4.18), (4.4.19) and (4.4.21) were used, with the following parameter values as default parameters: $\mu=4$, $K=20$, $k_1=1.5$.

Table 4.2: Ratio S_∞/X_∞ and ratio of eigenvalues for different cases

Case	τ^*	Mo	S_∞/X_∞	λ_1/λ_2	λ_1	λ_2
1	20	0.04	0.0032	0.0022	0.2	90
2	20	0.4	0.0323	0.0226	0.2	8.8
3	3	0.04	0.0306	0.0306	1.33	43.5
4	3	0.4	0.375	0.375	1.33	3.56
5	1.24	0.04	0.294	1	3.21	3.21
6	1.044	0.04	15	236	3.83	0.016

The results indicate that the supposed relationship between the ratio S_∞/X_∞ and the ratio of eigenvalues holds indeed. In the subsequent subsections, the cases are analysed more thoroughly according to Table 4.1.

4.4.2.2 Cases 1 and 2: Ratio S/X very low, τ^* very large

4.4.2.2.1 Direct

With the direct approach, we introduce scaled variables directly. In this case, from the supposed association of multiple timescales with a large concentration difference between the states, both states are scaled with their steady-state, assuming that S_∞/X_∞ is very small.

$$\dot{X}/X_\infty = \mu \frac{S/S_\infty}{K/S_\infty + S/S_\infty} X/X_\infty - DX/X_\infty \tag{4.4.23}$$

$$\dot{S}/S_\infty = -k_1 \mu \frac{S/S_\infty}{K/S_\infty + S/S_\infty} \frac{1}{S_\infty} X - DS/S_\infty + DS_{in}/S_\infty \tag{4.4.24}$$

In dimensionless variables we obtain with $k=K/S_\infty$:

$$\dot{x} = \mu \frac{s}{k+s} x - D x \tag{4.4.25}$$

$$\dot{s} = -k_1 \mu \frac{s}{k+s} \frac{X}{X_\infty} \frac{X_\infty}{S_\infty} - D s + D S_{in}/S_\infty \tag{4.4.26}$$

With $\varepsilon = S_\infty/X_\infty$ (4.4.26) becomes:

$$\varepsilon \dot{s} = -k_1 \mu \frac{s}{k+s} x - \varepsilon D s + D \frac{S_\infty}{X_\infty} \frac{S_{in}}{S_\infty} \varepsilon$$

$$= -k_1 \mu \frac{s}{k+s} x - \varepsilon D s + f_{in} \tag{4.4.27}$$

Now the problem is in standard form, and (4.4.25), (4.4.27) are the equations for the slow timescale. With the substitution $t_f = \varepsilon t$ the fast time equations are obtained:

$$\frac{dx}{dt_f} = \varepsilon\{\mu \frac{s}{k+s} x - D x\} \tag{4.4.28}$$

$$\frac{ds}{dt_f} = -k_1 \mu \frac{s}{k+s} x - \varepsilon D s + f_{in} \tag{4.4.29}$$

Note: To be able to arrive at (4.4.27), it must be shown that f_{in} is not very small, $O(\varepsilon)$, but of the same order of magnitude as the other non-negligible terms, and cannot be neglected. The result is given here as is without proof.

With the direct approach, we arrived at the equations in standard form. If the ratio S_∞/X_∞ is very small, this ratio can be used as a perturbation parameter to obtain the problem in standard form. In that case, biomass is the slow variable, substrate the fast variable.

The required physical knowledge to obtain the standard form in this case is the association of low S_∞/X_∞ with timescale multiplicity. However, the standard form obtained presupposes that S_∞/X_∞ be very small, but does not indicate whether this assumption indeed is valid. In the next two subsections, an alternative formulation of the standard form will be derived, which states the condition for timescale multiplicity directly in terms of (dimensionless) system parameters.

4.4.2.2.2 Timescale estimation for variables

The procedure described in Section 4.2 is applied to system (4.4.13), (4.4.14).

Step 1. Estimate initial timescales and select fast variables.
For estimation of the initial timescale for biomass X, the quasi-steady-state equation (4.4.30) for X with $S=S_0$

$$0 = \mu \frac{S_0}{K+S_0} \overline{X}^0 - D\overline{X}^0 \tag{4.4.30}$$

and the estimate (4.4.4) are used to obtain an approximation in the form of (4.4.7):

$$\frac{1}{\tau_{fX}} = \mu \frac{S_0}{K+S_0} - D\,. \tag{4.4.31}$$

For substrate S, we similarly obtain the estimate for the initial timescale:

$$\frac{1}{\tau_{fS}} = k_1 \mu \frac{K}{(K+S_0)(K+\overline{S}^0)} X_0 + D \tag{4.4.32}$$

with $\overline{S}^0$ the positive root of the quadratic quasi-steady-state equation of S:

$$0 = \quad -k_1\,\mu\frac{\bar{S}^0}{K+\bar{S}^0}X_0 - D\bar{S}^0 + DS_{in} \tag{4.4.33}$$

It is noted that in this form the timescales depend upon the initial state and thus have to be evaluated considering the initial condition. Consequently, here the timescales will be estimated numerically. This is a result of the nonlinearity of the model.

Results of fast time scale estimation for representative cases are given in Table 4.3. The default parameters given in Section 4.4.2.1 were used. As initial states, a value of half the steady-state value was chosen for both states

Table 4.3: Fast time scales for Case 1 and 2 (x(0)=0.5·x(∞)

Case	τ^*	Mo	λ_1/λ_2	τ_{fS}/τ_{fX}	τ_{fX}	τ_{fS}
1	20	0.04	0.0022	0.0022	10.3	0.023
2	20	0.4	0.0226	0.0213	10.3	0.22

Table 4.3 shows that the timescale estimation indicates multiplicity of timescales. S is selected as the fast state. The results obtained with the timescale estimation correspond well with the eigenvalue results. The advantage with time scales estimation is that the timescales are directly associated with variables.

Step 2. Estimate timescales of slow variables in the outer layer (quasi-steady-state).
As S is selected as the fast variable, X is the slow variable. Applying (4.4.9), the slow timescale for X is estimated with by substituting $\bar{S}^0$ obtained from (4.4.33).

$$\frac{1}{\tau_{sX}} = \mu\frac{\bar{S}^0}{K+\bar{S}^0} - D \tag{4.4.34}$$

Table 4.4 shows the results of the slow timescale estimates for Case 1 and 2.

Table 4.4: Slow time scales and error for Case 1 and 2 (x(0)=0.5·x(∞)

Case	τ^*	Mo	τ_{fS}/τ_{sX}	τ_{sX}	τ_{fS}	$\Delta X_0/X_0$
1	20	0.04	0.0042	5.0	0.021	0.0012
2	20	0.4	0.038	5.2	0.20	0.010

Step 3. Check the multiplicity of time scales.
From Table 4.4, it is seen that for both Case 1 and Case 2 the condition $\tau_{fS}/\tau_{sX}<<1$ holds.

Step 4. Estimate the error of the slow variables.
Applying (4.4.11), the error in the slow state X during the initial layer is estimated by (4.4.35) (X_0 can be eliminated).

$$\left|\frac{\Delta X}{X_0}\right| \approx \left|\frac{1}{2}\left(\mu\frac{S_0}{K+S_0} + \mu\frac{\bar{S}^0}{K+\bar{S}^0}\right) - D\right|\cdot\tau_{fs} \tag{4.4.35}$$

The errors are given in Table 4.4 and indeed the condition $\Delta X_0/X_0<<1$ holds. In Case 2, the error is approximately 1 %. It is concluded that time scale separation can be applied.

Step 5. Reduce model if preceding steps indicate that the QSSA applies.
From the preceding steps, we know that the QSSA applies because timescale multiplicity occurs and there is a separation into fast and slow states (see Step 5 in Section 4.4.1.2). Therefore, the system can be slow-mode reduced straightforwardly to:

$$\dot{X} = \mu \frac{\bar{S}^0}{K + \bar{S}^0} X - D\ X \tag{4.4.36}$$

with $\bar{S}^0$ the positive root of the quadratic quasi-steady-state equation for S (4.4.33). This describes the slow dynamics of the system that can be used for control of the biomass concentration. In this case, S reacts instantaneously to changes in e.g. S_{in}. For control of S_S, the fast mode reduction gives the fast dynamics, where the biomass concentration is considered constant.

4.4.2.2.3 Analytical scaling procedure

In this subsection, scaling is performed employing estimates based on the analytical solutions of the eigenvalues of the system, which leads to the standard form.

1. Estimate time scales

In Case 1 and 2, the large eigenvalue of (4.4.21) can be approximated as follows, because X>>S, S<<K, μ>>D (because τ^*>>1) and X≈S_{in}/k_1:

$$\lambda_2 = -D + \mu \frac{-k_1 XK + S(S+K)}{(S+K)^2} \approx -D - \mu \frac{k_1 XK}{(S+K)^2} \approx -D - \frac{\mu}{Mo} \approx -\frac{\mu}{Mo} \tag{4.4.37}$$

As the time constant is reciprocal to the real part of the eigenvalue, the fast time and slow time scales can be scaled as (4.4.38) and (4.4.39) respectively.

$$t_f = t \cdot \mu / Mo \qquad (4.4.38)\ ;\ t_s = t \cdot D \tag{4.4.39}$$

2. Test for QSSA necessary conditions

For the QSSA to be valid, $\tau_f << \tau_s$ must hold

$$Mo/\mu \ << \ 1/D, \text{ or } \quad \tau^*/Mo >> 1 \tag{4.4.40}$$

which is the same condition as was found before and which holds under the assumptions made.

3. Perform error analysis on initial condition for slow state.

For the fast time scale we have τ_f=Mo/μ. Assuming that S_0 and X_0 are in the same order of magnitude as S_∞ and X_∞ respectively and applying the (conservative) estimate (4.4.10) this is approximated by the estimate (ε is a small number O(Mo/τ)):

$$\left|\frac{\Delta X}{X_0}\right| \approx \left|\mu \frac{S_0}{K + S_0} - D\right| \cdot \frac{Mo}{\mu} \approx \left|\mu \frac{S_0}{K} - D\right| \cdot \frac{Mo}{\mu} = \left|\frac{S_0}{S_{in}} - \frac{Mo}{\tau}\right| = O(\varepsilon) \tag{4.4.41}$$

4. For time scales, choose state scaling and subsequently derive scaled equations and (try to) find perturbation parameter.

The states are scaled with their steady-state values, but instead of symbols S_∞ and X_∞, now expressions (4.4.18) and (4.4.19) are used to find the approximate steady-state values $X_\infty \approx S_{in}/k_1$ and $S_\infty \approx K/\tau^*$. Substitution of scaled variables $x=X\cdot k_1/S_{in}$ and $s=S\cdot\tau^*/K$ and for the slow time scale $t_s= t\cdot D$ yields:

$$D\frac{dx}{dt_s} = \mu\frac{sK/\tau^*}{K+sK/\tau^*}x - Dx \tag{4.4.42}$$

$$D\frac{dsK/\tau^*}{dt_s} = -k_1\mu\frac{sK/\tau^*}{K+sK/\tau^*}x\frac{S_{in}}{k_1} - Ds\frac{K}{\tau^*} + DS_{in} \tag{4.4.43}$$

Dividing (4.4.42) and (4.4.43) by D, multiplying numerator and denominator of the Monod term by K, using $Mo=K/S_{in}$ and introducing $1/\tau^*$ as a perturbation parameter yield the standard form with the outer equations (4.4.44) and (4.4.45).

$$\frac{dx}{dt_s} = \frac{s}{1+\varepsilon s}x - x \tag{4.4.44}$$

$$\varepsilon\frac{ds}{dt_s} = -\frac{s}{1+\varepsilon s^*}x\frac{1}{Mo} - \varepsilon s + \frac{1}{Mo} \tag{4.4.45}$$

The substitution $t_f= t\cdot\mu/Mo$ gives the inner equations (4.4.46) and (4.4.47).

$$\frac{dx}{dt_f} = \varepsilon Mo\left(\frac{s}{1+\varepsilon s}x - x\right) \tag{4.4.46}$$

$$\frac{ds}{dt_f} = -\frac{s}{1+\varepsilon s^*}x - \varepsilon Mo\ s + 1 \tag{4.4.47}$$

Thus the timescale estimation and knowledge of scaling of the variables enables a scaling of the variables which in turn has led to successful selection of a perturbation parameter $1/\tau^*$. This selection is in accordance with the cases studies, as here it is assumed that $\tau^* >> 1$, so that indeed $\varepsilon << 1$. Compared to the dimensionless equations obtained with the direct approach, equations (4.4.44)-(4.4.47) have the advantage of directly showing the physical prerequisite under which the model reduction with singular perturbation is allowed.

4.4.2.3 Case 3: τ^* intermediate, Mo<<1

4.4.2.3.1 Direct

The result obtained in 4.4.2.2.1 applies.

4.4.2.3.2 Timescale estimation for variables

Step 1. Estimate initial timescales and select fast variables.
The timescale estimation results (Table 4.5) indicate multiplicity of timescales. S is selected as the fast state.

Table 4.5: Fast time scales for Case 3 (x(0)=0.5·x(∞)

Case	τ^*	Mo	λ_1/λ_2	τ_{fS}/τ_{fX}	τ_{fX}	τ_{fS}
3	3	0.04	0.036	0.034	1.88	0.063

Step 2. Estimate timescales of slow variables in the outer layer (quasi-steady-state).
X is the slow variable; its timescale is estimated with (4.4.33). Table 4.6 shows the results of the slow timescale estimates.

Table 4.6: Slow time scales and error for Case 3 (x(0)=0.5·x(∞)

Case	τ^*	Mo	τ_{fS}/τ_{sX}	τ_{sX}	τ_{fS}	$\Delta X_0/X_0$
3	3	0.04	0.076	0.83	0.063	0.021

Step 3. Check the multiplicity of time scales.
From Table 4.6, it is seen that for both Case 1 and Case 2 the condition $\tau_{fS}/\tau_{sX}<<1$ holds.

Step 4. Estimate the error of the slow variables.
The condition $\Delta X_0/X_0<<1$ holds as the error is approximately 2 % (Table 4.6). It is concluded that time scale separation can be applied.

Step 5. Reduce model if preceding steps indicate that the QSSA applies.
The preceding results indicate that the QSSA is valid. The same comments as in Section 4.3.2.2.2 apply.

4.4.2.3.3 Analytical scaling procedure

In this subsection, scaling is performed employing estimates based on the analytical solutions of the eigenvalues of the system, which leads to the standard form.

1. Estimate time scales

In Case 3, S<<K no longer holds, because S= O(K). The approximation proceeds as follows. S is in the order of magnitude as S_∞, and with $S=K/(\tau^*-1)$, the term (S+K) is written as a·K, with $a=\tau^*/(\tau^*-1)$. Then, with X>>S and $X\approx S_{in}/k_1$ we obtain (4.4.48).

$$\lambda_2 \approx -D-\mu\frac{k_1 XK}{(S+K)^2}\approx -D-\frac{\mu}{a^2 Mo}\approx -\frac{\mu}{a^2 Mo} \qquad (4.4.48)$$

which is in the same order of magnitude as the estimate (4.4.38) for τ^* moderate ($\tau^*>2$).

2. Test for QSSA necessary conditions
3. Perform error analysis on initial condition for slow state

The same results as in Section 4.4.2.2.3 apply.

4. For time scales, choose state scaling and subsequently derive scaled equations and (try to) find perturbation parameter.

For S, now another scaling is used as S in O(K). Substitution of scaled variables $x=X\cdot k_1/S_{in}$ and $s=S/K$ and for the slow time scale $t_s= t\cdot D$ yields transformed equations. Dividing the transformed equations by D, multiplying numerator and denominator of the Monod term by K, using $Mo=K/S_{in}$ yield the standard form with the outer equations (4.4.49 and (4.4.50).

$$\frac{dx}{dt_s} = \tau^* \frac{s}{1+s} x \qquad - x \tag{4.4.49}$$

$$Mo \frac{ds}{dt_s} = \quad -\tau^* \frac{s}{1+s} x - Mo\, s + 1 \tag{4.4.50}$$

with Mo^* as a perturbation parameter. The substitution $t_f= t\cdot\mu/Mo$ gives the inner equations (4.4.51) and (4.4.52).

$$\frac{dx}{dt_f} = Mo\left(\frac{s}{1+s} x \qquad - \frac{1}{\tau^*} x\right) \tag{4.4.51}$$

$$\frac{ds}{dt_f} = \quad -\frac{s}{1+s^*} x - Mo\ \ s + 1 \tag{4.4.52}$$

Again, scaling has led to straightforward, successful selection of a perturbation parameter and reformulation of the problem in standard form. This selection is in accordance with the case studies, as here it is assumed that Mo<<1, so that indeed ε<<1.

4.4.2.4 Case 4: S and X comparable, τ^* moderate, Mo ≈ 1

In the subsequent cases, only the relevant steps of the respective procedures will be discussed. In Case 4, both the timescales estimated by the eigenvalues and the estimated timescales according to Procedure 2 indicate that the timescales are relatively close and no timescale multiplicity occurs (Table 4.7 and 4.8). This was also confirmed in simulation. Thus, the conjecture that timescale multiplicity is associated with large concentration differences is confirmed.

4.4.2.5 Case 5: τ^* close to critical, Mo << 1, $\tau_\varepsilon \approx Mo$

Case 5 is very interesting, as this is the situation of optimal biomass productivity in a chemostat. The eigenvalue ratio (evaluated in steady-state) indicates no difference in time scales (Table 4.7). Also the eigenvalue ratio in the initial state was computed, which was also close to 1 (1.56). This seems to be in agreement with the conjecture, because the ratio S_∞/X_∞ is close to 1 (Table 4.2).

Table 4.7: Fast time scales for Case 4, 5 and 6 ($x(0)=0.5\cdot x(\infty)$)

Case	τ^*	Mo	λ_1/λ_2	τ_{fS}/τ_{fX}	τ_{fX}	τ_{fS}
4	3	0.4	0.375	0.182	1.88	0.34
5	1.244	0.04	1.00	0.123	1.90	0.24
6	1.044	0.04	0.0042	0.040	6.45	0.26

Table 4.8: Slow time scales and error for Case 4, 5 and 6 (x(0)=0.5·x(∞)

Case	τ^*	Mo	τ_{fS}/τ_{sX}	τ_{sX}	τ_{fS}	$\Delta X_0/X_0$
4	3	0.4	0.227	1.50	0.34	0.022
5	1.244	0.04	0.118	2.01	0.024	0.0036
6	1.044	0.04	0.0020	129	0.26	0.019

However, the fast timescale estimates obtained with Procedure 2 indicate occurrence of timescale multiplicity, S being the faster variable (Table 4.7). This is confirmed by the ratio τ_{fS}/τ_{sX} in Table 4.8, which is much smaller than 1.

Figure 4.2 shows a simulation of Case 5, which shows that indeed a boundary layer in S occurs. Apparently, the eigenvalues in the steady-state and in the initial state do not reveal this timescale multiplicity, whereas the timescale estimation by Procedure 2 correctly indicated timescale multiplicity in this case.

The eigenvalues evaluated in the steady-state do not correctly reflect the timescale behaviour of the nonlinear model. The eigenvalue ratio in the quasi-steady-state was in better agreement with the timescale estimation (λ_1/λ_2=0.088; computation not shown) than the eigenvalue ratio in steady-state (λ_1/λ_2=1). An eigenvalue trace might better reveal the timescale properties of the model, as was observed by Steffens *et al.* (1997). However, this is less straightforward than the timescale estimation procedure and it is concluded that the proposed timescale estimation procedure is to be preferred.

The conjecture that stiffness is associated with large concentration differences is falsified in this case, as timescale multiplicity occurs when the ratio S_∞/X_∞ is close to 1 (see Figure 4.2).

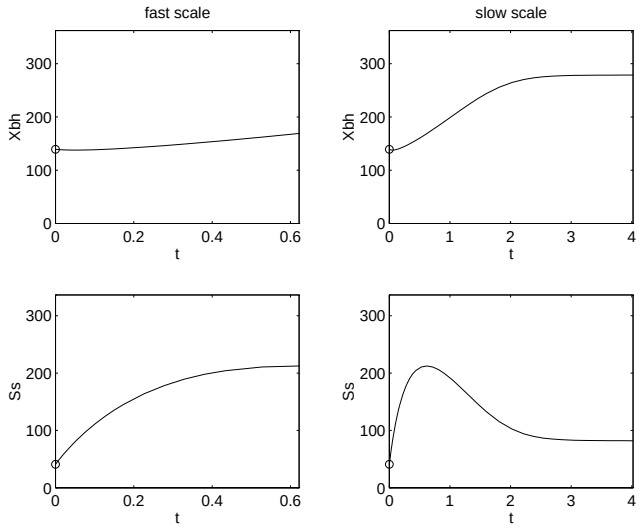


Figure 4.2: Timescale multiplicity at optimal τ^*

From the results the timescale and error estimates by Procedure 2, it is concluded that the QSSA applies in this case and S is the fast state. The model can thus be reduced. In the next subsection, for the situation that τ^* is close to critical, scaling will be applied to check whether this case can also be written in standard form and whether a perturbation parameter can be found.

4.4.2.6 Case 6: τ^* close to critical, Mo << 1, τ_ε << Mo

4.4.2.6.1 Direct

From the conjecture that a low ratio X_∞/S_∞ is associated with time scale multiplicity, both states are scaled with their steady-state, assuming that $\varepsilon=X_\infty/S_\infty$ is very small. With the scaled variables $x=X/X_\infty$ and $s=S/S_\infty$, the scaled equations (4.4.53) and (4.4.54) are obtained.

$$\dot{x} = \mu \frac{s}{k+s} x - D\,x \tag{4.4.53}$$

$$\dot{s} = -\varepsilon k_1 \mu \frac{s}{k+s} \frac{X}{X_\infty} - D\,s + D\,s_{in} \tag{4.4.54}$$

with $S_{in}= S_{in}/S_\infty$. This system is not in standard form however, so the direct scaling is not successful in this case.

4.4.2.6.2 Timescale estimation for variables

From Table 4.7 and Table 4.8, it is seen that the fast timescale for S (0.26) is much smaller than the fast timescale for X (6.45). The ratio of the fast timescale for S and the slow timescale for X (129) is even much lower (0.002). Also the ratio of the eigenvalues is very low. Clearly, multiple timescales are present. This is confirmed by numerical simulation, which shows a very short boundary layer for S (result not shown). Thus the QSSA holds and the system is in the form (4.4.2), (4.4.12) with ε very small and can be reduced.

4.4.2.6.3 Analytical scaling procedure

Finally, the analytical scaling procedure will be employed.

1. Estimate time scales

In Case 6, the nontrivial eigenvalue of (4.4.21) is approximated as follows. We have, with $\tau^*=1+Mo+\tau_\varepsilon$ and $\tau_\varepsilon<<1$,

$$\frac{S}{S_{in}} = \frac{Mo}{1+Mo+\tau_\varepsilon - 1} \approx 1 - \frac{\tau_\varepsilon}{Mo} \quad (4.4.55); \qquad X = \frac{(S_{in}-S)}{k_1} \approx \frac{\tau_\varepsilon}{Mo}\frac{S_{in}}{k_1} \tag{4.4.56}$$

which expresses the fact that conversion is very low and consequently the substrate concentration is close to the feed concentration S_{in}. With X<<S, and τ_ε<<Mo, after some manipulation and approximation we obtain (the result is given without proof):

$$\lambda_2 = -D + \mu \frac{-k_1 XK + S(S+K)}{(S+K)^2} \approx -D\,\tau_\varepsilon \tag{4.4.57}$$

The fast time and slow time scales can be scaled as (4.4.58) and (4.4.59) respectively.

$$t_f = t \cdot D \qquad (4.4.58)\ ; \quad t_s = t \cdot D \cdot \tau_\varepsilon \tag{4.4.59}$$

2. Test for QSSA necessary conditions

For the QSSA to be valid, $\tau_f << \tau_s$ must hold

$$1/D \;<<\; 1/D\cdot\tau_\varepsilon, \text{ or } \quad \cdot\tau_\varepsilon << 1 \tag{4.4.60}$$

which holds in the case studied.

3. Perform error analysis on initial condition for slow state: this is omitted here.

4. For time scales, choose state scaling and subsequently derive scaled equations and (try to) find perturbation parameter.

Substitution of scaled variables $x=X\cdot k_1\cdot Mo/S_{in}\tau_\varepsilon$ and $s=S/S_{in}$ and for the slow time scale $t_s= t\cdot D\cdot\tau_\varepsilon$ after some manipulation yields: (4.4.61), (4.4.62), which is not in standard form.

$$\tau_\varepsilon \frac{dx}{dt_s} = \tau^* \frac{s}{1+s} x \qquad - x \tag{4.4.61}$$

$$\tau_\varepsilon \frac{ds}{dt_s} = \; -\tau^* \frac{s}{1+s} x \frac{1}{Mo} - \varepsilon s + \frac{1}{Mo} \tag{4.4.62}$$

From this result and the scaling result in Section 4.4.2.6.1, it is concluded that for low ratio X_∞/S_∞ no simple perturbation parameter can be found. The results obtained with Procedure 2 clearly indicated timescale multiplicity for low ratio X_∞/S_∞, the fast timescale being associated with the substrate concentration S. From the conjecture, however, it was expected that for low ratio X_∞/S_∞,the fast timescale would be associated with the lower concentration, namely the biomass concentration X. Consequently, for low ratio X_∞/S_∞, the conjecture is falsified.

4.4.3 Other results

In Sections 4.4.2.2.1 and 4.4.2.3.1, direct scaling was applied to the system with Monod kinetics, which showed that the (small) ratio S_∞/X_∞ can be applied as perturbation parameter. It can be shown that is also possible for zero-order and first-order kinetics.

In addition to the simple system presented in Section 4.4.2, the same system but now extended with biomass retention was investigated, as biomass retention is the usually applied in activated sludge systems. Under typical operating conditions, the ratio S_∞/X_∞ is very small, which causes and even more pronounced timescale multiplicity between substrate and biomass in these systems (results not shown).

In addition to the simple system studied above, a slightly more complicated system was studied which included dissolved oxygen as an additional state variable. Here too occurrence of timescale multiplicity depends upon the operating conditions, especially the dilution rate and the oxygen mass transfer rate. The timescale estimation procedure was successfully tested to this system under operating conditions causing two timescales (Weijers and Weiss, 1999).

4.4.4 Conclusions

A simple bioreactor model of a chemostat with one biomass species and one substrate species was studied to obtain insight into timescale properties of bioprocess models and to test different procedures for model reduction. Starting point in the analysis was the conjecture that occurrence of multiple timescales is associated with a large concentration difference between the states. Three procedures to bring the problem into standard form were tested, namely a direct scaling procedure, a systematic, analytical scaling procedure and a procedure based on timescale estimation of variables.

At low substrate/biomass ratios, which occur at low dilution rate, the conjecture was valid. The direct scaling procedure showed that the problem can be brought into standard form and that the ratio substrate/biomass can be used as perturbation parameter in this case. The analytical scaling procedure enabled a more detailed analysis and showed that, depending upon the operating conditions, the Monod number or the reciprocal of the dimensionless residence time are suitable perturbation parameters. The substrate concentration was the fast variable in this case. The timescale estimation procedure correctly indicated the validity of the quasi-steady-state assumption for substrate.

For intermediate substrate/biomass ratios, the conjecture was falsified. At dilution rates with optimal biomass productivity, the ratio of eigenvalues evaluated in steady-state did not reveal timescale multiplicity, whereas the timescale estimation procedure correctly indicated timescale multiplicity in this case. The substrate concentration was the fast variable in this case, while the substrate concentration and biomass concentration were in the same order of magnitude. The timescale estimation procedure correctly indicated the validity of the quasi-steady-state assumption for substrate.

For high substrate/biomass ratios, the conjecture was also falsified. At high dilution rates close to washout, the ratio of eigenvalues evaluated in steady-state and the timescale estimation procedure correctly indicated timescale multiplicity. The substrate concentration was the fast variable in this case, while from the conjecture it was expected the biomass concentration would be the fast variable. Neither the direct scaling procedure, nor the analytical scaling procedure led to the standard form. The timescale estimation procedure correctly indicated the validity of the quasi-steady-state assumption for substrate, as confirmed by the clear boundary layer for this variable observed in simulations.

With respect to the procedures tested, it is concluded that the timescale estimation procedure is a helpful tool to detect timescale multiplicity and check validity of the quasi-steady-state approximation. The use of eigenvalues evaluated in steady-state or in the initial state can be misleading in nonlinear systems for this purpose. The analytical scaling procedure can be helpful to bring the problem into standard form and to obtain a perturbation parameter, thus providing insight into the cause of time scale multiplicity. Direct scaling is not a generally applicable procedure.

An important motivation to derive reduced nonlinear models is to obtain models that have a larger validity range than linear models. It is observed, however, that also nonlinear models obtained by reduction based on timescale separation have a limited validity range, namely for that operational range in state space or parameter space in which the assumptions for reduction are valid. A change of operating point may require a different reduced model, as states that were partitioned as slow may become fast or *vice versa*. This is probably the cause of the large error

induced in the reduction of ASM1 studied by Steffens and Lant (1997), discussed in Section 4.2.3. Thus, together with the reduced models, also a validity range should be indicated.

4.5 ASM1 Model reduction for interpretation of batch tests

4.5.1 Introduction

Development of easy-to-use methods for influent characterisation suitable for practical application is very important in the modelling of activated sludge processes, and has therefore received considerable attention over the last years. The Activated Sludge Model No. 1 (ASM1, Henze *et al.*, 1987) has become a standard model to describe the dynamics of wastewater treatment plants. An influent characterisation over different COD fractions that are distinguished in the model is required for most applications of the model. Examples of such applications are: checking of design under dynamic operating conditions (in designing new or upgrading existing plants), process analysis, design of control systems for process optimisation or as an aid in operation.

Different approaches for the COD characterisation task have been proposed in the literature. Frequently, batch tests are used in determining one or more of the biodegradable COD fractions X_{BH}, X_S and S_S. Typically, from the respiration rate (OUR) measured as a function of time, COD is estimated with a reduced model by curve fitting, with concomitant determination of one or more model parameters. Two relatively short batch tests were proposed by Kappeler and Gujer (1992) as discussed in Section 3.2.2. The simplifying assumptions and the reduced model used in these batch tests described below are given in Section 4.5.2, whereas below additional simplifying assumptions that have been made for the short batch tests are described.

Batch test A: wastewater/sludge. In this batch test, wastewater and sludge are added in a ratio of approximately 2:1. The test is relatively short and consequently biomass growth can be neglected. Dochain *et al.* (1995) employed a model different from ASM1 with the modification by Sollfrank and Gujer (1991), applying two hydrolysis processes that are first order in slowly biodegradable substrate X_S instead of one Monod type hydrolysis process. Kappeler and Gujer (1992) applied a similar approach, simplifying Monod type kinetics to first-order kinetics in X_S. If this reduced model is applied for identification, it can be shown that the identified hydrolysis parameter k_h' has another interpretation than the ASM1 hydrolysis parameter k_h, namely $k_h' = k_h/K_X$. Keesman *et al*. (1998) applied singular perturbation to analyse the endogenous respiration of this model, which corresponds to the slow timescale. In fact, the applied simplification of Monod kinetics can be applied only if $K_X >> X_S/X_{BH}$, a condition which is typically not satisfied. In fact, typically $K_X << X_S/X_{BH}$, which would allow simplification to first-order kinetics in X_{BH}. However, with this simplification, the resulting reduced model yields less identifiable parameter groups and no information on initial X_S is obtained.

Batch test B: wastewater only. In this type of experiments, biomass growth can not be neglected. In most cases, S_S is large, $S_S >> K_S$, and at the beginning of the batch test, the Monod kinetics can be simplified to first-order kinetics. This simplified model allows a straightforward identifiability analysis of the initial part of this batch test, the results of which are given in Section 3.2.3.

In a recent project (STOWA 96-08), biodegradable COD (COD_{BD}) was indicated the most important quantity for characterisation. BOD tests were suggested to determine this quantity. Measured BOD curves are well described by first-order kinetics (Metcalf & Eddy, 1991) and

total BOD (BOD_∞) is well estimated from measured BOD curves (Weijers, 1999; See Figure 4.3). In the experiment shown, BOD_∞ was estimated as 203 mg/l (the experiment corresponds to Sample 2 in Section 3.5).

$$BOD(t) = BOD_\infty (1 - \exp(-k\ t)) \qquad (4.5.1)$$

From the estimated BOD_∞, COD_{BD} is computed. Due to formation of inert products X_P assumed in ASM1, BOD_∞ observed in batch tests is lower than the initially present COD_{BD}. In Figure 4.4, a BOD curve is computed using ASM1 (Eqs.(4.5.3)-(4.5.5)). The parameter values and the initially present biodegradable COD (240 mg/l, straight line in Figure 4.4), were chosen such that the ASM1 curve describes the observed BOD in time, and especially its steady-state value, reasonably well. that The figure shows the initially present biodegradable COD is considerably higher than measure total BOD. This is due to formation of inert products, which are not respired. Therefore, a conversion factor between BOD_∞ and COD_{BD} is required (Eq.5.2). It is evident that an accurate conversion factor is required for accurate determination of COD_{BD}. However, the value of this parameter depends on the interpretation of BOD tests and is not unambiguous (Weijers, 1999a). Removing this ambiguity of the conversion factor f_C was an important motivation of the work in this section.

$$COD_{BD} = BOD_\infty/(1-Y_{H,BOD}) = f_C\ BOD_\infty \qquad (4.5.2)$$

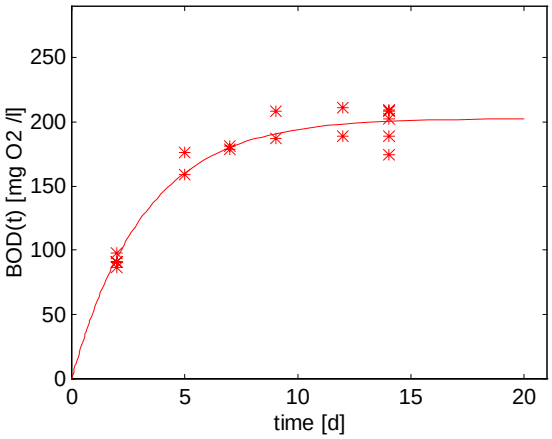


Figure 4.3: Measured BOD curves are well described by first-order kinetics.

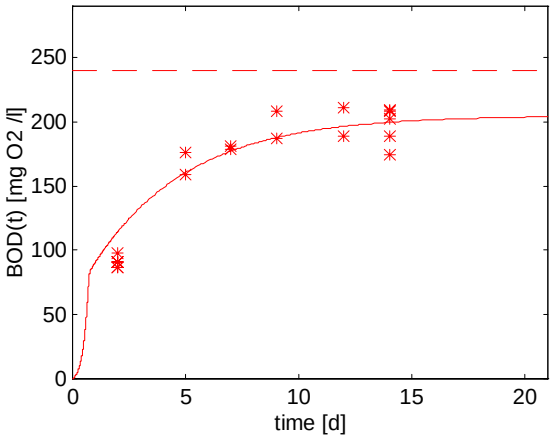


Figure 4.4: BOD curve simulated with ASM1; observed BOD_∞ is lower than COD_{BD} (straight line)

4.5.2 Theory and methods

ASM1 is reduced for aerobic conditions and without nitrification as a starting point for further model reduction. This initial reduction consisted of: 1) setting all Monod terms with dissolved oxygen (DO) limitation to 1; 2) setting all terms with DO inhibition to 0, thus neglecting denitrification and anoxic hydrolysis; 3) not considering inert components originally present in the wastewater (ASM1 component X_I), however including loss of biodegradable COD in the death-regeneration cycle due to inert product formation from biomass decay (X_P); 4) omitting alkalinity and 5) omitting nitrification (by setting X_{BA}=0). These assumptions lead to equations (4.5.3)-(4.5.5) (Note: X_P directly follows from a COD balance):

$$\frac{dS_S(t)}{dt} = -\frac{\mu_H}{Y_H}\frac{S_S(t)}{K_S + S_S(t)} X_{BH}(t) + k_h \frac{X_S(t)/X_{BH}(t)}{K_X + X_S(t)/X_{BH}(t)} X_{BH}(t) \quad (4.5.3)$$

$$\frac{dX_S(t)}{dt} = (1 - f_P) b_H X_{BH}(t) - k_h \frac{X_S(t)}{K_X + X_S(t)/X_{BH}(t)} \quad (4.5.4)$$

$$\frac{dX_{BH}(t)}{dt} = \mu_H \frac{S_S(t)}{K_S + S_S(t)} X_{BH}(t) - b_H X_{BH}(t) \quad (4.5.5)$$

with:

Y_H :	Heterotrophic yield	0.67	[-]
f_p :	Fraction biomass yielding inert products	0.08	[-]
μ_H :	Heterotrophic growth rate constant	6	[d^{-1}]
b_H :	Heterotrophic decay rate constant	0.62	[d^{-1}]
K_S :	Affinity constant for S_S	20	[mg l^{-1}]
k_h :	Hydrolysis rate	3	[d^{-1}]
K_x :	Hydrolysis affinity constant	0.03	[mg l^{-1}]
S_S :	Readily biodegradable COD		[mg l^{-1}]
X_{BH} :	Active heterotrophic biomass		[mg l^{-1}]
X_S :	Readily biodegradable COD		[mg l^{-1}]
X_P :	Particulate COD from decay		[mg l^{-1}]

The relationship between ASM1 and BOD tests is given by the oxygen consumption, expressed as OUR (Oxygen Uptake Rate, in mg O_2 l^{-1} d^{-1}), which upon integration gives BOD:

$$OUR(t) = \frac{(1 - Y_H)\mu_H}{Y_H} \frac{S_S(t)}{K_S + S_S(t)} X_{BH}(t) \quad (4.5.6)$$

$$BOD(t) = \int_0^t OUR(t)dt \quad (4.5.7)$$

4.5.3 Results and discussion

A further model reduction is obtained through applying a pseudo-steady-state assumption with respect to rapidly biodegradable COD. Central in ASM1 is the so-called death-regeneration concept, visualised in Figure 4.5. For typical parameter values used in ASM1 application, decay is rate limiting in the death-regeneration cycle. As a consequence, initially present S_S and X_S are (relatively quickly) degraded until a pseudo-steady-state is achieved (after a boundary layer δ), where S_S is constant (Figure 4.6). This is the case for many (realistic) ASM1 parameter values, as confirmed by extensive simulations.

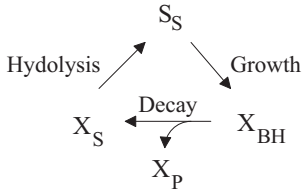


Figure 4.5: Death-regeneration concept in ASM1.

4.5.3.1 Pseudo-steady-state part

For the model reduction the following assumptions are postulated:

A.1: $\mu_H > k_h >> b_H$

A.2: S_S is constant ($\dot{S}_S = 0$) after $t=\delta$ (pseudo-steady-state assumption)

A.3: X_S/X_{BH} is constant =c (follows from A.2 and Eq. (4.5.3)).

A.4: $X_{BH}(t)=X_{BH}(\delta)\exp(-k\,t)$

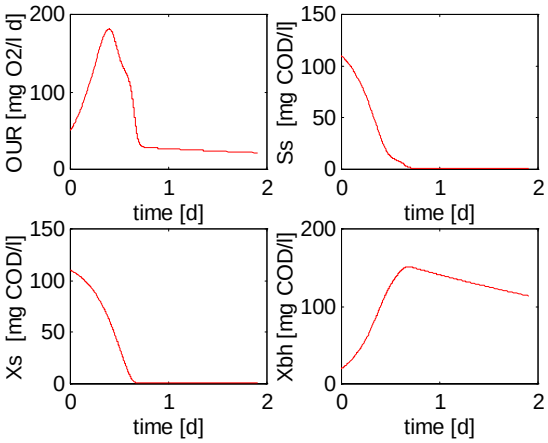


Figure 4.6.a: OUR and state trajectories in batch test, initial time (during boundary layer)

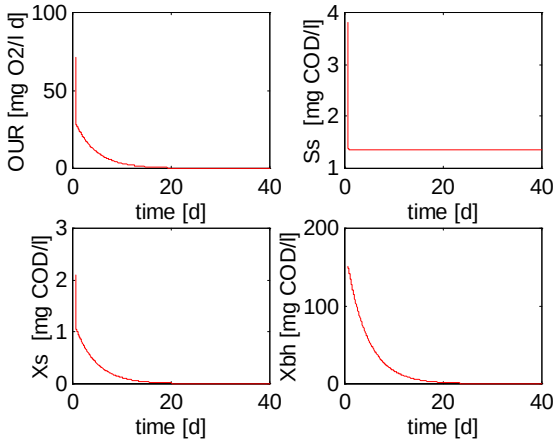


Figure 4.6.b: as 4.6.a, later time (after boundary layer)

Substituting A.3 and A.4 into (4.5.4) and (4.5.5), dividing left and right parts of the resulting equations by $X_{BH}(\delta)\exp(-k\,t)$ leads to a set of two algebraic equations (4.5.8) and (4.5.9).

$$-kc = (1-f_p)b_h - \frac{k_h c}{(K_X + c)} \tag{4.5.8}$$

$$-k = -b_h + Y_H \frac{k_h c}{(K_X + c)} \tag{4.5.9}$$

Solving (4.5.8) and (4.5.9) for c and k gives two roots for c and k. Selecting the positive root gives:

$$c=[b_H(f_p + K_X -1)-k_h + \sqrt{\{\, b_H^2\,((f_p+K_X)^2-2(f_p-K_X)+1)+b_H(2k_h(f_p-K_X-1)+ 4Y_H k_h K_X(1-f_p))+ k_h^2\,\}}]/2(Y_H k_h - b_H) \tag{4.5.10}$$

$$k = \frac{(1-Y_H(1-f_p))b_H}{Y_H c + 1} \tag{4.5.11}$$

The pseudo-steady-state value for S_S can be obtained by setting the derivative of S_S in (4.5.3) to zero which gives (4.5.12).

$$S_S(pss) = \frac{Y_H k_h K_S c}{Y_H k_h c - \mu_H (K_X + c)} \tag{4.5.12}$$

Thus, an analytical relationship is derived between ASM1 parameters and the first-order rate constant of the pseudo-steady-state part of batch BOD tests. Substitution of the default ASM1 parameter values into this expression gives k=0.23, which is the same as the typical value for the first-order rate constant in BOD bottle tests reported by Metcalf & Eddy (1991).

4.5.3.2 Complete BOD curve

Now the next step is to describe the complete BOD curve in ASM1 terms, including the initial part preceding the pseudo-steady-state. To compute the initial part of the BOD curve from (4.5.6) and (4.5.7), the initial state trajectories $S_S(t)$ and $X_{BH}(t)$ need to be known. In principle, it is possible to develop simplified expressions for these initial state trajectories. However, here we will make a stronger simplification, which is motivated by the fact that the pseudo-steady-state part is by far the largest part of the BOD curve and is attained relatively fast. Therefore, growth and hydrolysis are assumed to proceed so fast, that the pseudo-state is validly assumed to be attained (almost) instantaneously, within a very short boundary layer δ. During this (infinitesimally) small boundary layer δ, initially present S_S and X_S are converted to X_{BH}:

$$X_{BH}(\delta) = X_{BH}(0) + Y_H(S_S(0) + X_S(0)) \tag{4.5.13}$$

The initial BOD is then given by (it is emphasised that we are not concerned how this proceeds):

$$BOD(0+) = BOD(\delta) = (1 - Y_H)(S_S(0) + X_S(0)) \tag{4.5.14}$$

Finally, besides the rate constant and the initial value, we need the final value of the BOD curve, given by BOD_∞. Due to formation of inert products X_P assumed in ASM1, the total BOD observed in batch tests is lower than the initially present biodegradable COD_{BD}:

$$BOD_\infty = COD_{BD} - X_P(\infty) \tag{4.5.15}$$

with

$$COD_{BD} = S_S(0) + X_S(0) + X_{BH}(0) \tag{4.5.16}$$

Using ASM1, the rate of inert product formation is given by:

$$\dot{X}_P = f_p b_H X_{BH}(t) \tag{4.5.17}$$

The production of inerts is approximated using the fact that during the complete BOD curve biomass approximately decays exponentially from its value after the boundary layer and we write:

$$X_P(\infty) = \int_\delta^\infty f_p b_H X_{BH}(t)dt = f_p b_H X_{BH}(\delta)\int_\delta^\infty e^{-kt}dt = \frac{f_p b_H}{k} X_{BH}(\delta) \tag{4.5.18}$$

The complete BOD curve is now described by

$$BOD(t) = BOD(0+) + (BOD_\infty - BOD(0+))(1 - \exp(-kt)) \quad \text{for } t \geq \delta \tag{4.5.19}$$

4.5.3.3 BOD_∞ to CODbd conversion factor

To determine biodegradable COD from estimated BOD_∞, the conversion factor f_C is required. This conversion factor depends upon ASM1 parameters and influent COD fractionation and can be computed from (4.5.15), (4.5.16) and (4.5.18). However, a small correction is required, because a small amount of S_S (Eq. 4.5.13) is not respired. The conversion factor is therefore computed as:

$$f_C = \frac{COD_{BD}}{BOD_\infty} = \frac{COD_{BD}}{COD_{BD} - X_p(\infty) - S_S(pss)} \tag{4.5.20}$$

This analytic expression for f_C was tested against values obtained with ASM1 model simulations (Eqs. (4.5.3)-(4.5.5)). This was done for several values of ASM1 model parameters and different influent characterisations. Good correspondence was found for conversion factors with different values of ASM1 parameters, as all factors were within 1% from the exact values computed with ASM1. For default ASM1 parameter values and for low X_{BH}, it can be assumed that f_C=1.18 ± 0.01 (Weijers, 1999).

Of the ASM1 parameters, Y_H and f_p have the largest influence on the value of f_C. For non-default values of these parameters, f_C can be computed from (4.5.12), (4.5.13), (4.5.16), (4.5.18) and (4.5.20). The fraction X_{BH} of the initially present COD influences the value of f_C as well as the shape of the BOD curve during the boundary layer. If all initial COD is present as X_{BH}, a perfect first-order curve described by (4.5.1) without a boundary layer is obtained (Fig. 4.7.a). The value for f_C is then significantly higher than 1.18 (f_P=1.27).

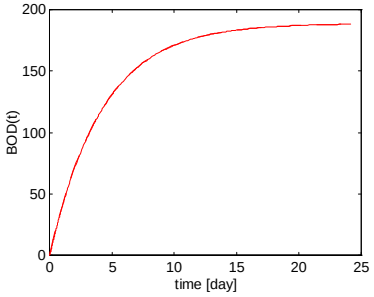


Figure 4.7.a: BOD curve, Only $X_{BH}(0)$

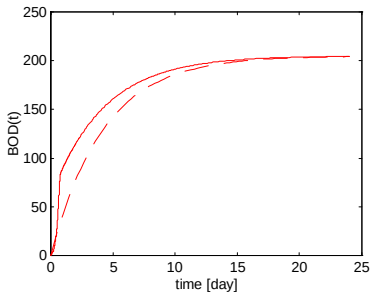


Figure 4.7.b: $S_S(0)$ high, $X_{BH}(0)$ low (5)

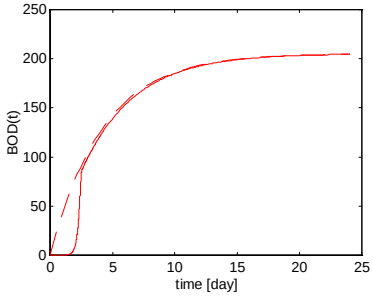


Figure 4.7.c: $S_S(0)$ high, $X_{BH}(0)$ very low (0.001)

For lower values of the X_{BH} fraction, but larger than approximately 10^{-3}, a boundary layer is obtained (Eq. 4.5.19) and an offset is present at t=δ (Fig. 4.7..b) , which does not correspond with experimentally observed curves (Eq. 4.5.1). However, for very low values of X_{BH} (lower than 10^{-5}), a lag in the BOD curve results and the boundary layer becomes larger, in the order of 1-3 days (Fig. 4.7.c). The BOD curve then has approximately the experimentally observed shape after the boundary layer, supporting the assumption of very low X_{BH} fraction as done in (STOWA 96-08).

4.5.4 Conclusions

Applying a pseudo-steady-state assumption, ASM1 has been reduced. Analytic expressions have been derived which provide straightforward interpretation of BOD curves in terms of ASM1 parameters as well as a quantitative basis to compute biodegradable COD from total BOD.

4.6 Conclusions and future perspectives

Rigorous models often must be reduced to low-order models as these are better suited for control, identification and are helpful to obtain a better understanding. The aim in this chapter was to develop a systematic reduction procedure to obtain nonlinear reduced models for controller design. First, reported reduction approaches and reduced models of ASM1 were reviewed. Several approaches are applied in ASM1 model reduction. Simplifying assumptions have been applied most frequently. Proposed models range from simple black-box zero-order kinetic models neglecting biomass dynamics, to the more complicated model of Jeppsson (1996), which includes biomass growth and decay and consequently has a larger validity range. Assumptions with respect to dynamics are also frequently usually applied for model order reduction. This is logical, as the stiffness of activated sludge process argues to develop models that are suited for different timescales. It appears that the reduction often is done heuristically. Relatively little systematic efforts have been done to analyse and understand timescale properties of ASM1.

It was concluded that singular perturbation is a promising candidate as a method to develop a systematic reduction procedure. It is a systematic reduction procedure and it can give more insight in dynamics of ASM1. Moreover, under certain condition, it retains the physical interpretation of the states in the order reduction, it provides an error estimate and it is suited for nonlinear model reduction, which is desired as it is an aim to obtain reduced models.

To apply the method, the model must be in the so-called standard form, which means that the states can be partitioned into fast and slow states. Obtaining this form or recognising that the model is in this form is the difficult part in the method. Therefore, it was decided to concentrate on this task.

First, methods the literature were reviewed. Bastin and Dochain (1990) suggested a simple rule for order reduction of (bio)process models through singular perturbation. This simple rule is not generally applicable, however, and can be applied in specific cases only, e.g. in the case of very low product solubility. Moreover, it does not yield the state partitioning or tell when the reduction can be made. Segel and Slemrod (1989) applied a methodology based on scaling to formally derive Michaelis-Menten kinetics via singular perturbation. This methodology was successful in detection of multiple timescales, to bring the model in the standard form and provided a suitable perturbation parameter that gave insight in the physical conditions that lead to timescale multiplicity. This procedure was therefore used as a starting point for the state partitioning (or detection of timescale multiplicity).

Three procedures were proposed, namely a direct scaling procedure, a procedure based on a mixed numerical / analytic timescale estimation and the analytical scaling procedure of Segel and Slemrod. The procedures were tested on a simple bioreactor model of a chemostat with one biomass species and one substrate species. Starting point in the analysis was the conjecture that occurrence of multiple timescales is associated with a large concentration difference between the states.

At low substrate/biomass ratios, occurring at low dilution rates, the conjecture is valid. The ratio substrate/biomass, the Monod number and the reciprocal of the dimensionless residence time are suitable perturbation parameters. For intermediate substrate/biomass ratios, the conjecture was falsified. The substrate concentration was the fast variable in this case, while the

substrate concentration and biomass concentration were in the same order of magnitude. For high substrate/biomass ratios at high dilution rates close to washout, the conjecture was also falsified. The substrate concentration was the fast variable in this case, while from the conjecture it was expected the biomass concentration would be the fast variable.

With respect to the procedures tested, the timescale estimation procedure is a helpful tool in model reduction, which is concluded from the fact that it in all cases correctly indicated whether the quasi-steady-state assumption was valid. The use of eigenvalues evaluated in the steady-state for timescale multiplicity however can be misleading in nonlinear systems. The analytical scaling procedure is helpful to bring the problem into standard form and to obtain a perturbation parameter in some cases, thus providing insight into the cause of time scale multiplicity. The direct procedure is not generally applicable.

In Section 4.5, a specific model reduction for interpretation of the batch test of Section 3.5 to determine biodegradable COD was carried out. Application of the QSSA to prolonged batch tests enabled reduction of ASM1 to a first-order model. This reduced model directly relates experimentally observed parameters to ASM1 parameters, and provides a quantitative basis to convert observed BOD to biodegradable COD. Moreover, the reduced model provides valuable insight into interpretation of BOD tests and the influence of influent COD fractionation.

It is expected that model reduction will remain an active research area in the next years, for application in control, identification and process optimisation. Singular perturbation provides the formal basis for quasi-steady-state assumptions and time scale separation and can be expected to play an important role. The procedure for timescale estimation of variables is a helpful tool for model reduction, as it provides a timescale to state association as well as an error estimate of the reduction. Scaling can provide additional insight into causes of timescale multiplicity.

In almost all reported cases of ASM1 reduction, the reduction was applied to lumped systems without concentration gradients, assuming the system to be either aerobic or anoxic. Thus reduction concentrated on reduction of the reaction kinetics, rather than reduction of transport and mixing in the reactor. However, many activated sludge systems are of the plug-flow type and exhibit gradients especially with respect to dissolved oxygen. This also holds true for full-scale bioreactors. Therefore, reduction of distributed systems may become an important topic in reduction of ASM1 and bioprocess models.

Chapter 5 Controller Design

They had well advanced in the project to look for possible benefits of an analytic design procedure. Together with project partners from the water boards, they had listed systematically all the performance specs they could think of, identified the disturbances and developed a plant model and an uncertainty description. Would possible performance improvement be high? The control engineer now had been working on implementation of the next design stage, which was to design the controller. He had expected this would be a straightforward step, because often modelling had proven to be the most time-consuming task in control system design. Now, however, he realised that this may be true to achieve some performance improvement but that guaranteeing optimality is much more involved. The available control theory and tools still were not able to deal with realistic objective functions and problem size. To finish the project within the time available, he had to decide either to apply well established methods that can only approximate the original performance specs or to apply brute force approaches that can not guarantee optimality. He set out to think for the best compromise.

This chapter focuses on controller design. Section 5.1 discusses possibilities and limitations of available control theory and tools in tackling practical controller design problems and motivates selection of Model Predictive Control (MPC) as a research tool in this chapter. Section 5.2 discusses state-of-art of control structure selection and control law selection in control of wastewater treatment plants, and introduces the case studies presented in Sections 5.3-5.5. Section 5.3 describes MPC application to a pre-denitrification plant. In Section 5.4, MPC application to a carrousel system is described. Section 5.5 investigates robustness of MPC controlled plants, using a structured uncertainty description. Section 5.6 gives conclusions.

5.1 Introduction

After definition of the control goal and modelling the plant, the actual control system is designed. If we apply an analytic design procedure for control system design as discussed in Chapter 2, we first list all design specifications as objectives and constraints of a multi-criterion optimisation problem and develop the required models of plant, disturbances and their uncertainties.

Stage	Action
1	Definition of the goal
2	Modelling of the plant
3	Input Output selection
4	Control Configuration
5	**Controller design**
6	Controller evaluation
7	Implementation, testing and commissioning

Figure 5.1: Control system design scheme. The focus in this chapter is on controller design. Control structure design (Stages 3 and 4) is only briefly addressed at.

It is assumed now that the uncontrolled system does not satisfy the specifications and that the task is to satisfy these through manipulating the system dynamics through control. The actual control system design then includes selecting the control structure, selecting the control algorithm(s) and tuning the controller(s).

In the idealised case of perfect knowledge of system and disturbances, an open-loop control approach could be applied for the control system design. In an analytic design procedure, a possible approach to solve the design problem would be to apply (off-line) dynamic optimisation to search for satisfactory system performance, employing trajectories of manipulated variables as decision variables. While such an open-loop approach provides useful insight in achievable performance and system behaviour, it is unsuccessful however to actually control systems due to uncertainty with respect to plant and disturbances.

Instead of open-loop control, feedback control is usually applied to reduce sensitivity to parametric uncertainty and to disturbances. The discussion below therefore starts from a general feedback scheme, comprised in the standard plant shown in Figure 5.2, which specifies the generalised plant *G* in Figure 2.1. The standard plant, originating from robust control theory, provides a powerful framework to systematically specify control system design problems.

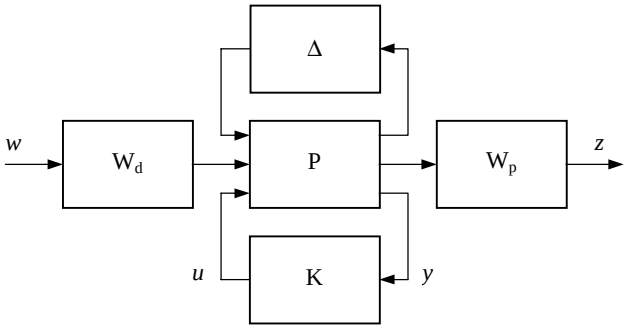


Figure 5.2: Standard plant, with controller K, uncertainty block Δ and the generalised plant that consists of the nominal plant P, disturbance weights W_d and performance weights W_p,

The standard plant includes performance specifications on the controlled variables signals *z* that are modelled in design filters W_p, models of reference signals *w* and disturbance and noise signals *w* that are included in W_d, a nominal plant model P and an uncertainty description Δ. To characterise performance in control system design, norms ("amplification measures") of the corresponding closed-loop (transfer) function matrix of *w* to *z* are used throughout the (modern) control literature.

While selection of inputs *u* and outputs *y* and their interconnections is an important part of design, this section will further concentrate on design of the controller K with given control structure[22]. Thus, the controller design problem is (Boyd and Barratt, 1991):

> Given a model of the system to be controlled (including its sensors and actuators) and a set of design goals, find a suitable controller, or determine that none exists.

A whole range of methods for controller design is available (see later in this section), where two extremes can be depicted. These two extremes are exact solution of an approximated design problem on one hand and approximate solution of the exact problem on the other hand. The first category consists of linear control methods, for which a well-established theory is

[22] Discussion of IO selection in feedback control system design is postponed until Section 5.2.1 to facilitate the discussion in this introduction.

available. In linear (robust) controller design, the specifications are translated into norms on transfer functions (system norms) and into design filters W_d and W_P, and model uncertainty into the (unstructured) uncertainty block Δ. Many design problems thus stated are convex and the corresponding optimisation can be solved guaranteed and with great efficiency (Boyd and Barratt, 1991). A fixed, linear, robustly stable controller K results. However, the original optimisation problem is only approximately solved because the controller design objective functions (norms) and models are only approximates of the actual problem.

In the second category, solving the actual optimisation problem approximately, several approaches are applied. One approach is parameter optimisation of fixed structure controllers, which can for example be linear controllers, rule-based controllers[23] and nonlinear controllers. A second approach is to apply dynamic optimisation of the actual optimisation problem and try to extract from the results sub-optimal, but easily implementable, control objectives[24]. A third approach is on-line optimisation, including feedback to reduce uncertainty[25]. Realistic problems that involve nonlinear models and/or objective functions can be dealt with in principle. However, as limited computation time is available on-line, approximations are required to reduce computational requirements of nonlinear optimisation methods, such as Sequential Quadratic Programming (SQP, Gill *et al*. 1981) or randomised approaches[26]. Several approximations are possible, e.g of the model (e.g. through model reduction), of the objective function or of the decision variables. While model reduction was treated in Chapter 4, here we concentrate on the controller.

Let us now return to wastewater treatment. Characteristics of chemical processes are interactions, stiffness, time delays and relative slowness, model uncertainty, time varying parameters (because of changing parameters), constraints and nonlinearity. Most of these characteristics also apply to bioprocess systems and wastewater treatment systems.

Many methods and approaches to control have been developed during the last few decades. An overview of methods is given in Table 5.1, in relation to the characteristics of the activated sludge process mentioned. Digital control was developed with the emergence of digital computing (Ragazzini and Franklin, 1958). Optimal control was developed as a rational, mathematically well-based design method, both for deterministic systems and for stochastic systems (Kwakernaak and Sivan, 1972; Sage and White, 1977), adaptive control for systems with varying parameters (Åström and Wittenmark, 1988; Wellstead and Zarrop, 1991), nonlinear control (Isidori, 1989; Slotine and Li, 1991), Model Predictive Control for optimal control of systems with constraints, large dead-times, non-minimum-phase behaviour and other inherent difficulties (Richalet *et al*. 1978, Morari *et al*., 1991, Bitmead *et al*., 1990), robust control theory to better understand and account for model uncertainty (Zhou *et al*., 1996), expert system control for crisp rule-based control and fuzzy control for fuzzy rules.

[23] For example, Kreisselmeier and Steinhauser (1983) determined optimal settings for a linear controller of an aircraft to operate in different operating points, thus incorporating robustness, whereas Schuetze (1998) optimised settings for rule-based controllers for integrated wastewater systems.
[24] For example, Ryckaert adopted this approach for optimal cyclic operation; see Section 5.2.2, Table 5.8.
[25] This is referred to as open-loop-optimal-feedback, see Section 5.2.3.
[26] A suitable approach for nonlinear optimisation is the application of randomised approaches. However, it cannot be guaranteed in general that the optimum found is indeed the global optimum; at most, an acceptance level can be indicated (Vidyasagar, 1997).

It was recognised in 1973 by Foss (Foss, 1973) that the important problems in chemical process control could not be coped with by one single all-embracing theory, while he indicated that it would be the theoretician to close the gap between actual problems and available theory. Still, no such single theory is available. With all the theoretical developments described above, several methods have well advanced, but it is still much of an art requiring significant application specific knowledge to select those pertinent for the application.

Table 5.1: System characteristics vs. control methods

System characteristics	**Control methods**
Interactions	1. Static/dynamic decoupling 2. Multivariable modern control LQG, IMC, MPC, H_∞
Stiffness	Hierarchical control Singular perturbation
Uncertainty	Robust control (design) methods, e.g. H_∞, Internal Model Control, Adaptive control
Time varying parameters	Adaptive control, Robust control
Lack of mathematical models	Rule-based control: Expert systems, Fuzzy control
Constraints	MPC
Nonlinearity	Several methods 1. Linearization 2. Piecewise linearization 3. Feedback linearization 4. Optimal control theory (dynamic programming) 5. Rigorous nonlinear optimisation (MPC)

In the line of the analytic design procedure discussed in Chapters 1 and 2, application of model-based on-line optimisation is a promising approach for control of wastewater treatment plants. Model Predictive Control is selected as a suitable framework, which we will further motivate in Sections 5.2.2 and 5.2.3. The characteristics of wastewater treatment processes may require MPC extension to adaptive and/or nonlinear MPC and possibly to include some way of dealing with stiffness. This chapter will investigate a few such aspects for MPC development for wastewater treatment. After discussing state-of-art in control structure selection (Section 5.2.1) and control law selection (Section 5.2.2) in wastewater treatment plant control, some aspects of MPC will be discussed into more detail in Section 5.2.3 and studied in the Sections thereafter.

5.2 State-of-art

5.2.1 Control structure design

This section treats control structure design. In the past, this stage has received relatively little attention in the control literature, while it has been indicated as very important already by Foss (1973). The situation is now improving and several scientists have been working on this topic (Morari and Stephanopoulos, 1980a,b; Morari, 1983; Hovd, 1992; Lee *et al.*, 1995; van de Wal, 1998). The task of control structure design is to (Skogestadt and Postlethwaite, 1996)

achieve satisfactory performance with minimal controller complexity.

Minimal controller complexity is required both for reliability reasons – design and maintenance are more prone to errors when the system is complicated[27] – and for economical reasons – a system with fewer sensors and actuators is cheaper to design and build[28].

Control structure design is especially difficult in large-scale systems, such as in control system design for chemical plants. This section will investigate whether control structure design is difficult also in wastewater treatment and if systematic methods for control structure selection are desirable. First, we will discuss IO selection and control configuration selection in wastewater treatment and then methods for these tasks and their applicability to wastewater treatment.

In the Input/Output selection step, one decides upon the number, place and kind of manipulated variables *u* and measured variables *y*. If the number of candidates for *u* and *y* is large, a large number of candidate IO sets typically remains. For large sets it is therefore impossible to design and test all candidate sets and systematic and quantitative pre-screening methods to reduce the number of candidate choices to feasible candidates are required to replace (or complement) engineering heuristics. A very desirable property of methods for IO selection is independence of the controller design method for two reasons. These are 1) to avoid computational effort of simultaneous control structure design and controller design and 2) to base the selection directly on the limits of performance imposed by the plant and the IO selection itself. Other desirable properties of IO selection methods have been listed and extensively discussed against existing methods in van de Wal (1998).

Table 5.2: Possible and suggested choices for *u*, *y* and *z* in control of WWTP's

Manipulated variables or **actuator inputs *u***	**Measured outputs** or **measured variables *y***	**Regulated outputs** or **controlled variables *z***
aeration (oxygen transfer k_La or DO setpoint)	Dissolved Oxygen DO	any of *y*
	ammonia NH_4	soluble COD
recycle rate Q_r	nitrate NO_3	total COD
waste flow rate Q_W	redox potential ORP	BOD
internal recirculation Q_{ic}	actual respiration rate r_{act}	MLSS
volume fraction aerobic	maximal resp. rate r_{max}	total amount of sludge
influent distribution	endogenous resp. rate r_{end}	biomass concentration X_B
influent buffering	StBOD	total biomass X
flow to clarifier‡	Total Organic Carbon TOC	sludge age SA
external carbon source	TAUC¶, [2]	dynamic sludge age DSA[1]
precipitants	turbidity in mixed liquor	specific oxygen uptake rate SCOUR[2]
	Sludge level in clarifier h_{sb}	food to mass ratio F/M[2]
	NAD(H)	
	sludge settleability SVI†	

†Not necessarily with a sensor, although also settlometers are also relatively well-developed (Grijspeerdt, 1996).
‡Only at very few plants. ¶ Total Area Under Curve. [1] Vaccari and Chritodoulatos (1989). [2] See Section 2.2.3.

Let us now consider the situation in wastewater treatment. Table 5.2 summarises possible choices for the manipulated variables *u*, measured variables *y* and controlled variables *z*. The table shows that many sensor types are available. Note that only the type of variables is listed,

[27] Addition of redundancy by extra actuators and sensors of course can improve system reliability.
[28] Thus control structure design itself is a multi-criterion problem, where performance is traded-off against reliability and cost.

not their location; moreover, only sensors that are relatively well developed have been included[29]. Section 2.2.3 summarises possible measurements including wet-analytical methods.

Before the actual IO selection is carried out, however, the controlled variables *z* should be selected and specifications defined. As discussed in Chapter 2, the choice of controlled variables in wastewater treatment is complicated, which is also seen from the list in Table 5.2. In fact, the conditions pertinent for reliable and optimal control are still insufficiently well known. Consequently, different choices for controlled variables are used or suggested in the literature as well as in practical applications.

Remark: In N-removal plants it is usually assumed that COD removal proceeds well if N-removal is well controlled[30].

After selection of the controlled variables, the IO selection can be carried out[31]. The typical approach adopted currently in WWTP design is to do static design and try out several sensor/actuator configurations by dynamic simulation. However, to guarantee successful selection this is not a feasible approach, and it is argued below why IO selection methods are desired.

Let us first consider input selection. In Section 2.3, it was shown that in plants for nitrogen removal there are more ways to act on the process than in conventional plants. Nevertheless, the abilities to act on the process are relatively limited when compared to the possibilities to measure. In Table 5.3, possible input selections are summarised for the types of N-removal systems considered in this thesis, for the most important classes of manipulated variables. For each manipulated variable, a list of measured variables is given as a summary of the literature. It is noted that the table is not an exhaustive overview of all possible selections.

Table 5.3: Some IO selections applied in wastewater treatment plant control

System	***u***	***y***
1,2,3	aeration (k_La or DO)	DO, NH_4, NO_3, ORP, r_{act}, TAUC, StBOD, TOC, R[at], NAD(H), SVI
2	Q_{ic}	NO_3, NH_4, ORP, Q_{in}
1,2,3	Q_r	MLSS, h_{sb}, X_B[at], R[at], R[profile], F/M, DO[ras], r_{div}†
1,2,3	Q_w	MLSS, h_{sb}, X_B[at], X_B[total], SA, R[ras], F/M, r_{div}[1]

1: Alternating systems, 1 tank (also includes carrousels with intermittent aeration);
2: Pre-denitrification systems, both with 2 CSTR's and plug-flow-like;
3: Carrousel systems (no intermittent aeration).
† r_{div}: different respiration rates can be measured. Several rates and combinations of rates are applied (Spanjers *et al.*, 1998). R = SCOUR, Specific respiration rate, r = respiration rate, F/M = Food to Mass ratio, [at]: in aeration tank, [ras]: in return activated sludge.

[29] Especially useful in control of WWTPs are sensors that employ cross-flow ultra-filtration in combination with automated laboratory wet chemistry methods. Reliable sensors for ammonia, nitrate and phosphorus based on this technology are now commercially available (Thomson and Kisbye, 1996; Longdong and Wachtl, 1996; Wacheux *et al.*, 1996). Also very useful are sensors based on respirometry. Several commercial respirometers exist; see Spanjers *et al.* (1998).

[30] This is a form of *partial control*. In partial control, only a subset of the controlled variables is actually controlled (Stephanopoulos, 1985).

[31] The tasks performed in Control Structure Design as defined in this thesis exclude the selection of controlled variables – this was supposed to be part of the control goal definition (See Chapter 2 and Section 2.4) – and the selection of the control law. This is different from Skogestad and Postlethwaite (1996) who include these tasks in Control Structure Design.

The table shows that output selection is more involved than input selection as the selection of the sensor type is nontrivial due to the large number of alternatives. Moreover, for many variables, different locations are possible, hereby significantly extending the number of candidates. In addition to insufficient understanding of the activated sludge process, it is often economically attractive to apply sensors for quantities closely related to the controlled variable ($y \neq z$) instead of measuring the controlled variables themselves[32].

Thus, on one hand, output selection has become more complicated as more sensor types must be chosen from, on the other hand, it has become more straightforward as several new sensor types have a closer relationship with the controlled variables. The overall result is that IO selection cannot be done by a candidate-by-candidate approach[33]. This is seen from the number of possible IO sets that can be derived from Table 5.3. This number amounts to several thousands, which, although it is much smaller than the numbers typical in large-scale problems such as in chemical plants, still is so high that a pre-screening is highly desirable.

In the control configuration stage, the structural interconnections between *y* and *u* are chosen. As discussed in Chapter 1, especially the trade-off between plant performance and controller complexity is made. Whether decentralised control can be applied, depends upon the occurrence of unwanted interactions. Such interactions do occur in activated sludge plants, which is discussed below. First, interactions in the bioreactor are considered, focussing on N-removal systems, then interactions are considered with the clarifier.

The following systems are distinguished here.

1. Alternating system (e.g. studied by Lukasse, 1999). Usually there is only one manipulated variable, namely the aeration intensity, and the system is not functionally controllable[34]: effluent ammonia and nitrate cannot be controlled independently
2. Predenitrification system. Often, two manipulated variables are applied, namely the aeration intensity and the internal recirculation flowrate Q_{ic}. Here, both ammonia and nitrate may be controlled. For example., Kayser (1990) suggested 2 SISO loops for control of ammonia by aeration and nitrate by Q_{ic}. Interaction may occur however, as was shown in a 2-reactor system (Weijers *et al.* 1995b; See Section 5.3).
3. Carrousel system. Usually aeration is used as a manipulated variable. If more than one aerator is present, there may be (limited) possibilities for independent control of ammonia and nitrate. However, interactions typically occur which was a reason to study application of multivariable control for these systems (van Schagen *et al*., 1995, Weijers *et al*., 1997c).

Interactions also occur in the system bioreactor plus clarifier. For example, control of the amount of the sludge concentration or of the sludge age will influence the concentrations of soluble components and vice versa. Sludge concentration control may interfere with sludge blanket level control in the clarifier. Unwanted interactions occurred between three SISO controllers for SCOUR profile, mean cell residence time and DO in an integrated control system for a step-feed activated sludge system (Vitasovic and Andrews, 1989).

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[32] This is referred to as *inferential control* (Stephanopoulos, 1985).

[33] In plants with N-removal, sensors for the pollutants of concern, NH_4 and NO_3, are available. One could argue that here output selection is much more straightforward than in conventional plants. However, in control of N-removal plants also inferential control is considered, e.g. for economical reasons (for example by using ORP as a cheap alternative for nitrate sensors) or to combine several objectives (as is the case in control of the Total Area Under Curve in respirometry). Consequently, the number of candidate choices is high also

[34] An m-input l-output system G(s) is functionally controllable if G(s) has full row rank. This is required to control all outputs independently (Skogestad and Postlethwaite, 1996).

From this brief discussion on interactions in activated sludge systems, it follows that in control system design for N-removal plants interactions must be taken into account. As interactions in activated sludge treatment systems have been hardly studied systematically, this topic requires further research. Depending on the wastewater treatment system of concern, the system specifications and the selected control inputs and outputs, multivariable control may be required. However, it is noted that while in mechanical systems and electrical systems functional control is required in most cases, in process control interaction may be acceptable in some cases (Foss, 1973), and the influence of interactions on the systems performance remains to be established.

From the discussion above, we conclude that selection of controlled variables has higher priority than IO selection. Improved insight in suitable controlled variables can well be obtained through dynamic optimisation studies. Optimal input, state and output trajectories and observed relations between different variables can provide valuable insight into the system and for deciding on suitable controlled variables.

An interesting option to include a control objective oriented approach would be to apply the procedure for selection of controlled variables described by Skogestad and Postlethwaite (1996, Section 10.3) to (dynamic) optimisation results. This procedure is based on selecting those controlled outputs that correspond to a plant transfer matrix with a minimum singular value that is as large as possible. The aim is to select the controlled outputs such that the inputs have a large effect on the outputs, the influence of disturbances on the optimum value is low and the control error is kept small. This procedure includes a scaling of inputs as well as of outputs.

We expect that IO selection will be more straightforward once a good selection of controlled variables has been made. For the IO selection and for the control configuration selection therefore, probably a basic analysis combined with engineering heuristics will suffice. Such a basic analysis for conventional activated sludge plants by studying step and frequency responses was carried out by van Straten (1993). Olsson and Jeppsson (1994) carried out a qualitative analysis of cause-effect relationships. These analyses can be extended towards a quantitative analysis of N-removal systems. Appropriate tools to start with are step and frequency responses. In addition, (dynamic) RGA (Relative Gain Array) as discussed in Skogestad and Postlethwaite (1996) may be helpful.

In this way, a limited number of promising IO candidates may be selected. Before the actual controller design, an analysis of Input/Output controllability on these IO candidates can indicate fundamental limitations imposed by the respective IO selections. A procedure for such an IO controllability analysis is given in Skogestad and Postlethwaite (1996, Section 6.11.1).

Should such a basic analysis be insufficient, more advanced methods can be applied. A combination of existing methods for IO selection may be required, as existing methods are still insufficiently powerful if applied individually[35]. Alternatively, better methods for control structure selection may be developed. An interesting option for this development would be to

[35] Methods for IO selection have been recently reviewed by van der Wal (1998). Existing methods were all judged unsatisfactory against the criteria defined. Especially promising were considered those based on robust performance, based on modern robust control theory. Both methods relying on sufficient conditions that employ unstructured uncertainty and on necessary conditions that employ structured uncertainty were studied. However, also these methods appeared to be still insufficiently suited for rigorous IO selection. The same conclusion was drawn with respect to control configuration selection methods.

use controllability analysis more rigorously for control structure design integrated with the controller design, instead of using it as a check afterwards. Possible methods for such an approach are mixed integer programming or combinatorial optimisation (e.g. de Jager *et al.*, 1999). The feasibility of such an approach remains to be established.

5.2.2 Control law selection

This section discusses state-of-art of control law selection in activated sludge plant control. An overview is presented of the literature in the form of summarising tables. Table 5.4 gives symbols used to present information on treatment systems and the type of studies in these tables.

Table 5.4: Abbreviations to indicate systems and studies in this section

Symbol	System
0	Conventional activated sludge
1	Alternating system
2	Pre-denitrification
3	Carrousel
-	Unspecified
s	Step-feed
p	Plug-flow
n	with Nitrification

Symbol	Study (status)
o	proposal only
d	under development
r	developed, but not tested
s	simulation
p	pilot plant
f	full-scale plant

Classical control

This category includes so-called classical control methods developed until the late 50's such as PID control, cascade control, ratio control etc. In addition, digital implementation of these methods is included. A large impulse to application of control in sewage treatment was given in the sixties with the progress of digital computers. Application of (PID) control of DO has become standard routine at many plants. Some examples are given in Table 5.5.

Table 5.5: Classical control examples

Reference	System	Study	Control	Remarks
Ruider and Schopper, 1974	0	o/p	SISO	several suggestions for DO and MLSS
Busby and Andrews, 1974	0s	s	SISO	P-control of h_{sb} with Q_w or Q_r Feed distribution (feedforward)
Stepner and Petersack, 1974	0	f	SISO	PID (velocity form, tuning with pole-placement)
Vitasovic and Andrews, 1989	0s	s	SISO	PI control of DO
Marsilli-Libelli, 1989	0	s	SISO PID	control of biomass by Q_r, 2 observers: for OUR and for substrate and biomass
STOWA 97-w05	2	f	SISO	PID control of NO_3 with Q_r (tuning with stepresponse; on-line retuning required)
STOWA 97-w03	3	f	SISO MISO cascade MISO cascade	PI on DO PI on NH_4 as master for DO slave PI on NO_3 as master for cascade NH_4

Rule-based (logic, expert system, and fuzzy control

While the selection of the control structure in classical control applications often is based on process engineering heuristics, for design, tuning and implementation of classical controllers, considerable control engineering knowledge and basic understanding of process dynamics is required. In rule-based control, process engineering heuristics can be directly applied. This can be particularly advantageous if considerable process knowledge in qualitative form, e.g. operator experience, is available and no or only poor mathematical models are available.

In its most simple form, rules are directly implemented in control logic, e.g. in PLC's. This approach is regularly applied in activated sludge control. If the number of rules is large, application of expert systems is more appropriate. Here, the knowledge and the logic are separated into a knowledge base and an inference engine respectively. This largely facilitates implementation and maintenance of the system.
In the late eighties expert systems were expected to become valuable operational tools in activated sludge plant control (Olsson *et al*., 1989; Barnett and Andrews, 1990) and several systems were proposed in the early nineties (see table 5.6). However, in the late nineties they were reported not successful (Olsson *et al*., 1998), at least in the Scandinavian countries. Reported causes of this are their complexity and the inability to capture available knowledge sufficiently well. Another cause is that construction of knowledge bases is a plant-specific task, requiring not only definition of rules but also of values for several parameters, which requires considerable tuning and thus is a costly task. It is noted that in most reported cases, expert systems were used for diagnostic (failure detection) and advisory tasks. No examples of direct expert control, which would also be a good possibility, are known to the author.

Table 5.6: Rule-based control examples

Reference	**System**	**Study**	**Control**†	**Remarks**
Vitasovic and Andrews, 1989	0s	s	SISO RB	rule based control of SCOUR profile on-off control of MCRT
STOWA 97-w01	3	u	MIMO RB	aerators switching based on NH_4 and DO
STOWA 97-w02	3	s/u	SIMO RB	aerators switching based on respirometry
Barnett and Andrews, 1990	-	o	ES	discussion of requirements for successful application (e.g. learning capability)
Koskinen and Viitisaari, 1990	-	p	ES	detect off-normal conditions
Maeda *et al*., 1990	-	f	ES	diagnosis and advise
Ladiges and Kayser, 1993	3	f o	ES	on-line system for failure detection off-line system as operational advisor (uses deterministic model predictions)
Ozgur, 1991	0n	o	ES (with 'fuzzy' terms)	refinery wastewater; diagnosis and advise (337 rules, 56 parameters) (uses deterministic model predictions)
Tong *et al*., 1980, Beck, 1984	0n	s	MIMO FLC	control of DO, Q_r and Q_w, 20 rules
Couillard and Zhu, 1992	0n	s	MIMO FLC	fuzzy supervisor for 2 PID loops for control of shock loading (16 rules)
Jager, 1995	0	s/f	FLC	industrial wastewater
STOWA97-32, Kalker *et al*., 1999	2p	s	MISO FLC SISO FLC	high-level (>6 rules) aeration control low-level (> 5 rules) aeration control

†RB: Rule-based; ES: Expert system; FLC: Fuzzy Logic Control; MCRT: Mean Cell Residence Time (=SA)

Fuzzy logic control (FLC) offers the possibility to implement vague linguistic rules. Its application to activated sludge control is under development. Rule bases for fuzzy control are often smaller than for expert systems[36]. Despite its attractiveness to engineers not familiar with control engineering theory and tools for its conceptual simplicity, successful implementation is hampered by time-consuming tuning of the fuzzy rule base, where, just as for expert system application, rules and parameter values must be defined. To achieve straightforward tuning, Kalker *et al*. (1999) determined fuzzy rules and sets for direct FLC based on an optimised PI-controller, according to a method described in Jager (1995). Such an optimal PI-like FLC can easily be combined with linguistic rules, which possibly improves performance. Besides its use

[36] The objectives and tasks of fuzzy control systems are correspondingly less ambitious, namely control of one or more outputs based on several inputs, for which a few rules usually suffice. In contrast to expert systems, fuzzy control often aims at direct control.

for direct (Table 5.6) and supervisory (see below, Table 5.10) control, other FLC possibilities are discussed in STOWA 97-32.

Improvement of application of artificial intelligence (AI) to control is expected from hybrid or integrated use of different techniques, referred to as multi-AI paradigms. Integrated use of different types of information and knowledge (deterministic models, physics-based or 'deep' knowledge, visual information, empirical (expert and fuzzy), 'shallow' knowledge, historical data, artificial neural nets) in a single environment is still under research. One approach would be to convert different types of knowledge and information into one another, in analogy to transformation between different model representations in linear systems. Examples are the translation of historical data via identification ('learning') to artificial neural nets (ANNs) and from trained ANNs via knowledge extraction to (fuzzy) rules.

Table 5.7: Hybrid or Integrated Artificial Intelligence techniques examples

Reference	System	Study	Control	Remarks
Baba *et al*., 1990, Enbutsu *et al*., 1993	¶	s	MISO ANN[2]	learning from historical data using ANN's and knowledge (fuzzy rules) extraction from ANN's
Ohtsuki, T. *et al.*, 1998	0[1]	f	MIMO	Agent-based AI system, including fuzzy expert, fuzzy control and model ASM1

¶ :Coagulant injection system; [1]High-loaded activated sludge with ultra-filtration; [2]ANN: Artificial neural network.

Another interesting - be it still rather crude - attempt to such an approach is the 'blackboard technique' (Krijgsman, 1993), applied to the activated sludge process by Ohtsuki *et al*. (1998). Here, different agents ('expert modules') consisting of different AI techniques consult each other via a common database ('blackboard') with a simple data type, without a central, co-ordinating system. The number of required transformations can be much more limited in this approach. Moreover, in such an agent-based type of approach, the complexity and related problems of expert systems can probably be avoided. It is noted however, that in such an agent-based or rule-based approach, optimality cannot be guaranteed as with model-based control.

Model based control

The availability of mathematical models for activated sludge processes has steadily increased and motivates application of model based control. Mathematical models are well suited for application of optimal control, which is defined here as mathematical optimisation of a performance index. Several studies of optimal control in ASP control have been reported and some examples are given in Table 5.8. For reviews on optimal control studies see Marsilli-Libelli (1984) and Kabouris and Georgakakos (1990).

Optimal control

In several studies, application of LQG has been investigated. This linear, time-invariant control technique is applied typically for regulation of a reference behaviour (a steady-state, a single operating point or a reference trajectory) where a linearized model is locally valid. In LQG, the output variance is minimised for Gaussian noise on the system inputs. The noise characteristics are often unknown, however, and are usually used as tuning parameters to achieve acceptable performance. Because usually not all states are measured, a state observer is applied. The robustness of the resulting LQG controller can be arbitrarily poor, in contrast to the full-state information controller (LQR) (Doyle, 1978).

To obtain the required reference behaviour, (off-line) dynamic optimisation can be applied. The resulting open-loop optimal reference behaviour is model dependent and cannot be

implemented as such. An alternative is to implement such dynamic optimisation on-line and include feedback, which is a form of MPC as discussed in Section 5.1. Another possibility would be to extract properties from the dynamic optimisation results that are not or little model dependent and are practically implementable. This approach was applied by Ryckaert (1998) for a cyclically operated process. The applicability of such an approach to other activated sludge systems remains to be established.

Table 5.8: Optimal control examples

Reference	System	Study	Control	Remarks
Hamalainen *et al*., 1975	0	s	MISO LQG	control S, X and X_r by Q_r[1] (+FF)
Marsilli-Libelli, 1984	1	s	SISO LQG[2]	control of DO by k_La
van Schagen *et al*., 1995	3	s	MIMO LQG	control NH_4 and NO_3 by k_La (2 aerators)
Lindberg, 1997	2	s	MIMO LQG	control NH_4 and NO_3 with DO setpoint, Q_{ic} and external carbon dosage; model by subspace identification (from ASM1)
Lukasse *et al*., 1998a	1	s/p	MISO RHOC[4]	control NH_4 and NO_3 by k_La (L_1-norm)
Lukasse, 1999	1	s/p	MISO state feedback (L_1)	L_1-norm optimal state feedback law (only for LTI systems with 1 input, 2 states and diagonal A)
Kabouris and Georgakakos., 1990, 1991	0	s	Open loop optimal	optimal control trajectories for Q_r and Q_w to suppress diurnal variations[5]
Kabouris *et al*., 1992	0	s	"	effect of sludge storage on performance
Ryckaert, 1998	cyclic[3]	s	Open loop	dynamic optimisation to derive implementable reference behaviour

[1] S: substrate, X: biomass, X_r: biomass in recycle. [2] Including integral action and converted to a transfer function representation; [3] Cyclic operation in the so-called Unitank system; [4] RHOC: Receding Horizon Optimal Control, a form of model predictive control; [5] In the 1991 study, output uncertainty resulting from input uncertainty was investigated as a means to estimate applicability of this open-loop approach.

Lukasse *et al*. (1998a) applied linear MPC for setpoint control (RHOC, Receding horizon Optimal Control) employing a L_1-norm[37], which was claimed more realistic than the usually applied H_2-norm[38]. In this specific case (alternating process), the global optimum could be found through enumeration. Moreover, the optimal RHOC could be approximated well by a state feedback controller (Lukasse, 1999). The solutions in these studies are specific for the L_1-norm and for alternating operation and can not be generalised to other criteria and other types of operation. It is noted that the performance in the pilot plant was not completely according to what was expected from simulation results, most probably due to model mismatch.

Robust, adaptive and nonlinear model-based control

Linear time-invariant control methods in fixed operating points have limited applicability to the activated sludge process for two reasons, namely nonlinearity and parameter variability. Due to the large disturbances, the system cannot be kept in a fixed operating point, and in fact, steady-state regulation cannot be expected to correspond to optimal performance and the nonlinearity of the system must be taken into account. Moreover, parameters of the activated sludge process change in time, for example due to temperature variations and to load and influent composition variations with corresponding changes in biomass composition and characteristics.

[37] For a description of signal and system norms, see e.g. Zhou *et al*. (1997) or Boyd and Barratt (1991).

[38] Deviations of effluent concentrations of NH_4 and NO_3 from setpoints were considered as a measure of performance. It was suggested to select setpoints equal to zero and use disposal costs as weight factors. This corresponds to an approximation of the actual costs. Actual costs relate to loads rather than concentrations.

Consequently, control systems that are robust against state and parameter variations are required in control of the activated sludge process. Possible approaches to achieve robust systems are to develop robust, adaptive and nonlinear control systems, which have been studied for activated sludge process control. Examples are given in Table 5.9.

For (low-level) DO control, SISO adaptive control will probably suffice. An alternative may be robust Model Predictive Control (Haarsma and Keesman, 1993).

For control of substrate and biomass, several combinations of techniques have been applied. Bastin and Dochain (1990) propose the application of nonlinear observers in combination with feedback linearization for bioprocesses. This approach was also adopted by Vanrolleghem (1994) for control of the sludge inventory. However, this feedback linearization alone is not an optimal control technique, it requires a reference behaviour and its linearizing effect is lost under hard constraints on the manipulated variables. MPC does not have these limitations. MPC has been investigated for DO control in conventional activated sludge plants (Haarsma and Keesman, 1993) and adaptive MPC for N-removal in alternating systems (Lukasse *et al*., 1997a). A very simple (reduced) model was used (see Chapter 4). An Extended Kalman Filter was applied for the adaptive part, and RHOC as described above for the MPC part. The methodology applied, including the controller criterion (L_1-norm), the model used and the solution method (through enumeration) are specific for alternating plants and cannot be applied to continuous plants such as predenitrification plants and carrousels.

Table 5.9: Robust, adaptive and nonlinear model-based control examples

Reference	**System**	**Study**	**Control**	**Remarks**
Marsilli-Libelli, 1989	0	s	implicit STC[1]	PID control of DO by (unknown) k_La
Holmberg, 1987	0	s	SISO adaptive	DO control by k_La with fb linearization
Lindberg, 1997	2	s p[4]	SISO (in)direct adaptive	control of external carbon by indirect (model based) adaptive PI and direct and indirect adaptive MV[2] control
Lindberg, 1997	2	p	SISO adaptive	nonlinear PI control of DO by k_La
Bastin and Dochain, 1990	0	s	SISO adaptive nonlinear	nonlinear observers and fbl[3]
Dochain, 1990	0	s	MIMO adaptive nonlinear	nonlinear observer and fbl[3], regulation of BOD and DO by k_la and Q_r
Dochain and Perrier, 1993	0	s	MIMO adaptive nonlinear	nonlinear observer and fbl[3], regulation of BOD and DO by k_la and Q_r
Vanrolleghem, 1994	0	s	MIMO adaptive nonlinear	nonlinear observer and fbl[3]; regulation of X and h_{sb} by Q_r and Q_w
Haarsma and Keesman, 1993	0	s/p	SISO robust MPC	Robust MPC with structured uncertainty; DO control by k_La and feedforward of OUR
Lukasse *et al*. 1997a	1	s/p	MISO adaptive MPC	Adaptive RHOC of NH_4 and NO_3 with aeration intensity (L_1-norm)

[1] STC: Self-tuning controller; [2]: MV: Minimum variance; [3] fbl: feedback linearization; [4]only direct adaptive control was evaluated on the pilot plant.

Plant-wide and supervisory control

Finally, supervisory or plant-wide control of the bioreactor in connection to the clarifier or other units of the wastewater treatment plant have been studied (Table 5.10). It is noted that in fact the expert system examples in Table 5.6 are to be considered as supervisory control, but they have been discussed under rule-based systems for ease of discussion. It is noted that several software tools for expert supervision are available, e.g. IC2S from Hydromantis Inc. (Patry and Takács, 1995) that includes a decision support system (DSS), deterministic models and

parameter estimators. However, many questions on the conceptual level with respect to their application and implementation remain to be studied.

A recent supervisory control study refers to application of fuzzy control (Müller *et al*., 1995). Application of an on-line optimisation based approach to control the conventional activated sludge process was suggested already in 1973 and later studied by Sperling and Lumbers in 1991 (see also Chapter 2). However, still no such studies have been carried out for control of N-removal plants.

Table 5.10: Plant-wide and supervisory control examples

Reference	System	Study	Control	Remarks
Patry and Takács, 1995	-	d	expert system	modular system with expert supervisor
Müller *et al*., 1995	0[1]	s/p	fuzzy control	fuzzy supervisor for COD overloads
Bowden and Wright, 1973	1	o	optimisation	ideas about on-line optimisation
von Sperling and Lumbers, 1991	3[2]	s	on-line optimisation	model-based; optimal cost or optimal performance by DO, Q_r and Q_w

[1]: four stages: anaerobic, aerobic, nitrification and denitrification; the study concerned the first two stages only;
[2]: oxidation ditch without N-removal, including clarifier

The overview shows that advanced control techniques are hardly applied on full scale. Only on-line applications of expert systems for diagnosis have been reported. In most of the recent full-scale examples given in Chapter 2, on-off control or PI control was applied. Still, pilot plant studies showed promising results, especially with adaptive predictive control.

A major motivation for application of advanced control is that expected performance is higher. A few comparative studies between rule-based and model-based control have been carried out, which we briefly summarise.

Rule-based control and model-based predictive control were compared by Isaacs and Thornberg (1998) for cycle length control in the Biodenitro process. In simulation studies, performance was comparable. If the results from the optimal controller were used for tuning of the rules of the rule-based controller almost similar performance could be obtained. The rule-based controller was more robust against different inlet wastewater and temperature scenarios than the model-based controller. This is not the case in general. Here it was most probably caused by the simplicity of the model-based controller at its stage of development at the time of study. For tuning the rule-based controller, four functions had to be defined. Although this offers a lot of freedom, it also leads to less straightforward and possibly even to conflicting tuning. The authors planned to study on adequate choice of these functions.

Lukasse *et al*. (1999) compared four controllers for switching aeration in a simulated alternating activated sludge process, namely 1) timer based; 2) switching at depletion of ammonia and nitrate; 3) switching when ammonia crosses predefined levels and 4) Adaptive MPC. The parameters of these controllers were tuned such that the time-average and weighted effluent quality with respect to ammonia and nitrate was optimised. Controllers 1, 3 and 4 had similar nominal performance. The sensitivity to suboptimal tuning was also investigated and was significantly less for the MPC controller. In addition, its tuning was more straightforward.

van Schagen *et al*. (1995) compared performance of an LQG controller with cascade PID control for regulation of the ammonia concentration in a carrousel system. In this study, simulations with different influent scenarios indicated that with LQG a better effluent quality could be achieved with lower energy consumption.

These studies show that optimisation based control does not necessarily lead to improved nominal performance. However, it generally leads to more straightforward tuning and provides

a guarantee that performance is good indeed. Moreover, advanced control may lead to better control system robustness, if designed to account for model uncertainty.

5.2.3 MPC, motivation of MPC evaluation and overview of case studies

In Sections 5.3-5.5, Model Predictive Control application to pre-denitrification plants and carrousels will be investigated. In this section, we motivate the selection of MPC. First, MPC technology is described. The selection of the studied MPC control algorithm is then motivated, followed by an outline of the cases studied.

Standard MPC technology

MPC is an ambiguous term. In a general sense, it refers to the (digital) control philosophy of Open-Loop-Optimal-Feedback, already suggested by Propoi (1963). The idea is to apply dynamic optimisation on-line, optimising an objective function that reflects desired process behaviour. The process behaviour is predicted using an explicit dynamic process model that describes the effect of future manipulated variable adjustments on the process outputs. Feedback is used to update the state of model. Only the first of the computed control moves is actually applied, after which the procedure is repeated at the next sampling instant. This idea is also referred to as receding horizon or moving horizon control.

In a more restricted sense, the term refers to linear MPC with a quadratic objective function and with constraints. In this class, we find several algorithms that have been very successful in the process industry, in particular algorithms based on impulse response models (Model Predictive Heuristic Control, MPHC, the software being known as IDCOM, Richalet *et al*., 1978) and step response models (Dynamic Matrix Control, DMC, Cutler and Ramaker, 1979, and Quadratic DMC QDMC, Cutler *et al*., 1983; Garcia and Morshedi, 1986). Over 2200 implementations of MPC have been reported (Qin and Badgwell, 1996). Several reasons for this success have been given:

- the philosophy has an intuitive attractiveness to industrial process control engineers;
- the use of impulse and time responses obtained via identification requires less modelling effort than physics-based models typically used in early LQG applications (Qin and Badgwell, 1996);
- the technique provides one general framework for complicated processes with time-delays, inverse-responses and interactions;
- the on-line optimisation allows economic operation;
- most importantly, it is the only methodology to handle constraints in a systematic way, which is required as economic operation is known to be on the intersection of process constraints (Garcia *et al*., 1989; Rawlings *et al*., 1994).

In its general form, MPC is not restricted in terms of model, objective function and/or constraints and consequently, several MPC algorithms exist.

In linear MPC, different model representations are applied, including several input/output descriptions as well as state space descriptions (Garcia *et al*, 1989; Lee *et al*, 1994), with correspondingly different identification methodologies. The optimisation problem is generally cast as a standard Quadratic Program (QP).

MPC extensions

Several MPC extensions have been developed. These include robust MPC, adaptive MPC and nonlinear MPC and other extensions. From academia, considerable efforts have been spent in

the last decade on robust MPC, attempting to apply results from modern robust control theory to understand MPC robustness properties. While some important results have been achieved, still many questions remain open, especially for the practically most relevant finite horizon MPC with constraints. Examples of results are the Linear Fundamental Control Problem as a design framework for linear MPC (Prett and Garcia, 1988), the Internal Model Control concept (Morari and Zafiriou, 1989) as a framework to analyse MPC robustness, robustness under hard (output) constraints (Zafiriou, 1990; Zaifiriou and Marchal, 1991), robust design via observer tuning (Lee and Yu, 1994), robust design via LMI's (Kothare *et al*, 1996) and several theoretical results concerning MPC robustness applying infinite horizon formulations (Rawlings and Muske, 1993), and more recently, finite prediction horizon with Lyapunov function arguments (Nevestic and Primbs, 1997).

Less numerous studies are reported on adaptive MPC. Most results have been obtained in an independent MPC branch from the adaptive control community, which mainly employs SISO black-box models and does not include constraints. Probably best known is Generalised Predictive Control (GPC) (Clarke *et* al, 1987a,b). Bitmead *et al*. (1990) revealed its links to Adaptive LQG. Their analyses within the state-space framework provide valuable insights. Unfortunately, the results are restricted to the unconstrained case.

In nonlinear MPC, a nonlinear internal model is applied. Reviews are (Bequette, 1991; Biegler and Rawlings, 1991; Rawlings *et al*., 1994; Schei and Johansen, 1997). An aerly example is Garcia (1984). In most cases, some form of repeated linearization is applied for computational efficiency (van Essen, 1998). Generally, a quadratic criterion is applied. More general objective functions are possible, but the resulting optimisation problems may be much harder to solve. Nonlinear MPC can be applied, but while several results on nonlinear MPC stability have been obtained (e.g. Rawlings *et al*., 1994; Zheng and Allgöwer, 1998), a lot of theoretical work remains to be done.

In third generation[39] MPC, a multi-objective formulation is applied as well as a primitive form of reconfiguration control. This is achieved by a controllability supervisor for on-line selection of controlled variables based on the condition number

While extensions to adaptive and nonlinear MPC exist, their application and analysis is less straightforward. Many technicalities remain to be resolved for each particular application. This holds especially for nonlinear adaptive MPC, which while attractive from the point of view of performance, includes many technical problems. Model selection and implementation, choice, implementation and tuning of suitable adaptive schemes and robustness analysis or, at least, thorough testing of the controller will require considerable efforts. Adaptive MPC should therefore be applied only if the application requires it.

Motivation of MPC application to activated sludge systems

From the above discussion, we see that linear MPC is a proven on-line optimising control technology in industrial process control, especially due to the ability to systematically handle constraints and to cope with time-delays, inverse responses and interactions. Moreover, industrially proven implementations in commercial software are available. This significantly facilitates implementation in practice, as much development and testing can be avoided.

From the activated sludge process characteristics, application of robust, adaptive and/or nonlinear MPC would seem desirable. While construction of adaptive and nonlinear systems is possible, in particular the state-of-art of adaptive and/or nonlinear MPC is such that a thorough

[39] First generation MPC was developed in the late seventies. (IDCOM, DMC). Second generation MPC included systematic constraint handling by applying a QP formulation (QDMC).

understanding of their stability and performance properties is not possible yet. Moreover, several design issues, especially model selection, are nontrivial and need thorough consideration. In fact, in the preceding chapters we have seen that while several models are available, suitable model selection for specific control goals remains a topic of further research. This also holds true for identifiability properties and suitable identification schemes for nonlinear models. In addition, implementation into software would be less straightforward than application of standard MPC techniques.

Rather than starting with developing adaptive and nonlinear MPC, we therefore decide to first study linear MPC with constraints as a first step towards developing a suitable type of on-line optimising control. This type of control is between the two extreme approaches to tackle realistic problems depicted in Section 5.1. Like linear controllers such as LQR and LQG, it employs linear models and quadratic criteria, but it constitutes a first step to include nonlinearity by dealing with constraints. Robust control theory enables us to perform an (approximating) analysis of robustness of the linear MPC controlled plant, at least in the unconstrained case. The studies should provide insight in linear MPC application to activated sludge process control and provide guidelines to define priorities for further MPC development.

Outline of case studies

In the case studies, MPC based on step responses (Section 5.3) and state-space methods (Sections 5.3-5.5) is applied as described by Morari *et al*. (1991) and Morari and Ricker (1994). Details of the algorithms and models are given in the corresponding sections.

In Section 5.3, MPC application to setpoint regulation of ammonia and nitrate concentrations in a predenitrification plant will be studied. In Section 5.4, different control objectives will be applied, corresponding to increasing operational freedom. The aim of this study is to investigate applicability of linear MPC to carrousel systems and to study objectives that are closer to the actual economic objectives than setpoint regulation. In both systems, instability occurred as a result of model mismatch. Rather than applying ad-hoc fix-ups of the MPC controllers, a more fruitful approach was felt to aim at a fuller understanding of robustness issues. These will be studied using robustness analysis tools in Section 5.5.

Of course, the linear MPC law and the corresponding quadratic criteria applied constitute an approximation only of the real problem. Industrial MPC is applied mostly on that level of the control hierarchy pyramid (Prett and Garcia, 1988) that corresponds to setpoint regulation or tracking, which are provided by a higher, plant optimisation layer. More interesting for activated sludge plants would be to apply MPC on this plant optimisation level, employing nonlinear MPC (Biegler and Rawlings, 1991), as was discussed in Chapter 2. In that case, other than quadratic criteria must be applied, with the problems as discussed in Section 5.1.

It is noted that the MPC control studied in Sections 5.3-5.5 is focused on control of the bioreactor, especially on ammonia and nitrate concentration. Control of the sludge inventory using MPC is not considered. Instead, this will be accomplished by separate control loops.

A note is also made with respect to the goals for the pre-denitrification plant in Section 5.3. It is stated in this section that, in priniple, the setpoints for effluent NH_4 and NO_3 concentrations would ideally be chosen equal to zero. Of course, this is not possible in the pre-denitrification plant studied, which is a poor design in the sense that 2 CSTRs are not suited to achieve NH_4 and NO_3 concentrations of (very close to) zero. In fact, a gradient is much more efficient if the concentrations must be (much) lower than the respective affinity constants (assuming Monod

kinetics). (In fact, setpoints of zero can under first order kinetics only be achieved by infinitesimally large plants, or achieved within measurement accuracy by very large plants). Thus the plant is not suggested as a good design, but, as this type of transport model is sometimes used to describe pre-denitrification systems, the system is used for a first analysis. It appears to show some typical difficulties for control (inverse response, additional inverse response and gain sign inversion at increased internal recycle flowrate).

A final note concerns the models applied in the studies. The state-space models are obtained through linearization of the nonlinear model in a steady-state. No order reduction is applied in these studies, as this is considered worthwhile only if the linear MPC appears successful, justifying the effort in finding good reductions. For actual implementation, reduction of the high-order state-space models of course would be desirable.

5.3 MPC applied to a pre-denitrification plant

Abstract[†]

The current situation in measuring and control of enhanced nitrogen removal wastewater treatment plants is briefly sketched, indicating a need for better control strategies. Control strategy is meant here to imply the main decisions or steps in control system design. The steps we believe are most important are discussed. Methods that might be helpful in selecting suitable control structures, that is the selection and pairing of sensors and actuators, are indicated. The second part will describe an application of linear Model Based Predictive Control, with a pre-denitrification plant as a model system, using the IAWQ Model No. 1 for modelling the plant. Application of a fixed, linear model in the controller on the nonlinear IAWQ Model is shown to have limitations, most probably as a result of model mismatch.

5.3.1 Control strategies for nitrogen removal activated sludge plants

As demands for nitrogen removal are becoming more stringent, process control is becoming more important. Recently, new types of sensors have become available, which creates more possibilities for control. Some important types of sensors that can be mentioned are FIA (flow injection analysis) based methods for ammonia and nitrate and respiration rate monitors, enabling measurement of active biomass or available organic substrate[20]. At the same time, control system design becomes more complex. The selection of sensors and actuators and their location is a difficult decision at the moment, because there is not enough knowledge and experience to indicate good choices. In the literature, several choices and suggestions for sensors and actuators and controlled variables can be found. An incomplete summary, which is however believed to include the most important options, is given in Table 1. For the discussion, a discrimination is made between measured and controlled outputs, and also between exogenous inputs and actuator inputs, according to the representation of closed loop systems[4] shown in Figure 1.

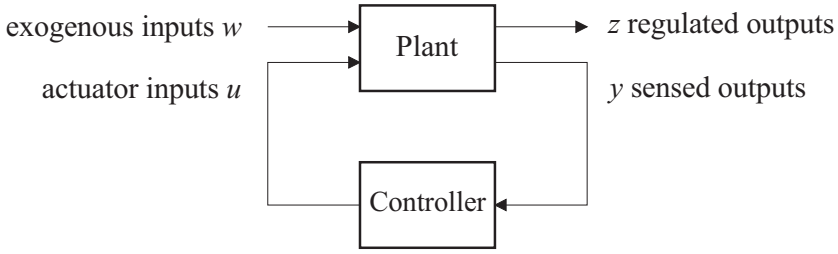

Figure 1: Closed loop system according to Boyd and Barratt (1991)

The exogenous inputs *w* include all inputs to the system, including disturbances and reference signals (setpoints). Although the scheme has been presented for linear control system design, in *w* also constraints might be included, *e.g.* on sludge age, plant loading, settler loading, return or internal recycle flows. The actuator inputs *u* coincide with the manipulated variables of the plant, and are exactly the signals leaving the controller. The measured outputs *y* are the process variables which are actually measured by sensors and input into the controller. The regulated

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outputs *z* include all variables which are important to us, which can be the measured outputs, but also the actuator inputs or other variables of interest which cannot be directly measured but are believed to be important. As an example, SCOUR control can be mentioned, where OUR and biomass are measured and SCOUR controlled[12].

Table 1: Possible and suggested choices for *u*, *y* and *z*

Manipulated variables or **actuator inputs *u***	**Measured outputs** or **measured variables *y***	**Regulated outputs** or **controlled variables *z***
oxygen transfer k_La or	Dissolved Oxygen DO	any of *y*
DO setpoint	ammonia NH_4	MLSS
recycle rate Q_r	nitrate NO_3	sludge height
waste flow rate Q_W	redox potential ORP	soluble COD, total COD, BOD
internal recirculation Q_{ic}	actual respiration rate r_{act} [10]	biomass concentration X_B
volume fraction aerobic	maximal resp. rate r_{max}	specific oxygen uptake rate SCOUR
influent distribution	endogenous rep. rate r_{end}	suspended solids MLSS
influent buffering	StBOD	food to mass ratio F/M
flow to clarifier	turbidity in mixed liquor	sludge age SA
external carbon source	sludge height in clarifier	sludge settleability SVI
precipitants		

This also has been represented in Table 1: the regulated outputs can be measured outputs, but can also be different from *y*. Looking at Table 1, a large number of possible combinations of choices for *u*, *y* and *z* can be made. These choices are related to definition of the goal (*z*) and the control structure selection, which comprises IO and control configuration selection.

Another development, the increasing use of dynamic modelling of wastewater treatment plants, together with developments in control theory, raises the question whether advanced, model based control can contribute to better plant performance. This point is related to control law selection and modelling the plant. The complete Control System Design scheme is depicted in Figure 2.

1. Definition of the goal
2. Modelling of the plant
3. Input Output selection
4. Control Configuration selection
5. Control law selection
6. Controller tuning and evaluation
7. Implementation and testing

Figure 2: Control System Design scheme

Steps 1-6 in the control system design will now be discussed, with emphasis on continuous systems for nitrogen removal, which are the main type of systems in The Netherlands.

1 Definition of the goal

Although at first sight the goal for a wastewater treatment plant might be stated quite simply, for example 'maximal treatment of wastewater against minimal costs', translating this to controller goals is not so straightforward. This is, amongst others, due to the fact that several

constraints are imposed onto the system. In the first place, constraints can be put upon safety and reliability, giving rise to a ranking in decreasing priority of goals as follows: safety, reliability, quality, economic optimization. An example: if aeration costs are included in a controller criterion function, this may lead to economic optimization as seen from the model in the controller, but may lead to impaired sludge sedimentation behaviour, which is not included in the model. This kind of effects might be eliminated by imposing constraints. The same applies to constraints on recirculation and internal recirculation flows and other variables[18]. If situations can occur where not all constraints can be met, a priority ranking can be used to ensure that the most important are dealt with first.

In the second place, it is not well known which choices have to be made for the controlled variables. This was especially true for conventional activated sludge systems, when no sensors for substrate were available. However, also in the case of nitrogen removal, where sensors are available for the outputs of interest (NH_4 and NO_3) and which are obvious candidates, one also has to control in some way or another the amount of sludge in the system and the distribution of sludge over biological unit and clarifier. It is however not clear which controlled output is the 'best' choice, although several suggestions have been put forward, including sludge age, MLSS, sludge height, SCOUR[12], SCOUR profile[22], maximum respiration rate[10] and others.

In the third place, the biological unit is not a stand-alone system, but interacts with the clarifier in the first place, and also with other process units within the plant, such as sludge treatment through internal recycles. To optimize plant operation, all units should be considered, giving rise to optimization problems that are more difficult to state.

In the last place, the plant receives its water from the sewer system and discharges its effluent on the receiving water. In addition, these interactions can in principle be taken into account, amongst which especially prediction of influent patterns from the sewer system may be of interest. The resulting optimization problems are more complex and more difficult to state and solve than those for the biological unit alone. Here, hierarchical optimization techniques might be used.

2 Modelling

A step which is always present in control system design is modelling. If no mathematical model is used, but heuristic rules concerning behaviour of the plant, we have a linguistic model. Here we will assume that the model is a mathematical model, linear or nonlinear. What kind of model we need, depends upon the step in the control system design and will be discussed in the appropriate sections.

3 Input Output selection

In this step, the number, place and kind of manipulated variables *u* and measured variables *y* are selected. Given the candidates for *u* and *y* in Table 1, in theory the possible number of choices is huge. In practice, heuristic guidelines significantly reduce the number of candidate choices, but still a large number remains. It is practically impossible to design and test all possible combinations, so methods to select good candidate choices are needed. Recently, a systematic inventory of cause-effect relationships has been established[18], based on qualitative knowledge of interactions in the system and an estimation of time constants involved. If models are available, more quantitative methods might be used. Several methods have been used. Steady-state performance for four different choices of controlled variables have been compared[19] for the conventional activated sludge system (to be more precise, this could better be classified as a method of choosing a goal). Steady-state computations were used in selecting sensor locations for DO control in a carrousel[21]. A dynamic measure based on observability has been used to select suitable sensor locations[1].

Together with the control configuration, the IO selection comprises control structure design. In control literature, more attention has been paid to control design than to control structure design. Nevertheless, a wrong control structure may put fundamental limitations on performance, which cannot be overcome by advanced control design. Recently, a survey has been given on this topic[23]. Some methods for IO selection are mentioned here: selection based on 1: control power and speed, 2: avoidance of Right Half Plane poles and zeros, 3: Cause and effect graphs, 4: Singular value decomposition, 5: Robust stability. Methods based on robust performance using μ-synthesis were reported to be especially promising[23].

4 Control Configuration selection

In this stage, the structural interconnections between *y* and *u* are chosen. This is often useful because a MAMS (Multiple Actuator, Multiple Sensors) system[4] does not necessarily have to lead to a MIMO (Multiple Input, Multiple Output) design, especially if there is no interaction between certain input and output combinations. In that case, decentralized control can be used, which is easier to design and implement than a fully centralized control. An example of a decentralized controller (three SISO loops) is the following system, where y_1 is controlled by u_1, y_2 by u_3 and y_3 by u_2.

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} x & 0 & 0 \\ 0 & 0 & x \\ 0 & x & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

If interaction is not accounted for in the design phase, unwanted interactions may occur, as could be observed in a 3x3 MAMS system [22]. The most widespread method for interaction analysis and controller configuration for fully decentralized systems is the Relative Gain Array. In its basic formulation it gives a static interaction measure, which is a major limitation of the method. More powerful methods exist, of which those based on performance degradation and robust performance seem most promising[23].

Although the number of possible control structures is huge, up till now only a limited number of them have been reported or suggested. Kayser suggested the following control structure to control a pre-denitrification plant: the internal recirculation is used as to control the nitrate concentration, the nitrification volume is used to control ammonia, and the air supply (k_La) is used to control DO, with an override control or cascade on ammonia[9]. The first aerator was used to control DO and the second to control ammonia in a full-scale carrousel[15] with two turbine aerators. Aeration was used to control nitrate in a full-scale carrousel[6]. In the same proceedings, aeration was reported to be used to control ORP in a full-scale carrousel and an oxidation ditch. Conventional DO (PI) control was compared with control of ammonia with aeration, and with controlling the ratio of the sum of ammonia and nitrate to ammonia by a (PI) master controller in cascade with a (PI) slave DO controller[13].

5 Control law selection

Many methods and approaches to control have been developed during the last few decades. Few of them are being applied, however. In most of the examples listed above, on-off control, eventually with a time delay, was applied. In the last example classical control, including PI(D) and cascade control, was applied. In the view of the characteristics of the process, which is nonlinear, time variant (as a result of changing parameters), multivariable and relatively slow, one might expect that application of more advanced control might give advantages over classical control. At the moment, thorough comparative studies have not been undertaken to

address this question. A possible approach to obtain an impression of possible benefits would be to compare what is optimally achievable theoretically to performance of currently applied controllers. For this approach, reliable models are required.
The model which has to be built in the model building step, is determined by the control law to be used (or *vice versa*). In general, models used for tuning and in model based controllers have to be relatively simple.

6 and 7 Controller tuning and evaluation and Implementation and testing

After tuning the controller, which is most often based on linear or simple models, before implementation it can be evaluated using more elaborate models. Here the IAWQ Models and relatively complicated sedimentation models can be used.

5.3.2 Model Predictive Control of a pre-denitrification plant

Model Predictive Control is a model based control method or philosophy which is becoming relatively well accepted in the process industries. One of the reasons for this success is that constraints can be incorporated in the control system in a systematic way. For reasons indicated above, this may also be an important issue in wastewater treatment. Here, the method is applied to obtain a first impression of possible benefits and limitations of application of model based control in nitrogen removal. It is being used to investigate what treatment performance can theoretically be achieved with a chosen control structure. In principle, this can also be done by dynamic optimization, but that approach supposes a priori knowledge of future disturbances, which is normally not available on-line. Although as a consequence a sub-optimal solution is obtained, this solution is representative for what can be achieved in on-line application. In this study, linear MPC is applied to control a prototype pre-denitrification plant, shown in Figure 3.

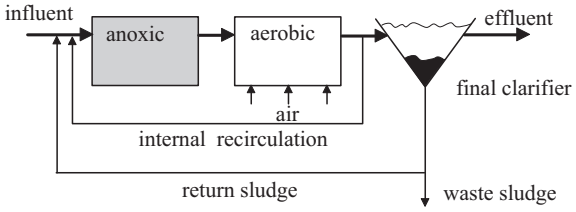

Figure 3: Scheme of pre-denitrification plant

Q:	influent flow	[m^3 d^{-1}]
Q_r :	recirculation	[m^3 d^{-1}]
Q_{ic}:	internal recirculation	[m^3 d^{-1}]
Q_w:	waste sludge flow	[m^3 d^{-1}]
V_i :	Volume reactor i	[m^3]
V_s :	Volume clarifier	[m^3]

$D_{in} = Q_{in} / V_1$;
$D_{Ti} = (Q + Q_r + Q_{ic}) / V_i$; $D_{ri} = Q_r / V_i$
$D_{SA} = 1 / SA$, with SA: sludge age

The plant is modelled by using the IAWQ Model No. 1. In addition to the assumptions of the IAWQ Model, it is assumed that reactions in the clarifier can be neglected, and that sludge storage in the clarifier can also be neglected. In that case, the model equations become:

$$\frac{d\xi_b}{dt} = \begin{pmatrix} K & 0 \\ 0 & K \end{pmatrix} \varphi(\xi_b) - \begin{pmatrix} (D_{T1} + D_{SA})I_x & 0 & -(D_{T1} + D_{SA}\frac{V_1}{V_2})I_x & 0 \\ 0 & D_{T1}I_s & 0 & -(D_{r1} + D_{ic})I_s \\ -D_{T2}I_x & 0 & D_{T2}I_x & 0 \\ 0 & -D_{T2}I_s & 0 & D_{T2}I_s \end{pmatrix} \xi_b + D_{in} \begin{pmatrix} I_x \\ \cdot I_s \\ 0 \\ 0 \end{pmatrix} \xi_{in}$$

with: $\xi_b{}^T = [\xi_1 \quad \xi_2] = \left[X_1^T \quad S_1^T \quad X_2^T \quad S_2^T \right]$;

K: stoichiometric matrix according to IAWQ Model No. 1;
φ: reaction rates according to Aqua-System (1991);
X: suspended components, $X^T=[X_I\ X_{BH}\ X_{BA}\ X_P\ X_S\ X_{ND}]$;
S: solute components, $S^T=[S_S\ S_{NH}\ S_{NO}\ S_{Alk}\ S_I\ S_{ND}\ S_O]$;
D: dilution matrix, containing all internal flows;
I_x and $I_{s:}$ identity matrices of appropriate size (6 resp. 7);
0: zero matrices of appropriate size.

1 Goal

The goal of the control is to achieve minimal effluent NH_4 and NO_3 concentrations despite disturbances in the influent, with more emphasis being put on NH_4 than on NO_3. In principle the reference or setpoint could then be chosen to be zero. The controller is linear, however, and the internal model is obtained by linearization around a steady-state. Therefore, as a first approach, the setpoints are set to the steady-state values. No constraints are defined. Sludge distribution in the clarifier is not studied here, and clarifier dynamics is neglected. This issue will be addressed in a later study.

2 Model

As controller, MPC based upon step response models is chosen. The internal step response model for the controller is obtained by doing simulations with the nonlinear plant model from an initial (steady) state, by applying steps to the manipulated variables.

3 Input Output and 4 Control Structure selection

The control structure is a modification of the control structure suggested by Kayser[9]. The manipulated variables are the DO setpoint in the aerobic reactor, which is assumed to be realized neglegibly fast by a cascaded control loop on DO, and the internal recirculation rate. The measured variables are the ammonia and nitrate concentration leaving the second reactor. As the system is expected to exhibit interaction, a MIMO configuration has been chosen. In addition, the sludge age is assumed to be kept constant by changing the waste flow rate. The control structure is as follows:

$$\begin{bmatrix} DO_{sp} \\ Q_{ic} \\ Q_w \end{bmatrix} = \begin{bmatrix} x & x & 0 \\ x & x & 0 \\ 0 & 0 & x \end{bmatrix} \begin{bmatrix} NH_4^+ \\ NO_3^- \\ SA \end{bmatrix}$$

5 Control law selection

Unconstrained linear MPC based on step response models is used. MPC uses a receding horizon strategy. At each sampling instant k, a prediction is made of the estimated future outputs over a prediction horizon P. The future outputs are computed from the free response, which is determined by the state of the system at instant k, plus the forced response, which is determined by the future control increments or moves which are varied over a control horizon M, which is equal to or smaller than the prediction horizon. After computing the optimal sequence of control moves, only the first move is implemented. The model prediction is corrected with the innovation signal and at the next time instant, the whole procedure is repeated.

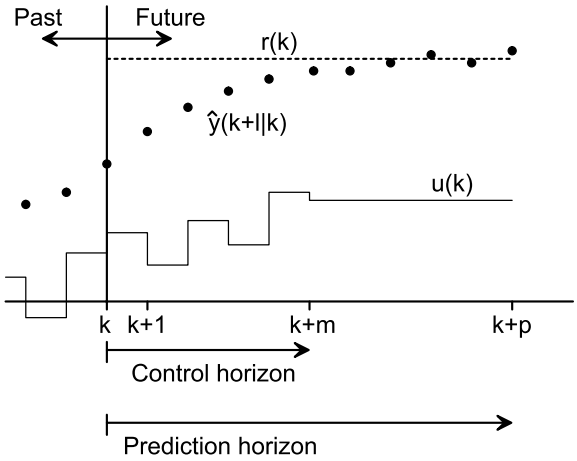

Figure 4: Prediction and control horizon

The following optimization problem is solved in MPC:

$$\underset{\Delta u(k)\ldots\Delta u(k+m-1)}{Minimize} \sum_{l=1}^{P}\left\|\Gamma_l^y\left[y(k+l|k)-r(k)\right]\right\|^2+\sum_{l=1}^{M}\left\|\Gamma_l^u\left[u(k+l-1)\right]\right\|^2$$

The first term, the predicted error, is weighted with a diagonal matrix Γ^y; the control moves are weighted by a diagonal matrix Γ^u. In the unconstrained linear case, the solution can be written explicitly as the product of a constant gain matrix and the predicted error. The most important tuning parameters are the prediction horizon P, the control horizon M, the weight matrices Γ^y and Γ^u and the observer gain. An important difference with LQG is the fact that the horizon is finite. A result of this is that stability with the computed controller gain matrix is not guaranteed. Another difference is that control increments themselves are weighted instead of control actions; in the case of perfect models, the steady-state error will be reduced to zero. In Figure 5, the step responses in the steady-state are shown.

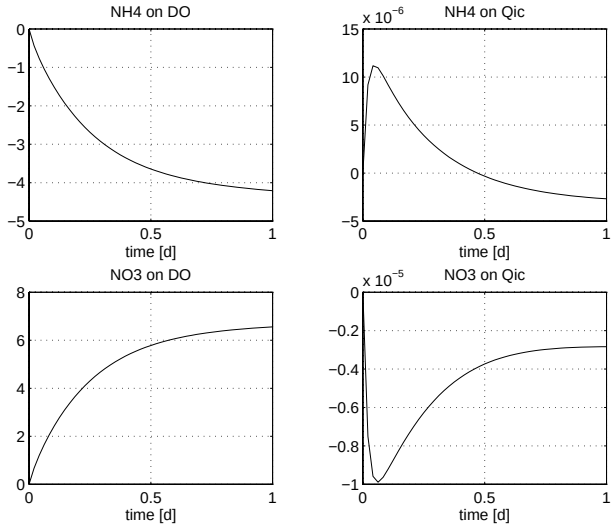

Figure 5: Stepresponses in steady-state

The step length is chosen one day, which seems to be long enough. The large difference in magnitude of the responses to DO and Q_{ic} is caused by the fact that the unit of the step on the setpoint for DO is 1 mg/l, which is rather large, and that for the internal recycle rate Q_{ic} is 1 m^3 d^{-1}, which is very small. An important observation that can be made, is that there is much interaction: both DO and Q_{ic} affect both the NH_4 and the NO_3 concentration. The RGA can be computed to be about 0.41, which indicates much interaction. Static decoupling is possible however. It can also be seen that the response of NH_4 to a step in Q_{ic} shows an inverse response. This is caused by the fact that first more ammonia from the first reactor enters the second reactor, giving rise to an increase; after this initial increase, the concentration drops because more ammonia is converted to nitrate. The control structure chosen thus introduces a

right half plane zero, which puts a fundamental limitation on performance, and this possibly indicates that the internal recirculation may not be the best choice as manipulated variable.

6 Controller Tuning and Evaluation

The goal is disturbance rejection; for this initial study a change of the reference signal has been used instead. A small step was applied first, because the system is nonlinear and it was expected that too large steps would lead to instability. First, the system has been tuned and simulated with a linear plant model, equal to the internal stepresponse model. Some tuning guidelines can be indicated: Decreasing P, increasing M and decreasing the control weight makes the response faster. The prediction horizon has to be chosen sufficiently large, particularly with inverse responses. Here 1 d was chosen, which with a sampling time of 0.5 h, gives a prediction horizon P=48. Setting M equal to P gave rise to unstable behavior for many combinations of the weighting factors. In the MPC implementation of Morari (1994), input blocking can be used. Here, a blocking was used, which keeps Δu constant over the first block of 5 samples, then over the second block of 5 samples and then constant. This choice gave good results. For the weighting factors there are three degrees of freedom, as one weight can be set to one. The weightings for the outputs ammonia and nitrate were chosen 4 resp. 1; this was done to reflect the greater importance attributed to the ammonia concentration and to obtain a sufficiently fast response for ammonia. The control moves have been weighted by the ratio of the steady-state gains, which gave 1 for DO and 5 10^{-7} for Q_i respectively. The results of this tuning with the linear plant are shown in Figure 6, with a requested change in setpoint of 1% (small for comparison with nonlinear plant). The response is rather slow; it takes two days before the concentrations reach their setpoints. This is probably a result of the right half plane zero, which impairs achievable performance. The same settings were applied to the nonlinear plant, with the same change in setpoint (1%). A stable response is obtained (Figure 7), which is somewhat slower than the response of the linear plant. With a requested change in setpoint of 2% however, the nonlinear plant became unstable after 8 days (results not shown). This appeared to be a result of model mismatch between the internal model and the controller. This was revealed by computing stepresponses at t=10 d, where the system was unstable. This linear model at t=10 also resulted in an unstable system, with responses which closely resembled those of the nonlinear system.

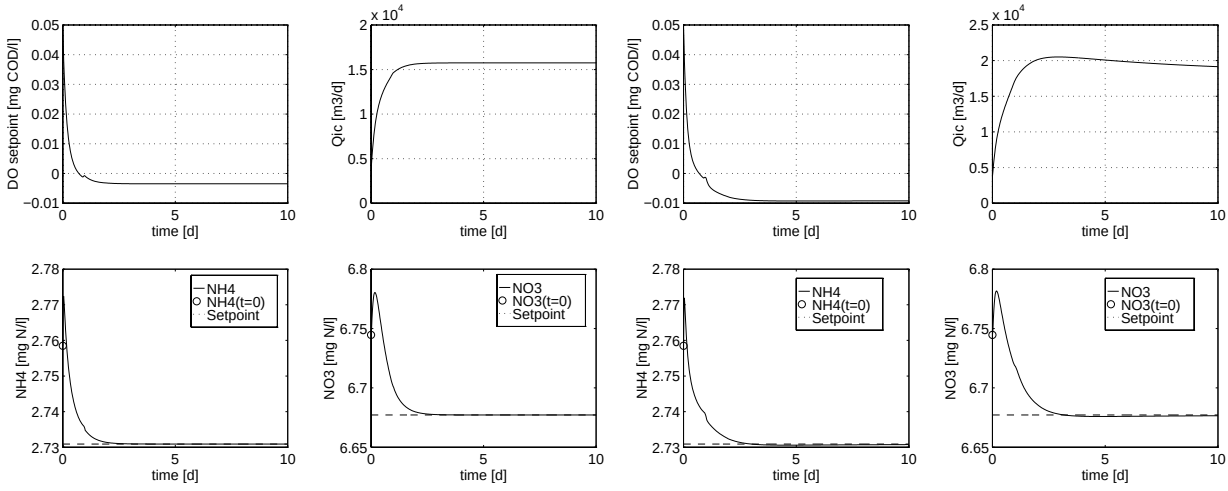

Figure 6: Response with linear plant

Figure 7: Results nonlinear plant

The stepresponses of the model at t=0 (the internal model) and the plant at t=10d are compared in Figure 8, over a period of 1 and 10 days. It can be seen that the gains of plant and model are different, that an additional inverse response is introduced for nitrate, and that the steady-state gain of the response of nitrate to Q_{ic} changes sign! At the high internal recirculation too much oxygen enters the first reactor, impairing denitrification; by setting constraints, this might be prevented. It can also be seen that the responses are not at their steady-state values at t=1; this was checked not to be a cause of instability. In the controller tuning, the estimator gain matrix has not been used for tuning; this is however an important factor in achieving robustness[3,11].

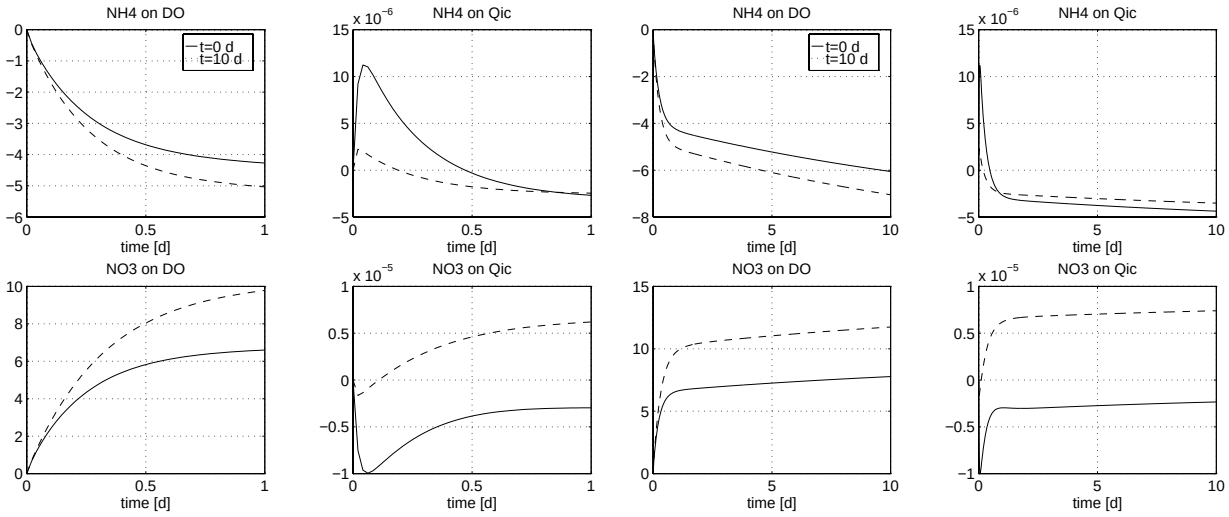

Figure 8: Step responses showing model mismatch and length of response

5.3.3 Conclusions and further research

In the definition of goals for wastewater treatment plants, objectives, constraints and interaction variables can be distinguished. Selecting appropriate control strategies may be facilitated and made more systematic by applying methods for control structure selection. Modern, model based control looks promising, but the benefits still have to be shown. Model Predictive Control may enable a systematic handling of constraints and off-normal conditions. Constant linear MPC seems to be limited in the case studied. Putting constraints on the manipulated variables possibly gives improvement in this case. MPC tuning is maybe more straightforward if criteria are used that ensure stability[16]. Tuning for robustness and applying nonlinear MPC will be investigated.

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5.4 MPC control of nitrogen removal in a carrousel system

Abstract[†]

More stringent demands with respect to nitrogen removal in wastewater treatment plants have created a need for improved process control. This has motivated significant research efforts to come up with better control strategies. In this section, the definition of the control goal and the selection of control laws or algorithms are addressed. Different control goals and corresponding controller criteria were defined, all aiming at disturbance rejection of ammonia and/or nitrate. With respect to the control law, linear Model Predictive Control was selected to investigate what advanced, model based control can contribute to improved nitrogen removal. For the evaluation, a model of a hypothetical carrousel type wastewater treatment plant was used, which was modelled using ASM1. The system performances obtained with MPC applying the different controller criteria are evaluated; subsequently MPC is compared with LQG control and classical controllers. The results indicate that advanced, model based control can contribute to better operation. It appeared difficult however to define goals and criteria that lead to better performance under all conditions studied. One criterion aimed at covering a wider range of conditions by imposing a setpoint for the sum of ammonia and nitrate; however, the validity range of the linear model appeared too limited for this criterion. It is concluded that it is necessary to formulate goals which rightly trade-off between ammonia and nitrate under various conditions. It remains to be established whether linear (MPC) controllers can be used for this purpose.

Keywords

Activated Sludge; nitrogen removal; control; Model Predictive Control; Optimal Control.

5.4.1 Introduction

With more stringent demands being put onto nitrogen removal from wastewater, process control is becoming increasingly important in operation of wastewater treatment plants. Conventional control based on DO control alone is often considered no longer sufficient and it is recognised that there is a need for improved control strategies. As the term control strategies is rather broad, it is more precisely defined here to include the main steps or aspects in control system design: 1) Definition of control system goal and specification; 2) Modelling the plant; 3) Selection of number, type and location of sensors and actuators and their interconnections; 4) Control law selection; 5) Controller tuning and, before implementing, 6) Control system evaluation. It is remarked that these steps are not necessarily taken in this order or in one go; in addition several steps are interrelated (e.g., the model to be used in design is dependent on the control law chosen).

Although over the last years considerable research efforts have been spent on control system design for nitrogen removal plants, still many questions remain to be answered. As an example, the selection of the control law or control algorithm can be mentioned: many control

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approaches have been developed over the last decades and for the wastewater engineer (and for the control engineer) it is not so obvious which method can best be chosen. In this section, especially the definition of the control goal and the control law selection are studied.

A carrousel type wastewater treatment plant was selected for this study, as many plants in the Netherlands are of this type. Simulation studies were done with a hypothetical plant, which was defined in accordance with the studies performed by Meinema *et al*. (1995): no primary clarifier, an oxidation circuit (volume of 13000 m^3) with one influent inlet point and two adjustable surface aerators with equal maximal aeration capacity and one final clarifier (3400 m^2).

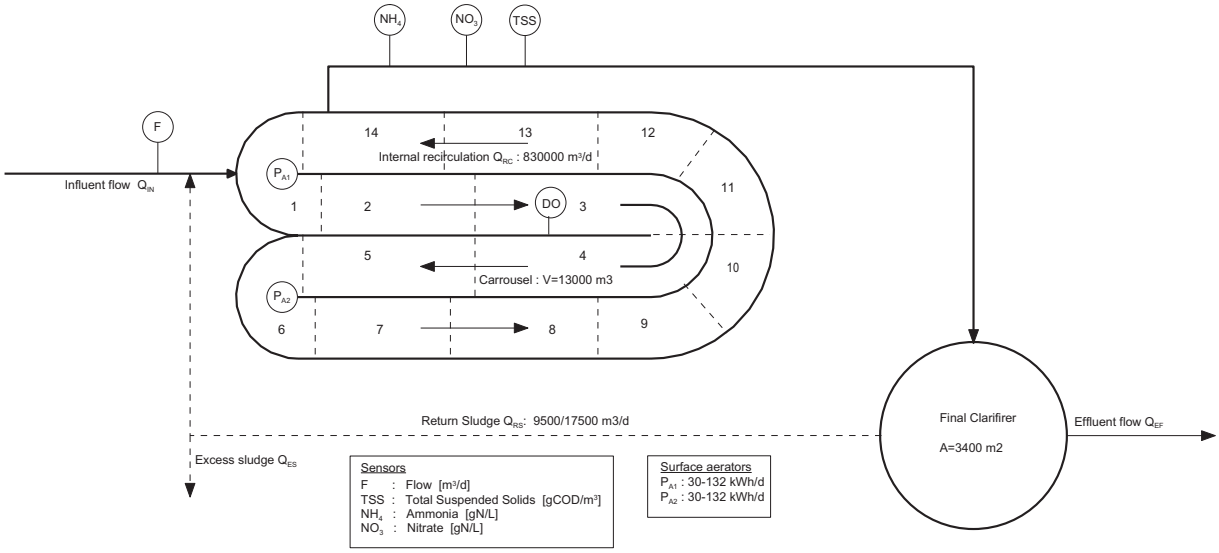

Figure 1: Oxidation circuit and final clarifier**.**

The sequel is organised along the steps indicated above, with the main focus on definition of the control goal and control law selection. First, different control goals are defined with the objective to investigate the influence of the definition of the controller goal on control system performance. After describing the modelling step, the sensor and actuator choices are motivated. Model Predictive Control was selected as the control law for evaluating the different control goals and to serve as a reference method to explore the possibilities and limitations of applying advanced, model based control methods. Then the tuning procedure applied is described. Subsequently, the performances obtained with MPC using the different control goals are evaluated and finally MPC is compared with results obtained by applying classical control and LQG in earlier studies.

5.4.2 Definition of the control goal

Starting point in control system design is the translation of legislative demands into control goals. This step includes the selection of and specifications for process variables to be controlled. This is an important and nontrivial task, as a poor decision in this basic stage will dramatically influence overall system performance.

For nitrogen removal, it is common practice to define setpoints for effluent ammonia and/or nitrate or their sum on the basis of heuristics or simulation studies, which may lead to

suboptimal performance. Legislative demands may be met with different choices for controlled variables and setpoints, but it is difficult to guarantee that a particular choice is optimal with respect to installed plant capacity, energy or cost.

An alternative approach to regulation of predefined, fixed and probably suboptimal setpoints is to apply (on-line) optimisation using mathematical models. The current knowledge in the wastewater community in the form of mathematical models suggests such an approach. However, although the goal for a wastewater treatment plant can be stated quite simply in verbal terms, e.g. 'maximal treatment at minimal costs'. it is more difficult to formulate this optimisation problem mathematically in technical terms fit for use in control, such that indeed an optimisation criterion is defined which makes sense. This is due to several reasons, amongst which the presence of process constraints and interactions (Weijers *et al*., 1995). Furthermore, it is difficult to attribute costs or weight factors to all relevant variables, especially for ammonia and nitrate, although efforts are being taken to come up with criteria entirely based on costs to enable objective benchmarking (Vanrolleghem *et al*., 1996).

The current study aims at assessing possibilities and limitations of applying optimal control, for which Model Predictive Control is used as a tool. In the Netherlands, the effluent requirement on total nitrogen has been set at 10 mg N/l as a yearly average. To study the influence of goal on system performance, this requirement was translated into three different control goals for MPC. Goal 1 was to keep both ammonia and nitrate on a constant level. Goal 2 was to keep ammonia at a constant level and at the same time minimise the sum of effluent ammonia and nitrate. The rationale for this second goal was to put more emphasis on ammonia, and allow for easier tuning. Goal 3 was to keep the sum of effluent ammonia and nitrate at a constant level of 10 mg-N/l, thus aiming at exactly meeting the requirements at all time instants. The choice of setpoints is motivated in Section 5.4.4; the values for the setpoints chosen are given in Section 5.4.6.

5.4.3 Modelling

Models are needed for control system evaluation as well as for controller tuning and, in the case of model based control, as internal model. Control system evaluation is carried out before control system testing on the real plant. For control system evaluation, typically large, mechanistic simulation models are applied. For the plant model to be used for evaluation in this study (step 6, see below) a nonlinear model was used for the oxidation circuit, which existed of 14 ideally mixed reactors in series as indicated in Figure 1, whilst the clarifier was modelled by a 10 layer Otterpohl model (Ifak, 1995).

For controller tuning, usually linear models or low-order, grey box nonlinear models are used; in some cases, neural networks are applied. Here, a linear model was applied for controller tuning and as internal model in the Model Predictive Controller. This model was obtained by linearizing a nonlinear plant model for the oxidation circuit which corresponded to the nonlinear plant simulation model used for evaluation, but using ASM1 according to Henze *et al*. (1987) instead of the model used in the plant simulator. For the clarifier, ideal and instantaneous clarification was assumed.

5.4.4 Control structure selection

This stage comprises the I/O Selection and the Control Configuration Selection. In the I/O Selection stage, the number, type and location of sensors and actuators is selected; in the Control Configuration Selection, their interconnections are decided upon (van de Wal, 1996).

Effluent ammonia and nitrate concentrations were chosen as measured variables, to be controlled by the power input into both aerators. A multivariable control configuration was chosen because of the system interactions. The choice to use both aerators was made because it had been shown that improved performance can be obtained if both aerators are used. This is due to the fact that the two aerators give different responses as a result of the location of the influent inlet point. Consequently, there is some, be it limited, freedom to control ammonia and nitrate independently.

Besides this MIMO control loop, the sludge concentration was measured and kept at a constant value by the waste sludge flow by a first order controller. The sludge recycle flow was switched to a higher flow rate when the influent flow rose above a certain limit for storm weather control.

5.4.5 Control law selection

As the control law for the multivariable control of the ammonia and nitrate concentration in the effluent, linear Model Predictive Control (MPC) was chosen. This model based optimal control method was used both as a tool to study influence of criterion definition on control system performance, as well as a reference method to compare achievable performance by (linear) model based control methods with classical control. The focus on model based control is motivated by the currently available knowledge in the form of quantitative, mathematical models, which allows for a relatively straightforward design and analysis of the control system. MPC is a control method which is becoming relatively well accepted in the process industries, one of the reasons for this success being that constraints can be systematically incorporated into the control system.

The principle of MPC is as follows (Figure 2). At each sampling instant k, a prediction is made of the estimated future outputs over a prediction horizon P. The future outputs are computed from the free response, which is determined by the state of the system at instant k, plus the forced response, which is determined by the future control increments or moves. The control moves are varied over a control horizon M, which is equal to or smaller than the prediction horizon. That sequence of control move is computed, which gives an optimal trajectory with respect to a defined optimisation criterion. Only the first move of this optimal sequence is then applied to the plant, after which the state estimation is corrected with the measured process output at the sampling

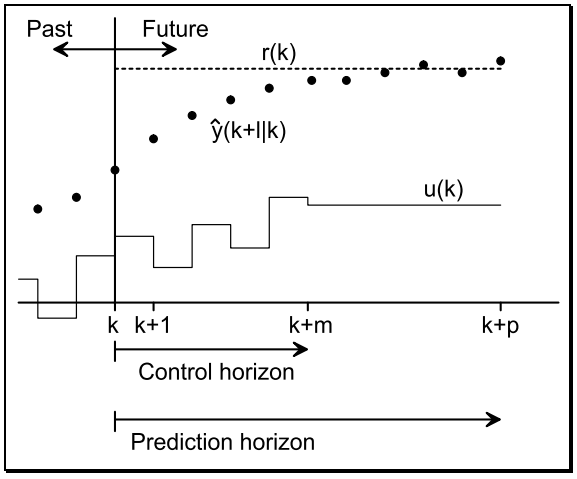

Figure 2: Principle of MPC.

instant. At the next time instant, the whole procedure is repeated. This repetitive procedure is referred to as receding horizon control. In this case, MPC according to Morari (1994) was used, with the following quadratic criterion, subject to linear constraints on the inputs and/or outputs:

$$\underset{\Delta u(k)\ldots\Delta u(k+m-1)}{Minimize} \sum_{l=1}^{P} \left\| \Gamma_l^y \left[\hat{y}(k+l|k) - r(k) \right] \right\|^2 + \sum_{l=1}^{M} \left\| \Gamma_l^u \left[\Delta u(k+l-1) \right] \right\|^2 \qquad (1)$$

subject to constraints on u, Δu and y.

The first term, the predicted error, is weighted with a diagonal matrix Γ^y; the control moves are weighted by a diagonal matrix Γ^u. With the weights Γ^y and Γ^u a trade-off can be made between trajectory following and control action.

Three criteria were formultaed corresponding with the three control goals defined. In the criteria, setpoints are defined for ammonia and/or nitrate. This choice was made, because a linear model is used in the controller which has a limited range of validity around the setpoints. Three criteria were defined with increasing freedom for the control system and with increasing ease of tuning.

1. Combined ammonia/nitrate criterion:
Both for nitrate and ammonia a fixed setpoint is selected. The model internally used in MPC is linearised around these setpoints. The idea is that by enforcing these setpoints, the state of the non-linear plant stays close to the linearisation point and thus in the validity region of the model. The combination of setpoints and weights will determine the performance of the controller. Due to limitiations of the plant, there is limited freedom to choose the setpoints so the feasibility of selected setpoints was checked with the nonlinear model.

2. Ammonia criterion:
A fixed setpoint for ammonia is selected, while simultaneously inorganic nitrogen is minimised, the inorganic nitrogen concentration being defined as the sum of the ammonia and the nitrate concentration. The idea for choosing this controller criterion function is that it is easier to tune than the previous, because only a setpoint for ammonia has to be chosen.

3. Inorganic nitrogen criterion:
Only a setpoint for inorganic nitrogen is imposed, which gives the controller the freedom to select the optimal ammonia and nitrate concentrations corresponding to this setpoint.

The current study was limited to linear control laws, and furthermore it was assumed that all process information such as plant parameters was available. Adaptive control including online parameter estimation was not studied, as the focus of this study was to first determine (theoretical) limits on performance.

5.4.6 Controller tuning

In the tuning step, weighting factors Γ^y for the controlled variables and Γ^u for the manipulated variables have to be chosen. Other important tuning parameters for MPC are the prediction horizon P, the control horizon M and the observer gain matrix. In the procedure followed here, also setpoints for the controlled variables have to be chosen. The performance is determined by the combination of the chosen setpoints and weights and other tuning parameters.

In the choice of setpoints and weights, a careful trade-off is to be made between ammonia and nitrate. This is because of the fact that often not only the sum of both components, corresponding to N-removal, is aimed at, but also simultaneously a goal is put onto effluent ammonia, which is consequently more emphasised than nitrate (or total-N). Putting too much emphasis on ammonia however can lead to a small decrease in ammonia at the cost of a large increase in nitrate, and thus may lead to poor nitrogen removal, especially at lower temperature, as was shown in preliminary studies with the same plant model (Veersma *et al.*, 1995).

A tuning strategy was developed in which as much quantitative knowledge was used as possible in order to obtain a relatively straightforward, systematic tuning procedure. First the setpoints were chosen. The sampling time was 15 minutes, based on typical sampling rates of ammonia and nitrate sensors. The prediction horizon P and control horizon M were both set at 35 samples (corresponding to 8h35min) which was chosen in relation to the time constants of the system. Weights for the inputs (aerator 1 and 2) were derived from steady-state gains and were 0.2458 and 0.7197, respectively. Weights for the outputs were determined by trial and error using the linear model of the plant. The minimum and maximum power input to the aerators were included as constraints on the inputs and were set at 30 and 132 kW respectively.. The values mentioned here were applied in the simulations, unless stated otherwise. The setpoints and weighting factors for the controlled variables are given below, at the corresponding results. For the observer gain, the standard DMC settings were applied (Morari, 1994).

5.4.7 Results: Control system evaluation

Evaluation of control goals with MPC

After tuning, the controllers were evaluated on the full nonlinear plant model by applying an influent pattern representing dry weather as well as storm weather flow conditions, all at 12 °C (Figure 3). On day 6, a storm event lasting 10 hours takes place During 1.5 hour all concentrations are kept unchanged, after which a concentration drop of approximately 80 % for the organic COD fractions and N fractions takes place, but not for ammonia and nitrate. The initial states for the simulations were obtained by simulating the dry weather pattern over a large number of days, until a repetitive pattern of the effluent concentrations was obtained.

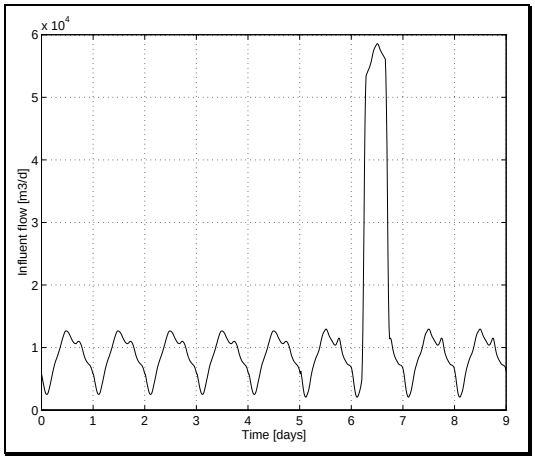

Figure 3: Applied influent flow.

First, the combined ammonia/nitrate criterion was studied. The setpoints for ammonia and nitrate were 3.5 and 7 mg/l, respectively and the weights 10 rep. 5. In Figure 4, in the left figure the effluent ammonia and nitrate concentrations are shown together with their setpoints and the total inorganic nitrogen effluent concentration, during one day. In the middle figure, the power input to the aerators is shown; in the right figure, the total power input to the aerators is shown. It can be seen that the controller is not able to keep the ammonia and nitrate concentration exactly at their setpoints, but that deviations occur up to 2 mg/l. In the open loop case (not shown), the nitrate

concentration would have risen to 15 mg/l on day 5, so the controller is effective in setpoint regulation. In the average, the deviation for ammonia is smaller than for nitrate, due to the higher weighting factor. What can also be observed, is that the aerators are operating against their constraints during a significant part of the time, and that most of the aeration is provided by aerator 2. This is caused by the location of the influent inlet point, which is close to aerator 1; by using aerator 2, the denitrification capacity is used more efficiently. What can also be observed in the right figure, is that the total aeration capacity is never used.

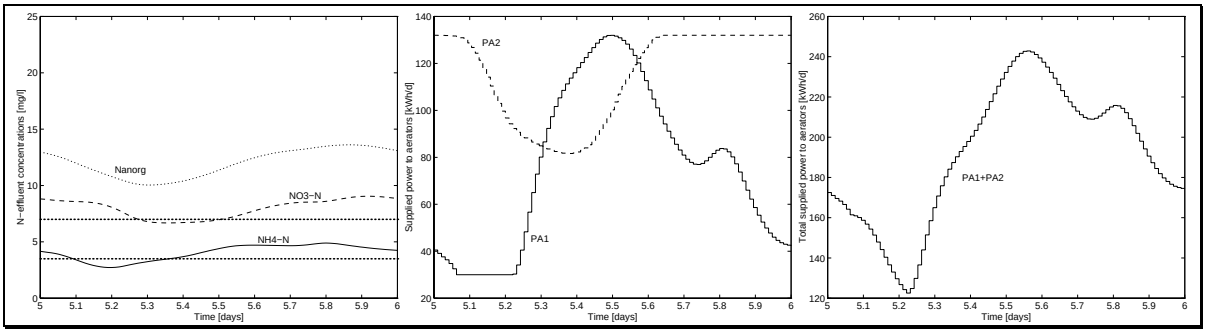

Figure 4: Combined ammonia/nitrate criterion, dry weather.

With regard to constraints on the power input to the aerators, it was observed that these constraints have a significant effect on performance (Figure 5). A better distribution of power input over the aerators leads to a better setpoint regulation with approximately the same total maximum capacity. The prediction horizon was chosen adequate, as no significant improvement was observed by doubling the prediction horizon.

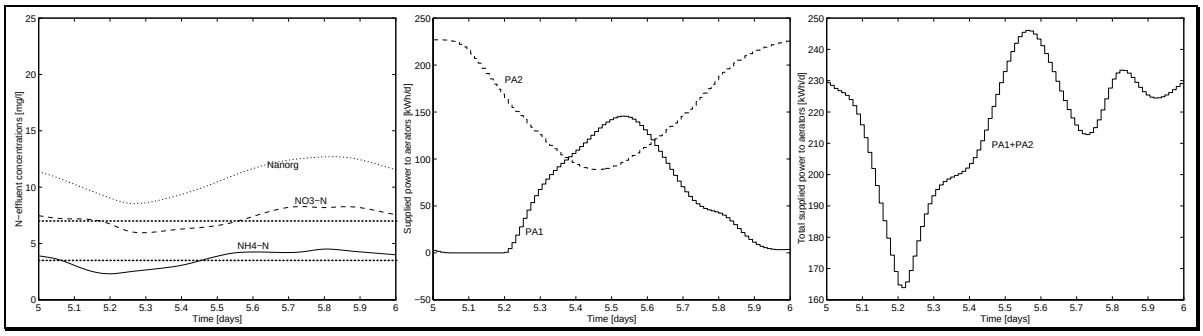

Figure 5: Combined ammonia/nitrate criterion, dry weather, no constraints.

Under storm weather conditions, the same cases were studied. The results for the last 4 days are shown in Figure 6 with constraints active. A temporary peak in effluent occurs and after the peak, there is a significant deviation from both setpoints. This was not avoided by releasing the constraints, although in that case the peak area for ammonia was slightly lower and the ammonia an nitrate concentrations were kept closer to their setpoints, be it at the expense of more than twice the peak aeration capacity (not shown).

To enable comparison with results obtained in earlier studies, tuning was carried out such that average ammonia under dry weather was 3 mg/l . In that case, the achievable nitrate concentration was 14 mg/l. The same cases were studied, showing similar results. For criterion 2, ammonia, performance comparable to criterion 1 could be obtained, whilst tuning was more straightforward.

With criterion 3, the sum of effluent ammonia and nitrate were to be kept at 10 mg/l. Under dry weather conditions, a constant sum at the setpoint value was obtained, with higher average ammonia and lower energy input. Thus, the total inorganic nitrogen concentration is significantly lower (10.0 vs. 17.3), at significantly lower aeration cost (182 vs. 201) than for the combined ammonia/nitrate criterion (with setpoints 3.0 and 14). Under storm weather conditions, at a certain time instant the controller became unstable (result not shown), which was due to the linear model which predicted negative concentrations.

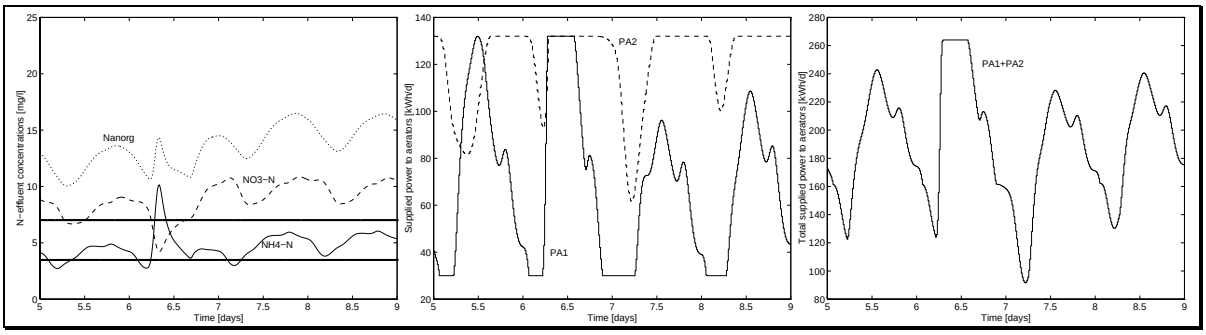

Figure 6: Combined ammonia/nitrate criterion, storm weather.

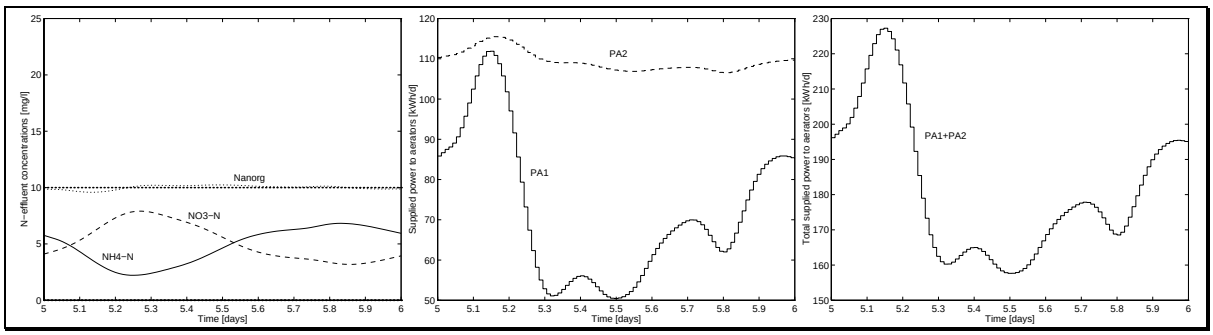

Figure 7: Inorganic nitrogen setpoint, dry weather.

In addition to these, in one case also feedforward control of the influent flow to the power input to the aerators was applied, using a model of the influence of the influent flow rate to the effluent ammonia and nitrate concentration. Applying this feedforward utilising the actual value of the influent flow showed only minor improvement in effluent quality (result not shown).

Comparison of MPC with other control laws

The results obtained by MPC were compared with LQG (Linear Quadratic Gaussian control), which is a well known optimal linear control law and three control structures with classical PI (Proportional Integral) controllers, namely only DO (Dissolved oxygen) control, ammonia control and ammonia control cascaded with DO control (Meinema *et al*., 1995, Schagen *et al*. 1995). To make a comparison possible, all these controllers were tuned such that the average ammonia concentration during dry weather flow was 3 mg/l. The controllers applied were as follows:

1. DO Control (PI): The power input to aerator 1 was selected as the manipulated variable, while aerator 2 was fixed at its maximal capacity. This choice was made for efficient utilisation of the denitrification capacity. The DO sensor was located in compartment 3 (Figure 1), and the setpoint was set at 1 mg/l.

2. Ammonia control (PI): Also aerator 1 was chosen, and the effluent ammonia setpoint was set at 3 mg/l.

3. Cascade/ratio control (PI/PI): For aerator 2, a two-speed aerator was chosen. In addition to the power input to aerator 1, the power input to aerator 2 was now also selected as manipulated variable. Two PI controllers were used in a cascade configuration: the master PI controller for maintaining a fixed ratio of (NH_4-N+NO_3-N)/NH_4-N at 6, with as output the DO setpoint for a slave PI controller.
4. LGQ control: The same manipulated variables are used as for the cascade controller. The goal is to minimise both ammonia and nitrate, while minimising aeration costs.

In Table 1, the results obtained are compared. For dry weather flow, the effluent concentration given in the table is the flow proportional mean over 1 day (day 5). For storm weather flow, the flow proportional mean over 4 days (day 6 - 9) is given. For MPC, the results are given for criterion 1, with setpoints for ammonia and nitrate 3 and 14 mg/l, respectively; also the results with a setpoint for NH4-N of 3.5 mg/l are given.

First, the systems were compared under dry weather conditions. If the same effluent NH4-N concentration of 3 mg/l is aimed at, similar or better effluent quality at lower energy consumption is obtained with MPC than with LQG, which in turn performed better than the classical controllers. DO control is least satisfactory. A setpoint for NH_4-N of 3.5 mg/l, which is slightly higher, lead to a significantly better N-removal at less aeration cost. It is to be remarked, that the improved performance of the advanced controllers is achieved at the cost of more instrumentation, which would however be very low compared to total investment costs.

To compare the controllers under conditions different from the tuning conditions, also storm weather conditions were applied. With the setpoint for NH_4-N of 3 mg/l, MPC performed slightly worse than LQG with respect to total inorganic nitrogen, as somewhat higher nitrate concentrations were achieved. Apparently, more weight is put onto ammonia, which also leads to a slightly higher energy consumption. Upon increasing the NH_4-N setpoint to 3.5, a significantly lower inorganic nitrogen concentration is achieved, at the expense of an increased NH_4-N concentration. This dramatic effect of setpoint choice and tuning on system performance complicates a clear judgement of control laws.

Table 1: Comparison of MPC with other control laws (D: dry weather flow, S: storm)

		Flow proportional [mg/l]			[kWh/d]
CONTROLLER	**INFLUENT**	**$N_{inorganic}$**	**NH_4-N**	**NO_3-N**	**P_A**
Influent	D	51.5	50.0	1.5	-
Open loop	D	18.8	3	15.8	202
DO (PI-type)	D	22	3	19	unknown
N-NH4 (PI type)	D	20	3	17	unknown
Cascade (PI-type)	D	19	3	16	213
LQG	D	18	3	15	200
MPC	D	17.2	3.1	14.1	201
MPC[1]	D	12.1	4.1	8.0	191
Influent	S	35.6	34.1	1.5	-
Open loop	S	20.2	3.6	16.6	202
N-NH4 (PI type)	S	20	3	17	unknown
Cascade (PI-type)	S	17	5	12	214
LQG	S	17	4	12	201
MPC	S	17.7	3.6	14.1	205
MPC[1]	S	13.5	4.7	8.8	191

[1]: Setpoint for NH_4-N is 3.5 mg/l, for NO_3-N 7 mg/l.

5.4.8 Conclusions

Treatment performance achieved by applying MPC indicates that this is a promising approach for control of nitrogen removal in carrousels. The fact that constraints can be taken into account adds another advantage to MPC over LQG and other linear control methods. Comparison of different control goals using MPC showed that the definition of the control goal has a large impact on control system performance. Both the setpoints and weighting factors influence the trade-off between ammonia and nitrate. Therefore, tuning is complicated and it is difficult to formulate criteria that lead to an appropriate trade-off under all operating conditions. Also the comparison of control laws is complicated. Therefore, it is worthwhile to formulate goals which are more general than setpoint regulation and which also allow for a flexible weighting of ammonia and nitrate; this would also enable a more objective evaluation of controller performance. This was aimed at by defining a criterion which imposed only a total inorganic nitrogen setpoint, which was unsuccessful under storm conditions due to the limited validity of the linear model used in the MPC controller. This may be improved by increasing controller robustness; another alternative may be the application of nonlinear MPC.

5.4.9 References

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5.5 Robustness analysis of MPC controlled activated sludge plants

Abstract[†]

Process control is considered an important means to meet the increasingly tighter demands that are being placed on sewage treatment in most western countries, especially with respect to nutrients. This section investigates stability robustness of a wastewater treatment plant controlled with Model Predictive Control (MPC). Aims of this model study are to study possibilities and limitations of advanced control application to wastewater treatment, to obtain insight in the process factors that affect control system robustness, and to find tuning rules to improve MPC robustness. A simple plant model was studied. A structured uncertainty description of parameter and state uncertainty was used to avoid conservative results. μ-Analysis was used to compute robustness bounds of the closed loop system. The results show that achievable robustness improvement by tuning is limited and indicate that nonlinearity has a stronger effect on stability than parameter errors.

Keywords

Bio control, Wastewater treatment, Predictive control, Robust control, Structured singular value.

5.5.1 Introduction

Increasingly stringent demands are being put onto nitrogen removal from wastewater. Municipal wastewater is treated biologically in so-called activated sludge plants. To meet the stricter demands, plants have to be upgraded and the treatment process becomes more complicated. Process control is generally considered as an important means to achieve stable operation under the typically large variations in load and temperature. This view and recent advances in modelling and sensor technology have been the motivation for significant research efforts in different countries to develop effective control strategies.

One particular question of interest is how and to which extent advanced control can contribute to improved plant operation and decreased investment costs. The activated sludge process is multivariable, nonlinear, time-variable and stiff, input constraints are present, and load and temperature vary considerably. It is difficult to find controllers that cope with all these characteristics, and currently different control laws are applied, proposed and investigated, ranging from classical control including cascade control, model based control such as LQG and MPC, adaptive control to rule-based control, including knowledge-based control and fuzzy control.

The currently available knowledge in the form of mathematical models, especially the well-known Activated Sludge Model No. 1 (ASM1, Henze *et al*., 1987) suggests the application of model based control. In previous work, application of MPC to different wastewater treatment systems was studied (Weijers *et al*. 1995, 1997) where MPC was used as a reference method to assess achievable performance with linear model based control. In some of the cases, instability occurred due to model mismatch as a result of linearization errors. In other studies that applied

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linear control (LQG), no instability was observed (van Schagen *et al*., 1995). This was probably due to the more limited operational range in these studies.

In this section, robustness of linear MPC control is investigated. The goal is to obtain physical insight in process factors that affect control system robustness, and to develop tuning guidelines for improving MPC robustness, if possible. Three main causes of uncertainty are studied, namely parameter uncertainty due to either identification errors (corresponding to small parameter errors) or parameter variation (large parameter errors), and linearization errors due to deviation of the states from the linearization point. The interest in the effect of linearization errors is motivated by results in the earlier studies. If linearization errors will be identified as a more severe cause of instability than parameter errors, this indicates that application of nonlinear MPC has preference over a parameter adaptive MPC controller.

For this study, a model is used that is as simple as possible but nevertheless exhibits some of the characteristics of the full ASM1 model, especially nonlinearity and stiffness.

The section is organised as follows. In Section 5.5.2, the applied state-space MPC controller is described and a closed loop expression for the MPC controlled plant that is used for the robustness analysis is given. Then, μ-analysis is outlined and the applied plant uncertainty model is described, followed by a description of the model system and the model studies. Section 5.5.3 presents the results and discussion and Section 5.5.4 gives the conclusions.

5.5.2 MPC, Robustness analysis tools, Modelling and Model studies

MPC

The principle of MPC is as follows (Figure 1). At each sampling instant k, a prediction is made of the estimated future outputs over a prediction horizon *P*. The future outputs are computed from the free response, which is determined by the state of the system at instant k, plus the forced response, which is determined by the future control increments or moves. The control moves over a control horizon *M* are used to compute an optimal trajectory with respect to a defined optimisation criterion. Only the first move of this optimal sequence is then applied to the plant, after which the state estimation is corrected with the measured process output at the sampling instant. At the next time instant, the whole procedure is repeated. This repetitive procedure is referred to as receding horizon control. In this case, MPC according to Morari and Ricker (1994) was used, with the following quadratic criterion, subject to linear constraints on the inputs and/or the outputs:

$$\min_{\Delta u(k+i),\, i=1,\ldots,m} J \tag{1}$$

with:

$$J = \sum_{i=1}^{p} \left\| \Gamma^{y} \left[r(k+i \mid k) - y(k+i \mid k) \right] \right\|_2^2 + \left\| \Gamma^{u} \Delta u(k+i) \right\|_2^2 \tag{2}$$

where $y(k+i|k)$ is the prediction of the outputs for time step $k+i$, done at time step k and $r(k+i|k)$ is the desired value of the outputs at time step $k+i$. The Δ-operator represents the change in the variable from the previous sampling time and $\Delta u(k+i)$ are the control moves at time step $k+i$.

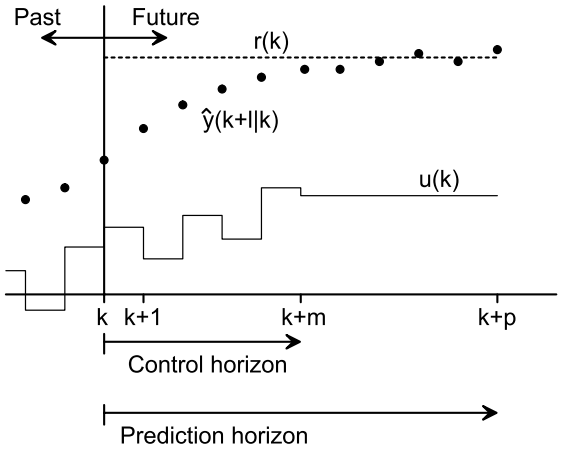

Figure 1: Receding horizon principle of MPC

The following time-invariant state-space difference equation is used as prediction model:

$$\begin{aligned} x(k+1) &= A^p x(k) + B_u^p u(k) + B_w^p w(k) \\ y(k) &= C^p x(k) + D_w^p x(k) \end{aligned} \tag{3}$$

with manipulated variables *u(k)* and measured disturbances *w(k)*. The measurement equation is:

$$\hat{y}(k) = C^p x(k) + D_w^p x(k) + v(k) \tag{4}$$

A closed loop expression is now derived for the controlled system to enable the robustness analysis, which holds if no constraints are active. The system and measurement equations (3) and (4) are rewritten in incremental form:

$$X(k+1) = \overline{A}X(k) + \overline{B}_u \Delta u(k) + \overline{B}_w \Delta w(k) \tag{5}$$

$$\hat{y}(k) = \overline{C}X(k) + v(k) \tag{6}$$

where:

$$X(k) = \begin{bmatrix} \Delta x(k) \\ y(k) \end{bmatrix} \tag{7}$$

$$\overline{A} = \begin{bmatrix} A^p & 0 \\ C^p A^p & I \end{bmatrix} \quad \overline{B}_u = \begin{bmatrix} B_u^p \\ C^p B_u^p \end{bmatrix} \quad \overline{B}_w = \begin{bmatrix} 0 \\ D_w^p \end{bmatrix} \quad \overline{C} = \begin{bmatrix} 0 & I \end{bmatrix} \tag{8}$$

For state estimation the following observer is used:

$$X(k \mid k-1) = \overline{A}X(k-1 \mid k-1) + \overline{B}_u \Delta u(k-1) + \overline{B}_w \Delta w(k-1) \tag{9}$$

$$X(k \mid k) = X(k \mid k-1) + K_f(\hat{y}(k) - \overline{C}X(k \mid k-1)) \tag{10}$$

If no constraints are active, the receding horizon control law reduces to a linear controller that is the sum of state feedback control and feedforward:

$$\begin{aligned}\Delta u(k) &= K_{MPC}(R(k+1|k) - Y(k+1|k)) \\ &= K_{MPC}(R(k+1|k) - L_{MPC}X(k|k) - K_{MPC}S^w\Delta w(k)\end{aligned} \tag{11}$$

where K_{MPC} is the (constant) MPC gain matrix, $L_{MPC} = K_{MPC}[S^x \quad S^p]$, *R(k+1|k)* is the reference trajectory over the prediction horizon and *Y(k+1|k)* the predicted output (free response):

$$Y(k+1|k) = [S^x \quad S^p]\begin{bmatrix}\Delta x(k) \\ y(k)\end{bmatrix} + S^w\Delta w(k) \tag{12}$$

with:

$$S^x = \begin{bmatrix}(C^pA^p)^T & \ldots & \sum_{j=1}^{p}(C^pA^{pj})^T\end{bmatrix}^T,$$

$$S^p = \begin{bmatrix}I_{n_y} & \ldots & I_{n_y}\end{bmatrix}^T$$

and

$$S^w = \begin{bmatrix}(C^pB_w^p)^T & \ldots & \sum_{j=1}^{p}(C^pA^{pj-1}B_w^p)^T\end{bmatrix}^T$$

K_{MPC} is an explicit analytical function of the system equations and the weights Γ^u and Γ^y. If there is no model-plant mismatch, then the plant is described with a state-space model with system matrices $\overline{A}^p$, $\overline{B}_u^p$ and $\overline{B}_w^p$ that are equal to the matrices A^p, B_u^p and B_w^p of the MPC prediction and observer model. The (nominal) closed-loop operator from the external inputs (measured disturbances $\Delta w(k)$, measurement noise *v(k)* and reference signals *R(k+1|k)* to *y(k)* can then be written as follows (Lee and Yu, 1994):

$$y(k) = \left[\begin{array}{c|c}A & B \\ \hline C & D\end{array}\right] \times \begin{bmatrix}\Delta w(k) \\ q \cdot v(k) \\ R(k+1|k)\end{bmatrix} \tag{13}$$

where

$$A = \begin{bmatrix}\overline{A} - \overline{B}_u L_{MPC} & \overline{B}_u L_{MPC} \\ 0 & \overline{A} - K_f\overline{C}\overline{A}\end{bmatrix}, \tag{14}$$

$$B = \begin{bmatrix}\overline{B}_w - \overline{B}_u K_{MPC} S^w & 0 & \overline{B}_u K_{MPC} \\ 0 & -K_f & 0\end{bmatrix},\ C = \begin{bmatrix}\overline{C} & 0\end{bmatrix},\ D = \begin{bmatrix}0 & 0 & 0\end{bmatrix} \tag{15, 16}$$

$$\left[\begin{array}{c|c}A & B \\ \hline C & D\end{array}\right] \stackrel{\Delta}{=} C(qI - A)^{-1}B + D \tag{17}$$

and q is the forward shift operator. A similar, more complicated expression was derived for the closed loop operator under plant-model mismatch for computation of the errors $\Delta A(\theta_i)$ and $\Delta B(\theta_i)$ the uncertainty description (see below).

Robustness analysis

In the robustness analysis of the MPC controlled plant, several parameters, including states, were considered as sources of uncertainty. The states were included to investigate the effect of linearization errors on the closed loop stability. In order to take different parameters and states into account and to avoid conservatism in the results of roust stability bounds, a structured uncertainty description was applied. The structured singular value (SSV) or simply μ) was used to compute robustness bounds.

The structured singular value is a matrix function denoted by $\mu_\Delta(\cdot)$. The value of $\mu_\Delta(M)$ does not only depend on M but also on the underlying structure Δ. One important question is how large Δ can be without destabilizing the feedback system. This can be found by the following analysis. The feedback system becomes unstable if

$$\det(I - M(s)\Delta(s)) = 0 \tag{18}$$

for some s. The structured singular value is defined such that $\mu^{-1}(M)$ is equal to the smallest $\overline{\sigma}(\Delta)$ needed to make (I-MΔ) singular:

$$\mu(M) = \frac{1}{\min\{\overline{\sigma}(\Delta) : \det(I - M(s)\Delta(s)) = 0\}} \tag{19}$$

If no Δ exists such that $\det(I - M(s)\Delta(s)) = 0$, then $\mu_\Delta(M)$=0.

Let $\gamma > 0$ be a number such that the closed-loop system is stable for all $\|\Delta\|_\infty < \gamma$. Increase γ until $\gamma_{\max}$ so that the system becomes unstable. So $\gamma_{\max}$ is the robust stability margin. The smaller $\sup(\mu_\Delta)$, the larger the robust stability margin:

$$\frac{1}{\gamma_{\max}} = \sup_{s \in C^+} \mu_\Delta(M(s)) = \sup_{\omega} \mu_\Delta(M(j\omega)). \tag{20}$$

In this section, robust stability is studied. The deltablock describes the differences between the true plant and the internal model. The analysis gives us the structured singular value for the frequency domain of interest. With the uncertainty blocks scaled such that $\overline{\sigma}(\Delta) \leq 1$, the structured singular value has to be smaller than 1 for all frequencies up to the sampling frequency to guarantee robustness.

An uncertainty description was developed for the closed loop system (nominal MPC controlled plant) in state-space format. For the uncertainty description, the general affine state space uncertainty according to Zhou was chosen (Zhou *et al*., 1996). This description is most suited for the application under study, because the model and controller are in state-space format, and

it allows for dealing with the type of nonlinearities involved in ASM1, be it that some approximations have to be made; these are described below. In the uncertainty description used, the linear system (here the closed loop system) is considered that is parametrized by *k* uncertain parameters, $\delta_1,...,\delta_k$. The nominal description of the system is given by known matrices *A*, *B*, *C* and *D* and the parametric uncertainty in the nominal system is reflected by the *k* scalar uncertain parameters $\delta_1,...,\delta_k$. The uncertain parameters can be specified by $\delta \in [-1,1]$.

The uncertainty description in state space can be written as a linear fractional transformation as shown in Figure 2.

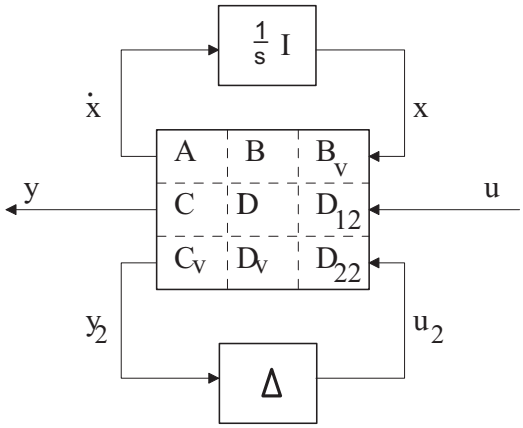

Figure 2: Linear fractional transformation representation of state space uncertainty

The deltablock Δ is a diagonal matrix that contains all the uncertain parameters:

$$\Delta = diag\{\delta_1 I, \delta_2 I, ..., \delta_k I\} \tag{21}$$

The uncertain state-space system is written as:

$$\dot{x} = (A + \underbrace{B_v \Delta C_v}_{\Delta A})x + (B + \underbrace{B_v \Delta D_v}_{\Delta B})u \tag{22}$$

$$y = Cx + Du \tag{23}$$

Now, the values of ΔA and ΔB of the system have to be found and split into Δ, B_v, C_v and D_v. Therefore, it is supposed that for all *k* uncertain parameters the uncertainty of the state space matrices can be written as:

$$\Delta A = \sum_{i=1}^{k} \Delta A(\theta_i) = \sum_{i=1}^{k} \frac{\Delta A(\theta_i)}{\Delta \theta_i} \Delta \theta_i \tag{24}$$

$$\Delta B = \sum_{i=1}^{k} \Delta B(\theta_i) = \sum_{i=1}^{k} \frac{\Delta B(\theta_i)}{\Delta \theta_i} \Delta \theta_i \tag{25}$$

For the nonlinear system, the terms $\frac{\Delta A(\theta_i)}{\Delta \theta_i}$ were computed with a difference approximation rather than by differentiation, as this will result in a better approximation of the uncertainty

when the parameter (or state) deviations are large. $\Delta A(\theta_i)$ is computed by subtracting the nominal value of A from the matrix A that is computed with all parameters equal to the nominal value, except parameter θ_i that is equal to an extreme (minimum or maximum) value of that specific parameter (or state). Inspection of the above equation leads to following matrices:

$$\Delta = I_{(k-n)\times(k-n)} \tag{26}$$

$$B_v = \begin{bmatrix} \Delta\theta_1 I_{n\times n} & \Delta\theta_2 I_{n\times n} & \dots & \Delta\theta_k I_{n\times n} \end{bmatrix} \tag{27}$$

$$C_v = \begin{bmatrix} \frac{\Delta A(\theta_1)}{\Delta\theta_1} & \frac{\Delta A(\theta_2)}{\Delta\theta_2} & \dots & \frac{\Delta A(\theta_k)}{\Delta\theta_k} \end{bmatrix}^T \tag{28}$$

$$D_v = \begin{bmatrix} \frac{\Delta B(\theta_1)}{\Delta\theta_1} & \frac{\Delta B(\theta_2)}{\Delta\theta_2} & \dots & \frac{\Delta B(\theta_k)}{\Delta\theta_k} \end{bmatrix}^T \tag{29}$$

With the uncertainty description thus derived, robust stability bounds were computed using the μ-toolbox (Balas *et al*. 1991).

Modelling

A simple model was derived with the following characteristics and assumptions: two states are considered, namely substrate and biomass; Monod growth kinetics ($\mu_m S/(K+S)$) are assumed; one measured output is selected, namely the concentration of the substrate; the reactor is described by one continuous stirred tank reactor; the volume of the final clarifier is neglected; in the final clarifier no reactions take place and clarification is ideal.

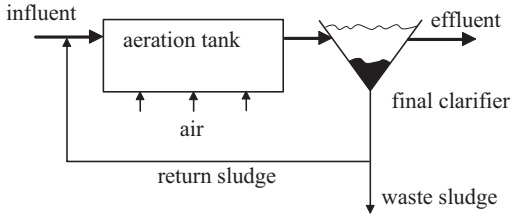

Figure 3: Process flowsheet for simple model

The nonlinear model then follows from component mass-balances:

$$\dot{X}_{bh} = \underbrace{\mu_m \frac{S_s}{K_S + S_S} X_{bh}}_{growth} - \underbrace{D_{SA} \cdot X_{bh}}_{out} \tag{30}$$

$$\dot{S}_S = \underbrace{-k_1 \cdot \mu_m \frac{S_s}{K_S + S_S}}_{substrate\ \ consumption} - \underbrace{D_{in} \cdot S_S}_{out} + \underbrace{D_{in} \cdot S_{s_{in}}}_{in} \tag{31}$$

The sludge age D_{SA} was chosen as the manipulated variable. Linearizing the differential equations for this configuration, with system $\xi = [X_{bh} \quad S_S]^T$ gives the following state space equations in deviation variables with $y = S_s$, $u = D_{SA}$ and $w = S_{s_{in}}$:

$$\begin{aligned} \dot{\xi} &= A\xi + B_u u + B_w w \\ y &= C\xi \end{aligned} \tag{32}$$

with:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix},$$

$$\begin{aligned} A_{11} &= \mu_m \frac{S_{s_0}}{K_S + S_{s_0}} - D_{SA}, \; A_{12} = \mu_m \left(\frac{X_{bh_0}}{K_S + S_{s_0}} - \frac{X_{bh_0} S_{s_0}}{(K_S + S_{s_0})^2}\right), \\ A_{21} &= -k_1 \mu_m \frac{S_{s_0}}{K_S + S_{s_0}}, \; A_{22} = -k_1 \mu_m \left(\frac{X_{bh_0}}{K_S + S_{s_0}} - \frac{X_{bh_0} S_{s_0}}{(K_S + S_{s_0})^2}\right) - D_{in}, \end{aligned} \tag{33}$$

$$B_u = \begin{bmatrix} -X_{bh_0} \\ 0 \end{bmatrix}, B_w = \begin{bmatrix} 0 \\ D_{in} \end{bmatrix}, \tag{34}$$

$$C = [0 \quad 1] \tag{35}$$

The nominal values of the kinetic and stoichiometric parameters (specific growth rate μ_m), half saturation coefficient for biomass K_s, yield for heterotrophic biomass $1/k_1$) were as follows:

k_1	=	3/2	[*g(COD)oxidized/g(COD)formed*]
μ_m	=	4	[d^{-1}]
K_s	=	20	[*g(COD)/*m^{-3}]

The values for parameters that describe the reactor model were as follows:

D_{in}	=	2	[d^{-1}]
D_{SA}	=	1/10	[d^{-1}]
$S_{s_{in}}$	=	20	[*g(COD)/*m^{-3}]

with D_{in} the dilution rate, D_{SA} the reciprocal of the sludge age and $S_{s_{in}}$ the substrate concentration in the influent. The dilution rate is the reciprocal of the hydraulic residence time (volume divided by influent flow rate) and the sludge age is the mean biomass residence time. For deriving the state-space model, the system is linearized at the equilibrium state. Setting the derivative terms in (30) and solving for X_{bh} and S_s gives two solutions for the equilibrium states, the nontrivial solution being:

$$X_{bh0} = \frac{D_{in} \cdot (-D_{SA} \cdot K_S + S_{S_{in}} \cdot (\mu_m - D_{SA}))}{k_1 D_{SA} \cdot (\mu_m - D_{SA})} \tag{36}$$

$$S_{s_0} = \frac{D_{SA} \cdot K_S}{(\mu_m - D_{SA})} \tag{37}$$

Substituting the numerical values of all parameters gives X_{bh0} = 659.8 [$g(COD)m^{-3}$] and S_{s0} = 0.5128 [$g(COD)m^{-3}$].

Model studies

With the linear model, a nominal tuning was carried out. The following controller tuning was applied: T_S = 1/48 [d], P = 48, M = 8, Γ^u = 0.1, Γ^y = 1 and K_f = [0 0 1]^T (standard DMC estimator). Nominal stability was checked by inspection of the closed-loop poles. With the nominal MPC controller, the nonlinear system was simulated over 10 d., with the initial state equal to the steady-state. At t=1 d., a step of +15% was imposed on the setpoint; at t=11 d., a setpoint 15% lower than the original concentration was imposed. The simulation was repeated with a small parameter deviation (K_s (-20%), μ_m (+20%) and k_1 (+20%)) and a large deviation (K_s (-50%), μ_m (+100%) and k_1 (+100%)). The state trajectories were used to determine the state deviations from the linearization point during the simulation. These were used for computation of the robustness bounds under state uncertainty. The initial states for the perturbed parameter cases were computed such that they corresponded to a situation where the output is at its desired setpoint.

The simulations and corresponding μ-plots were carried out for different values for the MPC tuning parameters to identify whether and which tuning improves robust stability. The following MPC tuning parameters were studied: prediction horizon P, control horizon M, input and output weights Γ^u and Γ^y and especially the observer gain matrix K_f, as suggested by Lee and Yu (1994).

5.5.3 Results and discussion

In Figure 4, the results of the different simulations are shown. It can be seen that the system with perturbed parameters responds faster at t=11 d. in downward direction than the nominal system, which is a result of the higher growth rate. The corresponding biomass concentrations in the perturbed case are much lower, which is understood from the larger growth rate and lower yield in this case. The system remains stable despite the large parameter variations.

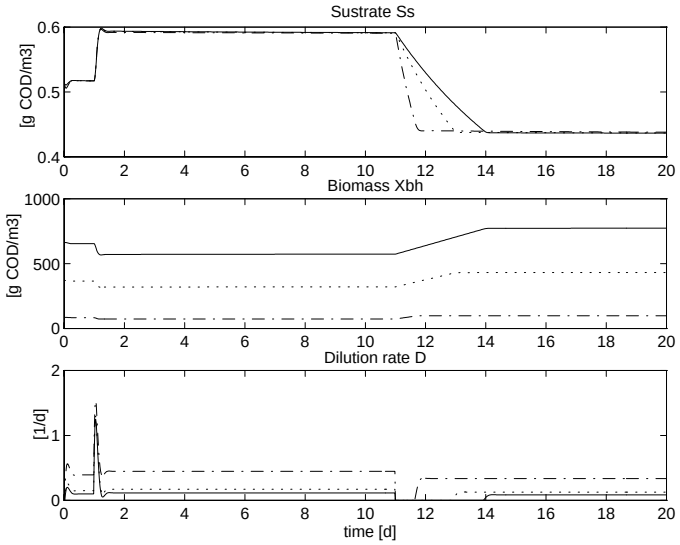

Figure 4: System with nominal parameters (-), slightly deviated parameters (·····) and stronger deviated parameters (-.-.).

Robust stability plots for the nominal and perturbed situations are given in Figure 5. From the μ-plots, the simulation with large parameter variation was expected to become unstable (μ>1), which is not in correspondence with the simulation results. This indicates conservatism in the μ-computation, which is probably a result of the fact that in the μ-computation unrealistic state and parameter combinations occur.

From the μ-plots of the total uncertainty and only parametric uncertainty, a large difference can be observed. The effect of parametric uncertainty alone is much lower than the total uncertainty. This result indicates that linearization errors due to state deviation have a larger effect than parameter errors. Due to the observed conservatism this is however not conclusive.

Finally, μ-plots were computed for different MPC tuning parameters. Most of the tuning parameters had a limited effect on stability robustness. The prediction horizon and control horizon had little influence on the robustness bounds. Increasing the input weights Γ^u did not always improve robustness as in the linear case. This is because too sluggish control due to large input weights leads to a large state deviation that deteriorates stability. Consequently, an optimal value for the input weights must be selected. The observer tuning has more effect. High

observer gains improved robustness; here a trade-off has to be made with noise rejection (which was not studied here).

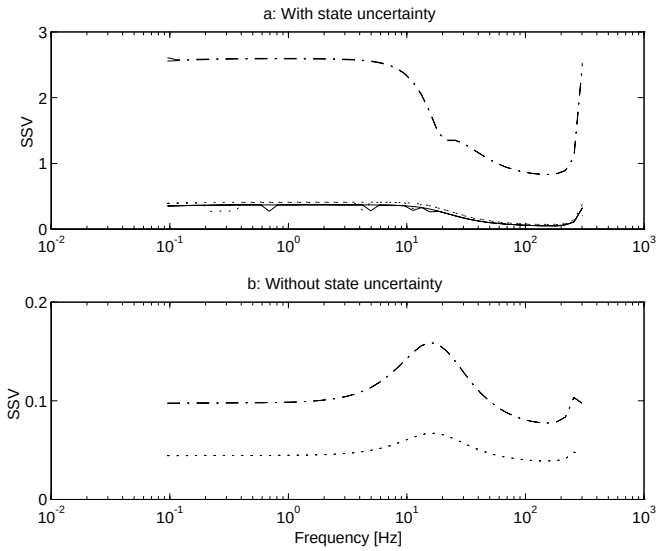

Figure 5: Upper μ-plot: total uncertainty (states and parameters);
lower μ-plot: only parameter uncertainty

5.5.4 Conclusions

A simple bioreactor system was used as a model for activated sludge plants. In simulations with a nonlinear plant model controlled by a nominally tuned MPC controller, no instability occurred, even under large parameter variations. Comparison with μ-plots indicated conservatism in the μ-computation. MPC tuning had a limited influence on robustness. A much larger value for μ was found for uncertainty including parameters and states when compared with uncertainty in parameters only. This result indicates that linearization errors have a more pronounced effect on stability robustness than parameter errors. Consequently, development of nonlinear MPC should have priority over parameter adaptive MPC for application in wastewater treatment. While the conservatism observed and the simplicity of the model applied prohibit completely solid conclusions, the results provide a good starting point for further insight in and development of robust control systems in biotechnology and wastewater treatment.

5.5.5 References

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5.6 Discussion and conclusions

Controller design was studied, including control structure design and the actual controller design. Because existing control design theories and methods cannot cope directly with realistic problems, approximations are required in problem formulation (criteria), plant model or controller and associated design method. Two extreme approaches were outlined, namely exact solution of an approximate design problem versus approximate solution of the exact problem. Application of on-line optimisation including feedback was concluded to be the most promising control approach.

Control structure design includes IO selection and control configuration selection. IO selection receives too little attention in the literature on activated sludge process control. Input selection for wastewater treatment is generally not a problem. Output selection is more difficult. Most difficult appears however to be selection of controlled variables. Output selection will be more straightforward once a correct selection of controlled variables has been made, and we expect a basic, quantitative analysis to be sufficient for output selection for activated sludge control. A methodology for selection of controlled variables was proposed.

With respect to control configuration selection, several interactions occur in the activated sludge processes that argue for MIMO control. Whether MIMO control is required from the point of view of the final control objectives remains to be determined, however.

Several advanced, model-based controllers have been suggested in the literature and tested in simulations and on pilot-scale. Adaptive model predictive control is a promising approach, which has been studied relatively well for alternatingly aerated systems. Few advanced control techniques however are being applied on full-scale. Comparative studies showed that advantages of model-based control are not necessarily in improved (nominal) performance, but in more straightforward design procedures and in providing an indication of achievable performance. Moreover, robustness can be higher if accounted for in the controller design.

For application to continuously operated systems, application of MPC to pre-denitrification and carrousels was investigated. Linear MPC with constraints, which is a standard technique, was applied as a starting point. In both systems, stability problems occurred, caused by model mismatch. In the cases studied, these problems might be circumvented by restricting models or by ad-hoc modifications, but this is not desirable in a generic methodology.

To find systematic remedies against the observed problems with model mismatch, robustness of MPC was investigated. A simple model and a structured uncertainty description were applied to study robustness against state vs. parameter uncertainty. The results indicate that state uncertainty has a larger effect than parameter uncertainty. Consequently, nonlinear control development should be given priority over parameter adaptation. However, these conclusions have to be drawn with caution, because the robustness results using μ-analysis are rather conservative.

MPC requires an accurate plant model. From experiences with controllers tuned based on a calibrated ASM1, one should avoid too optimistic expectations when employing existing calibration strategies if a calibrated ASM1 is used for controller tuning. For possible future application of nonlinear MPC, identifiable and reduced models are required.

Chapter 6 Conclusions and future developments

The aim of this thesis has been to study possible performance improvements of nitrogen removal activated sludge plants through application of advanced modelling and control techniques and to develop methodologies and tools to achieve improved operation. The emphasis has been on continuously operated carrousel systems and pre-denitrification plants, which are the most important systems in The Netherlands. In the preceding chapters, different topics were addressed along successive steps in control system design. In this concluding chapter, first general conclusions are formulated. Then, detailed conclusions are summarised per topic in the corresponding subsections. The final section formulates expectations for the future.

6.1 General conclusions

Stricter legislation calls for improved performance of activated sludge processes. Defining performance goals as a mathematical optimisation problem can guide performance improvement as it provides a clear judgement of performance. Moreover, the availability of advanced modelling and control techniques argues to develop straightforward, optimisation-based controller design procedures to close the gap between legislation and controller specifications. A good starting point is to minimise plant operating costs under quality and reliability constraints. The trade-offs between economy, quality and reliability can be analysed with a multi-criterion formulation.

Mathematical modelling based on Activated Sludge Model No. 1 (ASM1) is a very helpful tool for off-line application. Qualitative conclusions are well possible from comparative simulations, for example to compare alternative plant modifications or to compare performance and robustness of different controller types. Existing calibration procedures do not yield unique parameters, however. Consequently, one should avoid absolute, quantitative use of calibrated models, such as exact tuning of controllers. More insight is required in the prediction uncertainty and validity of calibrated models based on ASM1, especially if extrapolating beyond experimental conditions of calibration.

For on-line use such as in model-based control, direct application of ASM1 is less suited, due to its size, identifiability problems and stiffness. While several reduced models have been reported, there is a lack of reduced models for distributed systems, such as carrousels. Moreover, especially reduction based on timescale separation is interesting for control. Therefore, we studied techniques for understanding timescale properties of ASM1 and for systematic model reductions, which yielded valuable insight and tools that are useful for further research.

Advanced model-based control application to activated sludge processes is promising, but hardly applied on full-scale. On-line optimising control with feedback is the most suitable technique to approximate realistic objectives under constraints. From the activated sludge process characteristics, it is expected that best performance can be achieved with adaptive and nonlinear control. We studied linear Model Predictive Control application to a pre-denitrification system and a carrousel. The results indicate that nonlinear MPC is more suitable than linear MPC for operation over a larger operational range, which is required for economic operation.

The advantages of model-based over rule-based control must be further investigated. For this, model studies are invaluable, as is an optimisation-based analytic design procedure. It is here, where the value of models is most pronounced. Even if the actually applied controller is very simple, its development and design is greatly facilitated by a model-based approach, while its performance is much better guaranteed.

6.2 Goal formulation

A major task in controller design is formulation of consistent and sensible control system specifications. In Chapter 2, translation of legislation to control goals for wastewater treatment plants was analysed, which revealed that there is insufficient insight in the relationship between plant goals as derived from legislation and control goals. Consequently, a heuristic controller design approach is typically adopted, with trial-and-error design procedures that lead to time-consuming design and inability to recognise inconsistent specifications. Moreover, lack of standard, consistent criteria for plant performance evaluation complicates judgement of particular controller designs.

Instead of a heuristic approach, we suggest to apply an analytic design procedure, by formulating the design problem as a mathematical optimisation problem. In this approach, all plant objectives and constraints are explicitly formulated in a quantitative way. Trade-offs can be made explicit during design through mathematical optimisation and cumbersome trial-and-error and artificial objectives are avoided. Application of such a procedure requires availability of reliable models of specifications, disturbances and the plant and their uncertainties.

One possibility to define the control goal is to pose it as a minimisation problem of operating costs for the plant as a whole, treating quality and reliability as constraints. The operating costs should include costs of effluent disposal as imposed by national legislation, costs of energy consumption, costs of consumption of chemicals and sludge disposal costs.

A multi-criterion optimisation formulation that includes cost, quality and reliability is a more suitable paradigm for realistic definition of control goals than cost minimisation. This is because correct trade-off between different conflicting objectives is essential for a good controller design in wastewater treatment plants. In a multi-objective optimisation approach, these trade-offs can be analysed more transparently than in single objective optimisation.

Considering the treatment plant alone may lead to suboptimal solutions. This can be avoided in an integrated approach that considers the complete wastewater system, including sewer and receiving water.

6.3 Modelling, calibration and identifiability

For application of the analytic design procedure, reliable plant models are required. In Chapter 3, rigorous modelling and identification of activated sludge plants have been studied. The study focused on the bioreactor. Reactor modelling involves both biokinetic models and transport physical models. Biokinetics are typically modelled with Activated Sludge Model No. 1 (ASM1), while transport in the reactor is usually modelled with combined models from ideal model reactors. For accurate prediction of plant behaviour, both ASM1 parameters and transport model parameters should be calibrated, especially for distributed systems such as carrousels. The literature shows that most emphasis has been put on calibration of ASM1 model parameters, while transport model parameter calibration has been given little attention to.

Despite the observed emphasis on ASM1 calibration, still no clear, standard procedures for this task exist. To reveal how many and which ASM1 parameters can be uniquely obtained from

input-output data, ASM1 parameter identifiability was studied with practical identifiability analysis. A combined criterion based on the determinant and the condition number of the so-called Fisher information matrix proved effective to detect identifiable parameters.

A local identifiability analysis on a particular plant showed that at most eight parameters can be accurately estimated from realistic input/output measurements, assuming perfect knowledge of the transport model. This was confirmed by tests, estimating parameters from artificial data. From real plant data, only five to six parameters could be uniquely estimated. This lower number when using real data was most probably due to model mismatch of the transport model.

A procedure was proposed for global identifiability analysis, to investigate the dependency of the results of the local analysis towards the parameters values that must be assumed *a priori*. This procedure employs a so-called Latin Hypercube Sampling scheme, to efficiently select random parameter points. This procedure was successful in making a parameter identifiability ranking. It showed a limited dependency of results in the local analysis on the a priori selection of the parameter values. Moreover, the procedure showed that approximately fourteen parameters are important and must be calibrated. Other parameters may be fixed and taken from the literature. While the exact results obtained may differ from plant to plant, it is expected that the same trends will be observed for other continuously operated systems.

The results of the global analysis further lead to conclude that additional information is required to typical full-scale input/output measurements, as these measurements do not allow unique estimation of all required ASM1 parameters. To obtain additional information, an experimental test for determination of biodegradable COD was further refined and experimentally tested. The results show that total COD should be used as a basis to determine biodegradable COD. Interpretation of respirometry results should be done with care however because biological parameters in the tests can differ from those in the plant.

A special note is made with respect to the heterotrophic yield. This parameter is required for interpretation of respirometric experiments. It appears to be the best identifiable parameter from full-scale input/output data. Instead of using default values for this parameter, which has been suggested by several authors, one should consider to estimate this parameter from full-scale data to avoid bias in other parameters.

Existing calibration procedures do not yield unique parameters. Moreover, transport models in distributed systems are not adequately calibrated. Consequently, the physical (macroscopic) interpretation of parameters is unclear. One should avoid absolute quantitative conclusions when employing models tuned with existing calibration strategies.

6.4 Model reduction

Reduced models are better suited for identification, control and optimisation than high-order, rigorous models like ASM1. Model reduction of ASM1 was therefore studied in Chapter 4. Several approaches are applied in ASM1 model reduction, of which simplifying assumptions have been applied most frequently. For control, however, especially model order reductions into different timescales are interesting. Such reduced order models operating on a single timescale allow for reduced controller complexity, reduced computational requirements and for a hierarchical control approach. Understanding of timescale properties of ASM1 is insufficient however because few systematic studies have been done.

Singular perturbation theory has been studied to develop a systematic approach to derive reduced order models and to obtain understanding in timescale properties of ASM1. For model reduction by singular perturbation, the model must be into the so-called standard form. Usually the most difficult part in the reduction is to recognise if the model is in standard form or to bring it into this form, especially for nonlinear systems. Three procedures to obtain the standard form have been proposed, namely direct scaling, time-scale estimation and analytical scaling. They were tested on a simple model system with one biomass species and one substrate species.

The timescale estimation procedure proved a very helpful tool in model reduction. It correctly indicated whether the quasi-steady-state assumption was valid in all cases studied. Moreover, it is simpler to apply than eigenvalue analysis, because an ambiguous state-to-eigenvalue association is avoided. The analytical scaling procedure was helpful to bring the problem into standard form and to obtain a perturbation parameter in some cases, thus providing insight into the cause of time scale multiplicity. However, it was not always successful. The direct procedure is not generally applicable.

For interpretation of the BOD test for determination of biodegradable COD that was proposed in Chapter 3, ASM1 model reduction through application of the quasi-steady-state assumption led to a correct, reduced first-order model. This model provides a direct, analytical relation between experimentally observed parameters and ASM1 parameters, and thus gives valuable qualitative insight for interpretation of BOD tests. Moreover, it provides a quantitative basis to convert observed BOD to biodegradable COD, required to make the test useful in modelling.

6.5 Controller design

Chapter 5 treated control structure selection and the actual controller design. IO selection in activated sludge process control receives too little attention in the literature. Input selection for wastewater treatment is generally not a problem. Output selection is more difficult, but will be more straightforward once a correct selection of controlled variables has been made, so we expect a basic, quantitative analysis to be sufficient for output selection for activated sludge control. Most difficult is selection of controlled variables, and a methodology for their selection was proposed. With respect to control configuration selection, several interactions occur in the activated sludge processes that argue for MIMO control. However, it remains to be determined whether MIMO control is required from the point of view of the final control objectives.

Few full-scale applications of advanced control techniques have been reported. No single, all-embracing control theory or technique yet exists that can cope with realistic, nonlinear problems or with all process characteristics. A good approximation of actual optimisation problems is achieved by applying model-based optimisation on-line, including feedback, which is done in Model Predictive Control. The time-varying and nonlinear characteristics of the activated sludge process argue for adaptive and nonlinear control. Adaptive MPC has been studied for alternating systems in simulations and on pilot-scale, but not on full-scale.

We applied linear MPC with constraints to a pre-denitrification and a carrousel, which both are continuously operated systems. This was done to establish possibilities of this standard technique before investing in development of nonlinear and adaptive control application. In both systems, stability problems occurred, caused by model mismatch. In the cases studied, these problems can be circumvented by restricting models or by ad-hoc modifications, but this is not desirable.

To find remedies against the observed problems, MPC robustness against state vs. parameter uncertainty was investigated. A simple model and a structured uncertainty

description were applied. The results show that state uncertainty has a larger effect than parameter uncertainty. Consequently, nonlinear control development should be given priority over parameter adaptation. However, these conclusions are drawn with caution, because the robustness results using μ-analysis are conservative.

Comparative studies in the literature showed that advantages of model-based control over rule-based control are not always in improved (nominal) performance, but in more straightforward design procedures, in indicating achievable performance and in increased robustness. This also holds for application of an analytic design procedure versus a heuristic procedure.

6.6 Future developments

Goals

Performance improvement for wastewater treatment must be guided through clear goal formulation. A valuable starting point towards rational goal formulation within the wastewater community is the definition of an objective function based on operating cost in the control benchmark for activated sludge process control (Alex *et al.*, 1999). We expect that its use will stimulate further development of suitable goal formulation. The use of the objective function can be extended beyond control system evaluation, by using it more directly in controller design, using optimisation as outlined in this thesis.

Minimisation of individual plant operational costs neglects total impacts from the wastewater system and consequently leads to suboptimal solutions. An alternative is to apply an integrated approach that employs water quality oriented instead of emission based goals and that considers the whole wastewater system. Application of artificial, fixed setpoints or weight factors can be abandoned in such an approach. Such an approach may be feasible if the following approach is adopted. For receiving waters, generally a limited set of quality objectives can be selected, so that the required problem complexity is limited. Development of goal oriented models and decomposition into timescales will further reduce model and computational complexity.

Controlled variable selection is currently too heuristic. Models like ASM1 are helpful to obtain insight in relationships between process variables and process performance and should be more fully exploited to guide in selecting appropriate controlled variables.

Modelling

Calibration procedures of activated sludge models must be further developed if better extrapolation is desired. The role of transport model calibration in activated sludge plant calibration needs further attention. Transport and kinetics can be calibrated separately. For example, kinetics can be determined from optimally designed experiments in ideally-mixed lab-scale reactors, such as respirometers. For transport models, a combination of computational fluid dynamics, empirical relationships and tracer responses can be applied. Input/output measurements on full-scale can subsequently be used for fine-tuning.

Practical identifiability analysis based on the Fisher information matrix is a useful tool for selection and design of additional experiments for ASM1 calibration. For example, using the condition number, one might select to develop tests for determining those parameters that have the strongest interaction with the parameters identified from full-scale plants.

Model reduction

A model-based control approach that employs the process dynamics for economic optimisation requires internal control models that describe a larger operational range. This imposes stronger requirements with respect to model validity than operating with fixed setpoints. For possible future application of nonlinear MPC, reduced and identifiable nonlinear models are desired.

Model reduction will remain an active research area in the next years, for application in control, identification and process optimisation. Many activated sludge systems are of the plug-flow type. An interesting research area is model reduction of distributed systems, for example carrousels with gradients in the dissolved oxygen concentration. In almost all reported cases of ASM1 reduction, the reduction was applied to lumped systems without concentration gradients, assuming the system either aerobic or anoxic. In these cases, reduction concentrated on reduction of the reaction kinetics, rather than reduction of transport and mixing in the reactor.

Singular perturbation is a useful theory for model reduction studies. The procedure for timescale estimation of variables is a helpful tool for model reduction. It would be interesting to apply the procedure to the full ASM1 and its successors.

Controller design

In controller design, the great merit of models is that they enable application of an analytic design procedure by applying mathematical optimisation. This is possible despite the limitations of calibrated models. Even if the implemented controller is not model-based, then still a model-based design procedure offers significant advantages. We will now outline several options to apply optimisation and models, which are better or worse approximations of the actual problem.

First consider off-line application. If no model is available, precise formulation of system specifications into a mathematical optimisation criterion has a value in its own right as a performance measure, as this enables a more objective judgement of performance.

If reliable mechanistic models are available, mathematical optimisation can be applied. If a well-calibrated and validated model would be available, the result would be a tuned controller that can directly be used on the real plant. Due to the limitations of ASM1 calibration, this is generally not the case. Instead, only an approximate model is available. Still, such an approximate model can be used to study controller design and to compare different controller types and tuning procedures. Some approaches to apply optimisation are listed.

One possibility is single criterion optimisation. Dynamic optimisation with known disturbances will lead to optimal performance (under the assumed disturbances) that provides a reference for other, suboptimal approaches. One such suboptimal approach is parameter optimisation of fixed structure controllers, using the actual criterion. Another suboptimal approach is to approximate the problem as a linear control design problem.

Multi-criterion optimisation is useful for trade-off analysis, to determine suitable weight factors or constraints for on-line application. As this typically requires user interaction, this is limited to off-line application.

For on-line optimisation, standard linear MPC with constraints is the simplest option, while adaptive nonlinear MPC can give better performance as it better approximates the actual performance optimum. For economic operation over a larger range, some form of nonlinear MPC is required. Adaptation may lead to additional performance improvement. Its application to distributed systems requires suitable reduced models however.

An interesting option for MPC development is to develop MPC for stiff systems such as activated sludge plants. It would be interesting to apply singular perturbation theory to decompose the optimal control problem into slow and fast sub-problems. This allows a *divide*

et impera strategy with optimal results. The required theory is available and has been developed for greenhouse climate control, a problem that also has slow process dynamics and fast disturbances (van Henten, 1994).

Advantages of advanced, model-based controllers over simple rule-based controllers remain to be studied further. Besides for nominal performance, different control techniques and design approaches should be compared for robustness against model mismatch due to structural and parametric uncertainty, for sensitivity towards suboptimal tuning and for constraint handling. Such a study should also indicate which of the approximating design procedures is best. Here model studies will again be invaluable.

Appendix A Activated Sludge Model No. 1

On the next page, the stoichiometry matrix and the reaction rates as defined in Activated Sludge Model No. 1 (Henze *et al*., 1987) are given in matrix notation. The columns hereby represent the model components, the rows the processes that are distinguished in the model. The net reaction rate for each component is obtained by summation over the respective column.

The Task Group preferred to use COD for modelling for the following reasons. The COD is superior as it provides a link between electron equivalents in the organic substrate, the biomass and the oxgen utilized. Its use simplifies the stoichiometric coefficients and reduces the number of conversion factors required. Component balances can be checked for correctness by a continuity check. It allows calculating the oxygen requirement by a simple COD balance (Henze *et al*., 1987, 1987a).

Component → i / j Process ↓		1 S_I	2 S_S	3 X_I	4 X_S	5 X_{BH}	6 X_{BA}	7 X_P	8 S_O	9 S_{NO}	10 S_{NH}	11 S_{ND}	12 X_{ND}	13 S_{ALK}	Process Rate ρ_j
1	Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\mu_H \frac{S_S}{K_S+S_S}\frac{S_O}{K_{OH}+S_O}X_{BH}$
2	Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14\cdot 2.86Y_H}-i_{XB}/14$	$\mu_H \frac{S_S}{K_S+S_S}\frac{K_{OH}}{K_{OH}+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}\eta_g X_{BH}$
3	Aerobic growth of autotrophs						1		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\mu_A \frac{S_{NH}}{K_{NH}+S_{NH}}\frac{S_O}{K_{OA}+S_O}X_{BA}$
4	'Decay' of heterotrophs				$1-f_P$	-1		f_P					$-i_{XB}-f_P i_{XP}$		$b_H X_{BH}$
5	'Decay' of autootrophs				$1-f_P$		-1	f_P					$-i_{XB}-f_P i_{XP}$		$b_A X_{BA}$
6	Ammonification of soluble organic nitrogen										1	-1			$k_a S_{ND} X_{BH}$
7	Hydrolysis of entrapped organics		1		-1										$k_h \frac{X_S/X_{BH}}{K_S+X_S/X_{BH}}[\frac{S_O}{K_{OH}+S_O}+\eta_h\frac{K_{OH}}{K_{OH}+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}]X_{BH}$
8	Hydrolysis of entrapped organic nitrogen											1	-1		$\rho_7(X_{ND}/X_S)$
		Soluble inert inorganic matter	Readily biodegradable substrate	Particulate inert inorganic matter	Slowly biodegradable substrate	Active heterotrophic biomass	Active autotrophic biomass	Particulate inert products from decay	Dissolved oxygen	Nitrate and nitrite nitrogen	Ammonia and ammonium nitrogen	Soluble biodegradable organic nitrogen	Particulate biodegradable organic nitrogen	Alkalinity (molar units)	

Appendix B Simulation Model Description

The plant that was used to produce Figure 2.7 approximates a carrousel. The aerated part is modelled by 2 CSTRs in series, the anoxic part by 3 CSTRs in series (see Figure B.1). There is a large internal recycle.

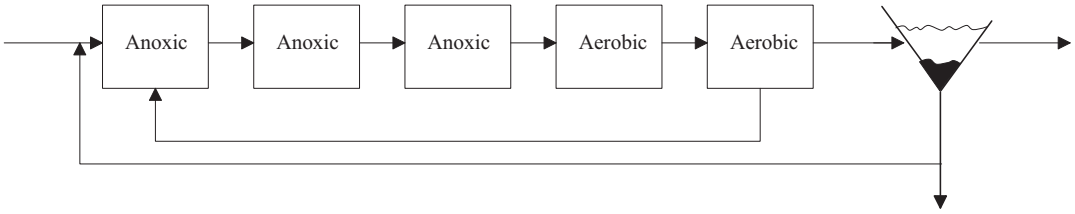

Figure B.1: Plant flow-scheme

Transport-physical model

Volume:	V :	10 000 m^3	(each reactor 2000 m^3)
Flows:	$Q_{in} = Q_r$:	10 000 m^3/d	
	Q_{ic} :	1000 000 m^3/d	
	Sludge age :	15 d	

The DO concentrations in the two aerobic reactors are controlled at the same setpoint.

Biokinetic model

Influent concentrations and characterisation into components:

Influent concentrations:

COD :	507.7	(kg m^{-3})
BOD	200.8	(kg m^{-3})
Nkj :	51.0	(kg N m^{-3})
NH_4-N :	40	(kg N m^{-3})

Influent characterisation into model components:

S_S :	46.7	Readily biodegradable COD	(kg m^{-3})
S_I :	32.9	Soluble inert COD	(kg m^{-3})
S_{NH} :	40.0	Ammonia and ammonium	(kg N m^{-3})
S_{NO} :	0	Nitrite and nitrate	(kg N m^{-3})
S_{ND} :	2.47	Soluble biodegradable organic N	(kg N m^{-3})
S_{ALK} :	5	Alkalinity	(Mol m^{-3})
S_O :	0.01	Dissolved oxygen	(kg m^{-3})
X_{BH} :	70.6	Heterotrophic biomass	(kg m^{-3})
X_{BA} :	0.1	Active autotrophic biomass	(kg m^{-3})
X_S :	234.0	Slowly biodegradable COD	(kg m^{-3})
X_I :	123.1	Particulate inert COD	(kg m^{-3})
X_{ND} :	0.03	Particulate biodegradable org. N	(kg N m^{-3})
X_P :	0	Particulate COD from decay	(kg m^{-3})

ASM1 parameters:

Stoichiometric parameters:

Y_H :	0.67	Heterotrophic yield	(-)
Y_A :	0.24	Autotrophic yield	(-)
f_p :	0.08	Fraction biomass yielding inert products	(-)
i_{xb} :	0.04	Fraction N in biomass	(kg N/kg COD)
i_{xp} :	0.04	Fraction N in inert products	(kg N/kg COD)

Kinetic parameters:

μ_H :	4	Heterotrophic growth rate constant	(d^{-1})
b_H :	0.62	Heterotrophic decay rate constant	(d^{-1})
K_S :	20	Affinity constant for S_S	(kg m^{-3})
K_{OH} :	0.25	Heterotrophic affinity constant for S_O	(kg m^{-3})
K_{NHH} :	0.1	Heterotrophic affinity constant for S_{NH}	(kg m^{-3})
K_{ALKH} :	0.1	Heterotrophic affinity constant for S_{ALK}	(mol m^{-3})
K_{NO} :	0.5	Affinity constant for S_{NO}	(kg m^{-3})
η_g :	0.8	Correction factor for anoxic growth	(-)
μ_A :	1.0	Autotrophic growth rate constant	(d^{-1})
b_A :	0.15	Autotrophic decay rate constant	(d^{-1})
K_{OA} :	0.5	Autotrophic affinity constant for S_O	(kg m^{-3})
K_{NHA} :	0.8	Autotrophic affinity constant for S_{NH}	(kg m^{-3})
K_{ALKA} :	0.25	Autotrophic affinity constant for S_{ALK}	(Mol m^{-3})
k_h :	2.4	Hydrolysis rate	(d^{-1})
K_x :	0.02	Hydrolysis affinity constant	(kg m^{-3})
η_h :	0.4	Correction factor for anoxic hydrolysis	(-)
k_a :	0.08	Ammonification rate	(d^{-1})

The following parameters were assumed temperature dependent with temperature dependency coefficients as follows:

μ_H b_H k_h K_x k_a	0.067
μ_A b_A	0.098
K_{NHA}	0.117

The temperature dependency is described according to (Gujer, 1985):

$$p(T) = p20*\exp((T-20)*f_{T,p}$$

with:
- p(T) : parameter at temperature T (in ºC)
- p20 : parameter value at 20 ºC
- $f_{T,p}$: temperature dependency coefficient for parameter p

The plots in Figure 2.7 were produced by performing simulations during 250 days to approximate steady-state. It was checked that the approximation was sufficiently accurate, which was the case. The steady-state concentrations of the ASM1 components were computed for a range of DO setpoints at 12 ºC and 8.4 ºC, from which plots 2.7.a and b were made, respectively. These temperatures were chosen such that at the lower temperature the minimal total effluent N concentration is 10 mg-N/l and thus meets the demands (at least in steady-state).

The sludge concentrations at the different DO setpoints were also computed to test if these were realistic and to check whether the sludge concentration difference between the two temperatures were not too different. The results are given in Figure B.1, which shows that the concentrations are comparable.

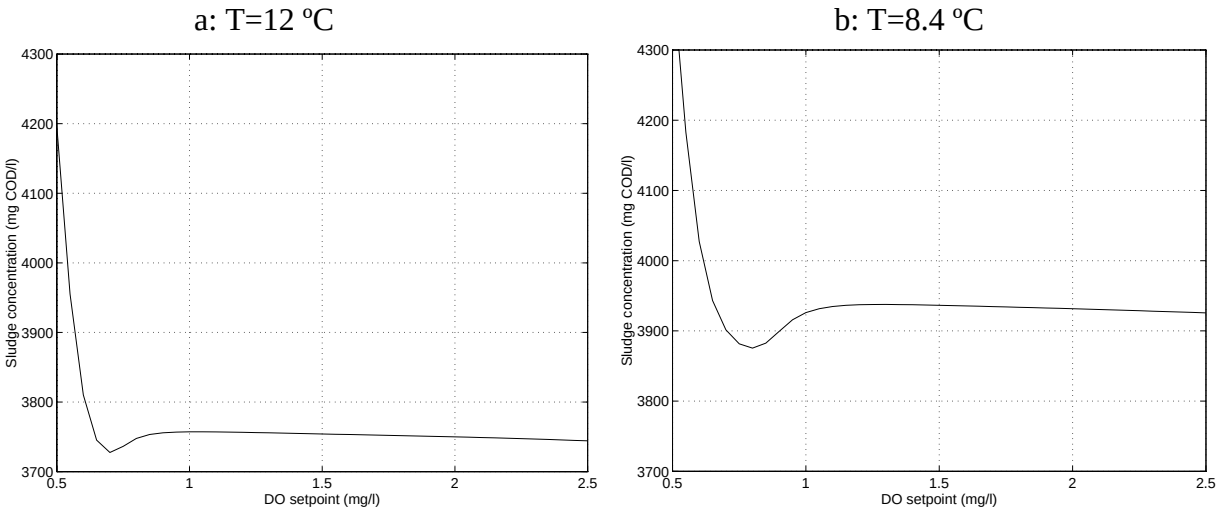

Figure B.1: Sludge concentration at different temperatures

It would be interesting to perform this type of studies under dynamic loading conditions, but this is beyond the scope of this thesis.

Appendix C Causes of ASM1 identifiability problems

This appendix indicates a few reasons why identifiability problems can be expected when calibrating Activated Sludge Model No. 1.

One reason is that Monod kinetics is applied for dependency of the growth rate on the concentrations of limiting substrates (Monod, 1942):

$$\mu = \mu_{max} \frac{S}{K_S + S} \tag{C.1}$$

The model parameters of Monod kinetics are the maximum growth rate and the affinity constant for the limiting substrate(s). These parameters are known to be poorly practically identifiable. Some important results from the literature are summarised here to support this claim.

If biomass and substrate measurements are available, the Monod model is theoretically identifiable (Aborhey and Williamson, 1978) (see Section 3.2.3 for a definition of theoretical or structural identifiability), but was found to be poorly practically identifiable (Holmberg and Ranta, 1982). They showed that different parameter combinations were obtained when estimating Monod parameters from a model response onto which different noise sequences were added. They concluded that 'the meaningfulness of comparing parameters and using them as biological characteristics should be critically reconsidered'.

It is emphasised that the practical identifiability problems occurred if the experiments were set up such that the substrate concentration was larger that the affinity constant. If this would not be the case, then Monod kinetics reduces to first order kinetics. Only the ratio μ/K_S can then be estimated, from which of course the separate parameters are not identifiable.

Dochain *et al.* (1995) studied theoretic identifiability of Monod kinetics (amongst others) when using only oxygen uptake rate data, which is the case when repirtomtry is used todetermine these parameters. They showed that three combinations of the five original parameters are theoretically identifiable.

Subsequently, practical identifiability of the Monod parameters was studied under the assumption that the yield, the initial substrate concentration and the biomass concentration are known. A contour plot of the object functional's (sum of squared errors) shape clearly indicated practical identifiability problems. This was also clear from the Fisher information matrix in the optimum and its trace and condition number. The practical identifiability could be improved significantly by an additional substrate pulse at the end of the batch experiments. The moment of pulse addition was determined by optimal experiment design techniques.

The model components for COD are only conceptual, and cannot be measured directly. This significantly complicates determination of model parameters of individual processes in the model.

Another reason for occurrence of identifiability problems is the fact that the model contains several loops, because of the death-regeneration concept. It is not possible to directly measure all the individual model components in these loops. For example, when using respirometry, the total loop effect is measured. Individual process rates and parameters can only be determined through careful experimental design. For example, through looking at different timescales, different processes may be identified.

For the very slow timescale in the order of days, this was done in Section 4.5 for the heterotrophic, aerobic death-regeneration cycle. Also short-term experiments have been designed to extract specific information from batch tests, see Spanjers and Vanrolleghem (1995) and the discussion in Section 3.2.2.

A final cause of possible identifiability problems is that the concentration of several components is the net result of several processes, e.g. production and consumption. An example is the nitrate concentration that is the result of nitrification and denitrification. If these two processes are separated in place or in time, then the course in time of the nitrate concentration is informative for each of these processes. With simultaneous denitrification, this is not the case. Separate additional experiments then must be designed to obtain the required information. A similar situation occurs for the DO concentration, which is determined by aeration on one hand and consumption on the other hand. See for example Holmberg and Olsson (1985) and Sollfrank and Gujer (1990) as efforts to estimate both the oxygen transfer rate and the oxygen uptake rate from DO measurements.

Identifiability is required for (classical) point estimation of parameters. It can be argued that, especially for prediction of ill-defined systems with complex models, regional parameter estimation techniques that make estimates of parameter distributions instead of values are preferable, and that Bayesian techniques may be even better (Omlin and Reichert, 1998). The computational requirements for such Bayesian estimation are very large and typically require Monte-Carlo simulation, usually according to a Latin Hypercube Sampling scheme for computational efficiency. Bayesian estimation is therefore less suited for on-line application such as in adaptive control. A procedure to reduce computational requirements by combining classical estimation with Bayesian techniques has been suggested by Reichert and Omlin (1997). More research is required to reveal if such a combined procedure will eventually be suitable for on-line use for control of activated sludge plants.

Figure C.1: Death-regeneration loops in ASM1

Component → i / j Process ↓		4 X_S	2 S_S	5 X_{BH}	8 S_O	6 X_{BA}	10 S_{NH}	11 S_{ND}	12 X_{ND}	9 S_{NO}	1 S_I	3 X_I	7 X_P	13 S_{ALK}	Process Rate ρ_j
7	Hydrolysis of entrapped organics	-1	1												$k_h \frac{X_S / X_{BH}}{K_S + X_S / X_{BH}} [\frac{S_O}{K_{OH} + S_O} + \eta_h \frac{K_{OH}}{K_{OH} + S_O} \frac{S_{NO}}{K_{NO} + S_{NO}}] X_{BH}$
1	Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$	1	$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$							$-\frac{i_{XB}}{14}$	$\mu_H \frac{S_S}{K_S + S_S} \frac{S_O}{K_{OH} + S_O} X_{BH}$
2	Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$	1			$-i_{XB}$			$-\frac{1-Y_H}{2.86Y_H}$				$\frac{1-Y_H}{14 \cdot 2.86Y_H} - i_{XB}/14$	$\mu_H \frac{S_S}{K_S + S_S} \frac{K_{OH}}{K_{OH} + S_O} \frac{S_{NO}}{K_{NO} + S_{NO}} \eta_g X_{BH}$
4	'Decay' of heterotrophs	$1-f_P$		-1					$-i_{XB} - f_P i_{XP}$				f_P		$b_H X_{BH}$
5	'Decay' of autootrophs	$1-f_P$				-1			$-i_{XB} - f_P i_{XP}$				f_P		$b_A X_{BA}$
3	Aerobic growth of autotrophs				$-\frac{4.57-Y_A}{Y_A}$	1	$-i_{XB} - \frac{1}{Y_A}$			$\frac{1}{Y_A}$				$-\frac{i_{XB}}{14} - \frac{1}{7Y_A}$	$\mu_A \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_O}{K_{OA} + S_O} X_{BA}$
6	Ammonification of soluble organic nitrogen						1	-1							$k_a S_{ND} X_{BH}$
8	Hydrolysis of entrapped organic nitrogen							1	-1						$\rho_7 (X_{ND} / X_S)$

Symbols

ASM1 symbols

Stoichiometric parameters:

Y_H ::	Heterotrophic yield	(-)
Y_A ::	Autotrophic yield	(-)
f_p ::	Fraction biomass yielding inert products	(-)
i_{xb} ::	Fraction N in biomass	(kg N/kg COD)
i_{xp} ::	Fraction N in inert products	(kg N/kg COD)

Kinetic parameters:

μ_H ::	Heterotrophic growth rate constant	(d^{-1})
b_H ::	Heterotrophic decay rate constant	(d^{-1})
K_S ::	Affinity constant for S_S	(kg m^{-3})
K_{OH} ::	Heterotrophic affinity constant for S_O	(kg m^{-3})
K_{NHH} ::	Heterotrophic affinity constant for S_{NH}	(kg m^{-3})
K_{ALKH} ::	Heterotrophic affinity constant for S_{ALK}	(mol m^{-3})
η_g ::	Correction factor for anoxic growth	(-)
μ_A ::	Autotrophic growth rate constant	(d^{-1})
b_A ::	Autotrophic decay rate constant	(d^{-1})
K_{OA} ::	Autotrophic affinity constant for S_O	(kg m^{-3})
K_{NHA} ::	Autotrophic affinity constant for S_{NH}	(kg m^{-3})
K_{NO} ::	Affinity constant for S_{NO}	(kg m^{-3})
K_{ALKA} ::	Autotrophic affinity constant for S_{ALK}	(Mol m^{-3})
k_h ::	Hydrolysis rate	(d^{-1})
K_x ::	Hydrolysis affinity constant	(kg m^{-3})
k_a ::	Ammonification rate	(d^{-1})
η_h ::	Correction factor for anoxic hydrolysis	(-)

Components:

S_S ::	Readily biodegradable COD	(kg m^{-3})
S_I ::	Soluble inert COD	(kg m^{-3})
S_{NH} ::	Ammonia and ammonium	(kg N m^{-3})
S_{NO} ::	Nitrite and nitrate	(kg N m^{-3})
S_{ND} ::	Soluble biodegradable organic N	(kg N m^{-3})
S_{ALK} ::	Alkalinity	(Mol m^{-3})
S_O ::	Dissolved oxygen	(kg m^{-3})
X_{BH} ::	Active heterotrophic biomass	(kg m^{-3})
X_{BA} ::	Active autotrophic biomass	(kg m^{-3})
X_S ::	Slowly biodegradable COD	(kg m^{-3})
X_I ::	Particulate inert COD	(kg m^{-3})
X_{ND} ::	Particulate biodegradable org. N	(kg N m^{-3})
X_P ::	Particulate COD from decay	(kg m^{-3})

Other symbols:

BOD_5 ::	Biological Oxygen Demand measured after 5 days	(kg m^{-3})
BOD_{st} ::	Short term BOD	
COD_{BD} ::	Biodegradable COD	
F	Flow rate	
G ::	Generalised plant	
K ::	Controller	
k_La ::	Mass transfer rate for oxygen	
M ::	Fisher Information Matrix	
N_{KJ} ::	Kjeldahl nitrogen concentration	(kg N m^{-3})
NH_4 ::	Ammonia	(kg N m^{-3})
NO_3 ::	Nitrate	(kg N m^{-3})
Ntot ::	Total nitrogen	(kg N m^{-3})
OUR ::	Oxygen Uptake Rate	(kg O_2 m^{-3} d^{-1})
p ::	number of parameters	
Q_{ic} ::	internal recirculation flowrate	(m^3 d^{-1})
Q_k ::	measurement error covariance matrix	
Qr ::	sludge recycle flowrate	(m^3 d^{-1})
Q_w ::	sludge wastage flowrate	(m^3 d^{-1})
R_k ::	weighting matrix	
u ::	manipulated variables	
V ::	Volume	(m^3)
V_{aer} ::	aerobic volume	(m^3)
w ::	weight factors	
w ::	external inputs to general system	
y ::	output (column vector)	
y_p ::	measured output (column vector)	
y ::	measured variables	
z ::	external outputs	

Greek symbols:

Δ ::	Model uncertainty
α ::	influent flow distribution
β ::	return sludge flow distribution
λ ::	eigenvalue
μ ::	structured singular value
θ ::	parameter vector

Glossary

Terms

Activated sludge	Suspended material consisting of inert material, biodegradable material and active biomass. This active biomass degrades pollutants in wastewater.
Aerobic	With (abundant) oxygen
Anaerobic	Without oxygen or other inorganic electron acceptor
Anoxic	Without oxygen, with nitrate
Clarifier	Sedimentation tank in wastewater treatment system which separates sludge from wastewater
Mixed liquor	Liquid-sludge mixture in the activated sludge reactor

Acronyms

AI	Artificial Intelligence
AMvB	Algemene Maatregel van Bestuur (General Enactment of Administration)
ANN	Artificial Neural Network
ASM1	Activated Sludge Model No. 1
ASM2	Activated Sludge Model No. 2
ASM3	Activated Sludge Model No. 3
ASP	Activated Sludge Plant
ATU	Allylthioureum, a nitrification inhibitor
BNR	Biological Nitrogen Removal
BOD	Biological Oxygen Demand
COD	Chemical Oxygen Demand
CSD	Control System Design
CSO	Combined Sewer Overflow
CSTR	Continuous Stirred Tank Reactor
DMC	Dynamic Matrix Control, MPC based on step responses
DO	Dissolved Oxygen
DOF	Degrees of freedom
ES	Expert System
FLC	Fuzzy Logic Control
GPC	Generalised Predictive Control
IAE	Integral of Absolute Error
IAWQ	International Association on Water Quality (formerly IAWPRC, now IWA)
ICA	Instrumentation, Control and Automation
IDCOM	Identification and Command (an MPC implementation)
ISE	Integral of Squared Error
LHS	Latin Hypercube Sampling
LQG	Linear Quadratic Gaussian
LQR	Linear Quadratic Regulator
LTI	Linear Time Invariant
MAMS	Multiple Actuator Multiple Sensor
MFD	Matrix Fraction Description
MIMO	Multiple Input Multiple Output
MISO	Multiple Input Single Output

MLSS	Mixed liquor suspended solids
M(B)PC	Model (Based) Predictive Control
NAP	North Sea Action Program
NVA	Dutch Society for Water Quality
ORP	Oxidation-Reduction Potential
OUR	Oxygen Uptake Rate
p.e.	Person Equivalent
PSSA	Psuedo-steady-state Assumption
QDMC	Quadratic Dynamic Matrix Control
QP	Quadratic Program
QSSA	Quasi-steady-state Assumption
RAP	Rhine Action Program
RAS	Return Activated Sludge
RB	Rule based
RHOC	Receding Horizon Optimal Control
SA	Sludge Age
SCOUR	Specific Oxygen Uptake Rate
SISO	Single Input Single Output
SIMO	Single Input Multiple Output
SQP	Sequential Quadratic Programming
SS	Suspended Solids
STOWA	Stichting Toegepast Onderzoek voor Water en Afvalwater
STP	Sewage Treatment Plant
SVI	Sludge Volume Index
TKN	Total Kjeldahl nitrogen
TOC	Total Organic Carbon
VSS	Volatile Suspended Solids
WWTP	Wastewater treatment plant

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Curriculum Vitae

3 juli 1961	Geboren te Utrecht
1973 – 1980	Gymnasium β aan het College Blaucapel te Utrecht
1980 – 1987	Studie Moleculaire Wetenschappen, oriëntatie Biotechnologie aan de Landbouwuniversiteit te Wageningen
september 1984	Kandidaats Milieuhygiëne, oriëntatie Waterzuivering (met lof)
mei 1986	Kandidaats Moleculaire Wetenschappen, oriëntatie Biotechnologie (met lof)
21 september 1987	Ingenieursdiploma Moleculaire Wetenschappen (met lof) Afstudeervakken: Proceskunde, Systeem- en Regeltechniek (bij de vakgroep Regeltechniek, Faculteit Elektrotechniek, TU Delft), Biochemie, Informatica (bijvak)
1988 – 1989	Vervulling militaire dienstplicht als ROAG officier. Gedetacheerd als wetenschappelijk vertaler Russisch bij TNO-PML
eind 1989	Toegevoegd onderzoeker bij de Sectie Proceskunde, LU Wageningen
1990	Milieuadviseur bij TAUW Infra Consult b.v. te Deventer
1991 – 1994	Wetenschappelijk medewerker bij TNO Technisch Physische Dienst, Delft
1994 – heden	Universitair docent bij de Vakgroep Systeem- en Regeltechniek, Faculteit Technische Natuurkunde, Technische Universiteit Eindhoven

In Anglo-American terms:

Stefan Weijers was born July 3, 1961 in Utrecht, The Netherlands. From 1973 until 1980, he went to secondary school at the College Blaucapel in Utrecht.

In 1980, he started studying Environmental Sciences, orientation Wastewater Engineering, at the Wageningen Agricultural University. After two years, he combined this study with Biotechnology, which was a new orientation within Molecular Sciences. He finished the bachelors of both studies (cum laude) and graduated cum laude in Biotechnology in September 1997 on three main Master's projects. The first thesis was on bioprocess engineering, the second thesis on biochemistry. The third thesis was on control of biotechnological processes. This project was carried out at the Control Laboratory of the Electrical Engineering Department of Delft University of Technology. An additional project was carried out on Computer Science.

After his studies, in 1988 he went into military service where he learned Russian at the School of the Military Intelligence Service to become scientific translator at TNO-PML. After military service, he worked several months at the Process Engineering section in Wageningen.

In 1990, Stefan Weijers worked about one year as environmental consultant at TAUW Infra Consult b.v. in Deventer. Then he joined TNO-ITP (later TNO-TPD) to work as a process control engineer. In 1994, he became assistant professor at the Systems and Control group of the Faculty of Applied Physics, Eindhoven University of Technology. His main research areas are modelling, identification and control of wastewater treatment plants, Model Predictive Control, process control and sustainable wastewater treatment.

Samenvatting

Huishoudelijk afvalwater wordt doorgaans biologisch gezuiverd in zogenaamde actief-slib installaties. Strengere wetgeving in de EG ten aanzien van nutriëntverwijdering bij afvalwaterzuivering vereist een verbeterde prestatie van actief-slib systemen. Deze moeten daarom worden aangepast om aan nieuwe lozingsnormen voor stikstof (N) te voldoen. Doel van dit proefschrift is het bestuderen van mogelijke prestatieverbeteringen van actief-slibsystemen door toepassing van wiskundige modellering en geavanceerde regeltechniek en het ontwikkelen van methodologieën om verbeterde procesprestatie te bereiken. De nadruk ligt op continu bedreven carrousel systemen en pre-denitrificatie systemen, omdat deze in Nederland het meest worden toegepast. Verschillende aspecten worden belicht aan de hand van achtereenvolgende stappen in regelsysteemontwerp, namelijk formulering van de regeldoelen, procesmodellering en –identificatie en regelaarontwerp.

Een literatuurinventarisatie toont dat onvoldoende inzicht bestaat in de relatie tussen wetgeving en regeldoelen. Indirecte en vage regeldoelen worden toegepast. Deze leiden tot tijdrovende ontwerpprocedures die gebaseerd zijn op trial-and-error en bemoeilijken beoordeling van ontworpen regelaars. De beschikbaarheid van geavanceerde modellering en regeltechniek pleit ervoor om systematische, doelgerichte ontwerpprocedures te ontwikkelen die gebaseerd zijn op wiskundige optimalisatie om zodoende de kloof tussen wetgeving en regeldoelen te dichten. Een dergelijke zogenaamde analytische ontwerpprocedure wordt gekenmerkt door wiskundige modellering van doelstellingen, verstoringen en procesgedrag en door inzet van mathematische optimalisatietechnieken. Hierbij worden kwalitatieve doelstellingen voor actief-slib procesvoering vertaald naar formulering als een (multi-criterium) optimalisatieprobleem. Afwegingen tussen verschillende doelstellingen en de keuze van de systeemgrenzen dienen zorgvuldig te geschieden voor een adequate doelstelling.

Voor toepassing van een analytische ontwerpprocedure voor regelsysteemontwerp zijn betrouwbare procesmodellen nodig, onder meer voor de evaluatie van het ontworpen regelsysteem. Modelvorming en identificatie worden daarom bestudeerd, in het bijzonder het IAWQ Actief Slib Model No. 1 (ASM1), dat de biologische reacties beschrijft. Om het gedrag van een praktijkinstallatie te beschrijven, is calibratie van modelparameters vereist. Hiervoor bestaan echter nog geen eenduidige standaardprocedures. Daarom wordt nagegaan of voldoende parameters kunnen worden geschat op basis van een realistische verzameling van in- en uitgangsmetingen aan praktijkinstallaties. Dit wordt onderzocht via analyse van de praktische identificeerbaarheid. Een gecombineerd criterium dat gebaseerd is op zowel de determinant als het conditiegetal van de Fisher informatie matrix blijkt hiervoor effectief. Zowel een locale als een globale identificeerbaarheidsanalyse is uitgevoerd voor een bepaalde installatie, onder de aanname dat het transportmodel dat de menging beschrijft perfect is. De resultaten tonen dat in- en uitgangsmetingen onvoldoende zijn voor het uniek schatten van alle benodigde ASM1 parameters en dat daarom additionele informatie nodig is. Een test om dergelijke aanvullende informatie te krijgen, namelijk voor het bepalen van de concentratie van biodegradeerbaar CZV (Chemisch Zuurstofverbruik) in het influent, een belangrijke grootheid voor de modellering, wordt daarom nader onderzocht en experimenteel getest.

Het volledige ASM1 model is minder geschikt voor identificatie, als intern model bij regeling en regelaarontwerp, vanwege de hoge orde, identificeerbaarheidsproblemen en stijfheid, dat is

het voorkomen van zeer uiteenlopende tijdschalen. Daarom wordt onderzocht in hoeverre modelreductie op basis van tijdschaalseparatie met singuliere perturbatietheorie mogelijk is. Drie procedures voor het testen of tijdschaalseparatie mogelijk is worden voorgesteld, namelijk tijdschaalschatting, directe schaling en analytische schaling. Deze procedures worden getest met een algemeen, eenvoudig, continu bioprocesmodel. De tijdschaalschatting blijkt een goed hulpmiddel voor modelreductie. Deze procedure is directer dan eigenwaarde analyse, omdat een niet-eenduidige toestand-eigenwaarde associatie niet nodig is en omdat de procedure tevens voorziet in een schatting van de fout die de reductie introduceert. De analytische schaling verschaft inzicht in de oorzaakvan het optreden van tijdschaalmultipliciteit. Deze procedure is echter slechts in een beperkt aantal gevallen succesvol en is minder algemeen toepasbaar. De directe schaling blijkt niet algemeen toepasbaar.
Voor de bovengenoemde test voor bepaling van biodegradeerbaar CZV is via een quasi-steady-state aanname een eerste-orde model afgeleid. Dit gereduceerde model verschaft inzicht en kwantitatieve relaties voor interpretatie van de test.

De volgende stap in regelsysteemontwerp is de regelaarstructuurselectie en het eigenlijke regelaarontwerp. Regelaarstructuurselectie omvat in-/uitgangsselectie (de selectie van actuatoren en sensoren) en de regelaarconfiguratie (de interconnecties ertussen).

Voor in-/uitgangsselectie voor regeling van actief-slibsystemen is een basale modelanalyse waarschijnlijk voldoende, wanneer eenmaal een goede selectie van te regelen grootheden is gedaan. Selectie van te regelen grootheden is een moeilijker stap. Een mogelijke methodologie voor deze selectie gebruikt de minimale singuliere waarde van de overdrachtsmatrix, die bijvoorbeeld met een model op basis van ASM1 wordt gemaakt. Wat betreft de regelaarconfiguratie wordt opgemerkt dat in het actief-slibproces meerdere interacties optreden. In hoeverre multivariabele regeling nodig is gezien vanuit het perspectief van de uiteindelijke doelstellingen dient echter nog te worden vastgesteld.

Het eigenlijke regelaarontwerp, met name de regelwetselectie, wordt onderzocht met Model Predictive Control als een prototype regeling. MPC voert on-line optimalisatie uit, en is zeer geschikt om realistische optimalisatieprolemen onder beperkingen aan te pakken. Lineaire MPC met beperkingen op de ingangen wordt toegepast op een model van een pre-denitrificatiesysteem en van een carrousel. In beide systemen deden zich stabiliteitsproblemen voor ten gevolge van discrepantie tussen model in de regelaar en model van het te regelen systeem. De resultaten tonen dat MPC met een niet-lineair model beter geschikt is voor economisch bedrijf omdat het interne model dan over een groter bereik geldig is. Daarnaast pleit de tijd-variantie van het proces voor het toepassen van adapterende regelsystemen. Om de noodzaak van niet-lineaire regeling en adapterende regeling na te gaan, is robuustheid van MPC geregelde systemen onder parameter- en toestandonzekerheid onderzocht. Hiervoor is een eenvoudig procesmodel gebruikt en is een gestructureerd onzekerheidsmodel opgesteld en mu-analyse toegepast. De resultaten toonden dat vooral fouten ten gevolge van linearisatie bepalend zijn voor het optreden van instabiliteit. Daarom dient ontwikkeling van niet-lineaire regeling prioriteit te hebben boven parameteradaptatie. Deze conclusies worden echter met enige reserve getrokken vanwege de conservativiteit in de robuustheidsanalyse.

Bij de huidige stand van kennis in modellering van actief-slib systemen dient men absolute, kwantitatieve conclusies te vermijden wanneer men deze baseert op modellen die gecalibreerd zijn met bestaande calibratiestrategieën. Deze resulteren namelijk niet in unieke parameterwaarden, zodat de fysische interpretatie van de parameters onduidelijk is en daardoor de predictienauwkeurigheid van het model beperkt is. Verdere ontwikkeling is nodig van methodologieën voor calibratie van ASM1 of andere actief-slibmodellen. Dit is ook het geval

voor ontwikkeling en calibratie van transportmodellen, in het bijzonder voor carrousels en andere gedistribueerde systemen.

Modellen zoals ASM1 zijn ondanks deze genoemde beperkingen uiterst nuttige hulpmiddelen voor het ontwikkelen van directere procedures voor regelaarontwerp. In combinatie met wiskundige optimalisatietechnieken bieden ze een referentiepunt voor haalbare procesprestatie en maken een eenduidige beoordeling mogelijk van het effect van alle ontwerpstappen en van modelonzekerheid op de totale procesprestatie. Daarmee zijn modellering en optimalisatie van onschatbare waarde om tot procesverbetering te komen en om te beslissen over geschikte regelstrategieën.

STELLINGEN

behorende bij het proefschrift

Modelling, Identification and Control of Activated Sludge Plants for Nitrogen Removal

van

Stefan Weijers

Eindhoven, 20 juni 2000

1. Toepassing van modelgebaseerde regeling en een systematische ontwerpprocedure op basis van mathematische optimalisatie is een veelbelovende weg om de doelstellingen voor regeling van actief-slib systemen dichter bij de werkelijke doelstellingen, bijvoorbeeld economische, te kiezen en zodoende tot een verbetering van de totale systeemprestatie te komen.

   Dit proefschrift, Hoofdstuk 2.

2. Indien men modelparameters identificeert met het doel om een bestaande praktijkinstallatie te beschrijven met gebruikmaking van Actief Slib Model No. 1, bijvoorbeeld ten behoeve van procesanalyse en/of regelaarontwerp, dan dient men dit te doen op basis van het gemeten in-/uitgangsgedrag van de betreffende installatie, om zodoende het menggedrag van de betreffende installatie te verdisconteren in het model. Omdat bij deze werkwijze echter de biologische parameters oneigenlijk worden gebruikt, verdient het in plaats van deze werkwijze de voorkeur om meer aandacht te besteden aan het menggedrag dan tot dusver gebruikelijk is en dit expliciet experimenteel te bepalen en te identificeren.

   Dit proefschrift, Hoofdstuk 3.

3. Bij parameteridentificatie van Actief Slib Model No. 1 is het aan te bevelen de opbrengstcoëfficiënt van de heterotrofe biomassa niet, zoal wel gesuggereerd wordt, bekend te veronderstellen, maar te schatten uit gemeten in-/uitgangsgedrag van de te identificeren installatie. Hiermee worden afwijkingen in schattingen van andere parameters ten gevolge van een onjuiste waarde van de opbrengstcoëfficiënt vermeden.

   Dit proefschrift, Hoofdstuk 3.

4. Het toepassen van een probabilistische benadering bij regelaarontwerp is voor veel systemen een realistischer benadering om regelsystemen te ontwerpen die robuust zijn voor parametersonzekerheid dan H_∞-optimaal regelaarontwerp en μ-synthese, omdat deze de conservativiteit van de worst-case benadering in laatstgenoemde methoden en de daarmee gepaard gaande prestatiedegradatie vermijdt. Een worst-case benadering kan wel een adequate benadering zijn indien absolute garanties geëist worden ten aanzien van systeemgedrag onder onzekerheid, bijvoorbeeld vanuit het oogpunt van veiligheid.

   M Vidyasagar (1997) *Statistical learning theory and its applications to randomized algorithms for robust controller synthesis,* Proceedings European Control Conference 1997, pp.162-189.

   Y. Boers (1998) *Average Performance Control for Systems with Parametric Uncertainty,* Proefschrift, Vakgroep TU Eindhoven.

5. Het is opvallend dat veel regeltechnische problemen die in het verleden ofwel als triviaal werden beschouwd ofwel als wetenschappelijk niet interessant (vaak te moeilijk), inmiddels flinke wetenschappelijke belangstelling genieten. Dit is bijvoorbeeld gebeurd voor regelen van systemen onder beperkingen en voor hybride discrete-event / continue systemen. Te verwachten valt dat dit ook gaat gebeuren onder meer voor het ontwerp van fout-tolerante systemen zoals reconfigureerbare regelsystemen, welke ook grotere processtoringen zoals sensoruitval kunnen opvangen. Dit geldt eveneens voor de verdere ontwikkeling van

software gericht op integratie van modelvorming, simulatie en regelsysteemontwerp voor complexe systemen in diverse applicatiegebieden, om hiermee het modellerings- en regelaarontwerpproces te verbeteren, zowel qua snelheid als qua eenduidigheid en consistentie.

J. Maciejowski (1987) *Reconfigurable control using constrained optimization*, Proceedings European Control Conference 1997, pp.107-130.

F.E. Cellier (1996) *Object-oriented modelling: means for dealing with system complexity*, Proc. 16th Benelux Meeting on Systems and Control, March 6-8, 1996, Mierlo, The Netherlands, pp.53-64.

H.A. Preisig (1994) *MODELLER -- A Computer-Aided Modelling tool*, FOCAPD 94; Snow-mass, Colorado.

6. Binnen het regeltechnisch onderwijs zou er, naast het beheersen en begrijpen van diverse technieken, meer aandacht moeten zijn voor de beperkingen van huidige ontwerpmethoden en voor het belang om product- of processpecificaties te vertalen naar regeltechnische specificaties, de regeldoelstelling.

7. Terwijl op korte en middellange termijn het optimaliseren van bestaande waterzuiverings-installaties en afvalwatersystemen een goede weg is voor het verbeteren van de waterkwaliteit, is het voor de lange termijn belangrijk om grondig te onderzoeken of decentrale, kleinschalige waterzuivering niet een duurzamer optie is, onder meer met het oog op eindigheid van fosfaatvoorraden. Essentieel hierbij is een juiste keuze van systeemgrenzen en van het begrip duurzaamheid. Multi-criterium optimalisatie kan ook voor dit probleem een nuttig hulpmiddel zijn om tot een transparante afweging van alternatieven te komen.

   A.J. Balkema, S.R. Weijers and A.J.D. Lambert (1998) *On methodologies for comparison of wastewater treatment systems with respect to sustainability*, Proc. International WIMEK congress 'Options for closed water systems: sustainable water management', Wageningen, The Netherlands, March 11-13, 1998.

8. Het gebruik van de term 'afvalwater' geeft een attitude aan welke historisch is gegroeid. Het produceren van 'afvalwater' dient te worden vermeden door de afzonderlijke waardevolle componenten niet door menging nutteloos te maken voor hergebruik. Om een verandering in attitude te stimuleren is tevens een alternatief gewenst voor de term 'afvalwaterzuivering', bijvoorbeeld 'water- en mest kringloopsluiting'. Voordat dit laatste echter positieve associaties oproept zullen grote veranderingen in de landbouwsector noodzakelijk zijn.

9. Galileo Galilei beschouwde wiskunde als een gids die hem hielp de bewegingen van hemellichamen te begrijpen. Voor het hanteren van wiskundige modellen als gids moet de gebruiker echter goed doordrongen zijn van de uitgangspunten en beperkingen van het model, omdat deze modellen anders dwaalgids in plaats van leidgids zijn.

10. Water van voldoende kwaliteit is een eerste levenbehoefte van de mens en wordt een steeds schaarser goed. Om deze reden is het, bij een vrij marktmechanisme, te verwachten dat de

prijs zo hoog zal worden dat het voor een toenemend aantal mensen een onbereikbaar want onbetaalbaar goed wordt. Het is daarom naïef te denken dat hier heil van alleen marktwerking is te verwachten en zal de rol van overheden essentieel zijn, waarbij zij *op zijn minst* monopolievorming dienen te voorkomen.

11. Het toenemend gebruik van beeldschermwerk doordat steeds meer taken achter de PC kunnen worden uitgevoerd, de toenemende werkdruk en toenemende taakcomplexiteit vereisen een pro-actieve aanpak van RSI om te voorkomen dat een groot gedeelte van de toekomstige beroepsbevolking straks door deze ziekte geveld is. Investeringen in goede werkplekergonomie, inzet van spraakherkenningssoftware en ergonomische training en begeleiding van medewerkers dienen tegen deze achtergrond te worden bezien.

12. Zolang gewelddadige films als normaal vermaak worden beschouwd en al door kinderen worden bekeken, zijn overheidsacties tegen zinloos geweld dweilen met de kraan open.

13. Kleine stappen vooruit zijn ook stappen vooruit.

14. Beter is de vijand van goed.