A Pragmatic Approach to Wastewater Treatment Modelling: The Källby Wastewater Treatment Plant as a Case Study

Marco Fezzi

Water and Environmental Engineering
Department of Chemical Engineering
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Marco Fezzi

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Department of Chemical Engineering
Lund University

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Supervisor: **Professor Jes la Cour Jansen, Associate Professor Paola Foladori**
Co-supervisor: **Tobias Hey**
Examiner: **Associate Professor Åsa Davidsson**

Picture on front page: Källby WWTP. Photo by VA SYD.

Postal address	**Visiting address**	**Telephone**
P.O. Box 124	Getingevägen 60	+46 46-222 82 85
SE-221 00 Lund, Sweden		+46 46-222 00 00
Web address		**Telefax**
www.chemeng.lth.se		+46 46-222 45 26

Preface

The present master thesis is original, unpublished, independent work by the author, Marco Fezzi.

This last effort represents the conclusion of a two-years master program in Environmental and Land Engineering with focus on Reclamation and Managing of Environmental Resources at the University of Trento (Italy).

All of the work presented in this master thesis was conducted at Water and Environmental Engineering at Chemical Engineering department at Chemical Center (Lund University, Sweden) and was accomplished with the support of VA SYD.

It is the result of my experience as an exchange student there from September 2014 to February 2015. Coming to Lund represented the last part of my course of study.

Regarding the acknowledgements, first of all I would like to thank my family that gave me the chance to attend university and made my dream of completing my course of study abroad come true.

Secondly I would like to thank my co-supervisor Tobias Hey for his constant support and for providing me with relevant measured data from the VA SYD database, indispensable to carry out the project.

Thirdly I am really grateful to Jes la Cour Jansen and Paola Foladori for their support as supervisors and to Åsa Davidsson for her contributions as examiner of this thesis project: All of them promptly answered to my questions.

Fourthly I would like to thank Marika Murto, current process engineer at Källby wastewater treatment plant, for providing me with some relevant informations regarding the operation of some treatment units.

After I would like to appreciate Christoph and Carlos, my office mates at Chemical Center, that made time spent there more delightful, as well as all

the people that it was a pleasure to meet in the department.
Last, I thank also the University of Trento that provided me with a licence for WEST®, the software used to accomplish the present work.

Summary

The present study focused on the evaluation of the possibility of simulating the wastewater treatment lines at Källby wastewater treatment plant. The work was accomplished by the use of a commercial available software incorporating wastewater treatment models, WEST® by DHI.
It should be underlined that the thesis has not an advertising purpose, instead the intention was to use the software to achieve the scope of modelling.

To generate the inputs for the model, *i. e.* initial and boundary conditions, only available measurement were used, without any additional measurements campaigns.
Primary settlers, biological stage, secondary settlers, chemical precipitation and polishing steps were included in the used model. Activated sludge modelling was used to evaluate the treatment capacity for nitrogen removal and outputs from the model were compared with real measurements from the existing plant. Chemical precipitation was also simulated at the corresponding existing step.
First this was achieved by:

- Setting the size data (tanks volumes, areas, heights)
- Providing and fixing the correct flow data (incoming flow data series, correct partition between the treatment lines, correct amount of recycles, etc.)
- Feeding the software with the actual nutrient concentrations (*e.g.* carbon, nitrogen) and other boundary conditions (*e.g.* temperatures, TSS concentration in the activated sludge units, sludge volume index).

Secondly a troubleshooting step was performed. In this the mismatches between model and measurements outputs were analysed, discussed and

when possible solved. During this phase the actual plant operation was more deeply understood and the knowledge achieved was used to adjust the model settings.

To succeed in finding the best possible model, a trial and error approach with an iterative procedure was performed. Every time a relevant discrepancy between model outputs and measurement was found, causes were investigated and solutions found.

Two biological treatment lines were well represented by the model after the initial set-up, while the other two required a calibration stage to improve the match model-reality. After calibration the representation of these two lines improved.

Annual variation of the nitrogen and phosphorus concentration in the outlet of the plant are shown by the calibrated model.

Available data proved to be enough for the modelling of the wastewater treatment lines, especially regarding nitrogen removal in lines B1 and B2 and phosphorus removal.

The result of this thesis is a deeper understanding of the actual behaviour of the plant, allowing adjusting in operation of the plant, simulations and evaluations of new scenarios and possible future changes of the operation. Knowledge achieved in this work could also be used by plant operators to troubleshoot or to find better control strategies.

Contents

Introduction

General background on wastewater treatment

Sewage treatment is the removal of impurities from raw wastewater, which includes physical, chemical and biological processes (Tschobanoglous *et al.*, 2003) .

The wastewater treatment aims to achieve a treated effluent and a treated sludge. The first is a fluid waste that must be environmentally safe for the receiving water body and the second is a solid waste that must be safe for later reuse *e.g.* as a fertilizer. The distinction between clean water and polluted water is only based on the type and concentration of pollutants: Water is polluted when the concentration of certain pollutants is so high that it is unfit for particular usages *e.g.* drinking, bathing, fishing. The word pollution is usually connected to water usage by humans.

Oxygen depletion may occur if too large amount of organic substances are released in the effluent. The reason for this is that a lot of oxygen is consumed when the organic substances are decomposed. The low oxygen concentration has to be prevented, as it is a vital substance for many water organisms.

From a historical point of view, the first basic sewer systems were used for waste removal by Mesopotamia, Indus Valley, Crete, Greece and Romans ancient civilisations. The sewer systems fell into disuse in the middle ages and the wastes were collected in cesspools that were periodically unfilled and used as a fertilizer (therefore described as sanitary dark ages), as reported by Henze *et al.* (2008).

As reported by Ashton (1991), in the mid-nineteenth century the first modern sewage systems were built as a reaction to the aggravation of sanitary conditions caused by heavy urbanisation due to industrial revolution in London *e.g.* cholera outbreaks. In the latest nineteenth century the precursor of the

modern septic tank was discovered and the first experiments about filtration of sewage through porous gravel (forerunner of the modern contact bed) were conducted, leading to the modern concept of wastewater treatment, *i. e.* treating the effluent breaking it down biochemically (Melosi, 2010).

In the early twentieth century secondary treatment were developed and this brought significant improvement in public health and environment in urban areas. The first aerated sewage treatment in sequencing batch reactor were discovered and the process was named "activated sludge" (Benidickson, 2011). The process produced highly treated effluents, achieving a complete nitrification and subsequent understanding of the process and improvements in technologies made the activated sludge the most widespread treatment method.

Due to the further enlargement of the cities, the increase of the population and the necessity of preserving the self purification of natural streams, the removal efficiency of pollutants needed to be incremented. Furthermore,from the mid-twentieth century the role of nitrogen and phosphorus in eutrophication was clarified. In fact high nitrogen and phosphorus emissions can result in eutrophication of the receiving water body and cause algal bloom Therefore denitrification and phosphorus removal treatments were developed.

The understanding of wastewater treatment increased constantly during the twentieth century: Monod equation (1949) and bioenergetic principles developed by McCarty (1964) were basic for the comprehension of denitrification, carbon and nitrogen biological removal processes. For example by applying Monod equation, Downing *et al.* (1964) discovered that the sludge age has to be long enough in order to attain low ammonium in the effluent. Another fundamental step in developing of wastewater treatment were post-denitrification in an anoxic tank with addition of methanol (Wurhmann, 1964) and pre-denitrification (Ludzack and Ettinger, 1962).

Phosphorus removal was initially performed only by chemical precipitation and it is still the most commonly applied, but then biological phosphorus removal was developed and spread (van Haandlen *et al.*, 2012).

A whole range of new processes were developed to respond many different requirement such as the need for more compact treatment options, *e.g.* MBR, and energy saving technologies, *e.g.* anaerobic processes development.

In the latest decades, growing environmental awareness led to the consciousness that the developing of modelling and simulation of wastewater treatment is important. Moreover, increasing costs and scarcity of water drive to the study of innovative treatment technologies and approaches for reusing wastewater (Grau *et al.*, 2010). For this purpose models can be a worthwhile tool.

As a result, nowadays models are considered to be crucial for the design, operation and optimisation of wastewater treatment systems (Alalewi *et al.*, 2010). Furthermore it is a quick and inexpensive device. Furthermore, it is a valuable tool to evaluate different control strategies. In fact it is technically the most feasible and maybe least costly way of attaining a sustainable improvement in performance (Rustum *et al.*, 2012). It can help plant operator to test some corrective actions without the need to test them in pilot or full scale plant. Even with the limitation that calibration of wastewater treatment model is particularly hard, the application field for wastewater treatment models is promising. Therefore it was selected to deeply understand the wastewater inner processes in the case study.

Aim of the study

The present master thesis is a compilation of work regarding mathematical modelling of wastewater treatment.

The Master Thesis investigates the feasibility of setting up the Källby wastewater treatment plant into a dynamic wastewater treatment model by using a commercial software. The model is based only on the commonly available construction, operational and measured data, without performing specialized measuring campaigns for more accurate plant characterization .

The model outputs are compared with respect to the measurement in the outflow from the existing plant, in order to evaluate the quality of the model achievable only by using practical data.

Some research questions need to be answered by the present thesis:

- Are these data good enough to build up the model?
- How accurate is the simulation going to be?
- For what purpose can the achieved model serve?

The latter includes the evaluation of possible future applications of the model, such as assess whether the model is suitable just for educational purposes or also to *e.g.* process optimisation.

Furthermore it should be evaluated whether further measuring campaigns are needed, identifying which units and parameters in the treatment plant are more important to be investigated from this point of view.

Outline of the thesis

The present thesis is structured as follow:

Chapter 1 contains a literature overview about modelling of wastewater treatment modelling

Chapter 2 presents the actual Källby wastewater treatment plant layout and operation as a case of study

Chapter 3 concerns the methods followed to accomplish the model for the case of study, such as data treatment to create the needed input files

Chapter 4 shows the achieved results for a first set-up step and a following calibration of the model

Chapter 5 incorporates conclusions of the master thesis work

Chapter 6 contains suggestions for future works.

Chapter 1

Dynamic modelling of wastewater treatment plants with nitrogen removal

1.1 Pragmatic approach vs. scientific approach

Once the design of wastewater treatment plants was based on a pragmatic approach, *i. e.* a concept founded on the experience acquired from trial and error method to operate and design the plants. Such empirical model is based on the selection of the essential parameters to describe the behaviour of interest and establishing proper links through empirical relationships. In accordance with the observation-established black-box approach, the design of wastewater is based on recommended loading figures and rules of thump, a simple approach that will always appeal to the practitioners.

Nowadays the design and operation of wastewater treatment plants is founded on a scientific concept, based on cause-effect relationships, generally expressed via mathematical formulations. Compared to other disciplines of engineering, the scientific approach in treatment plants design had a late development, due to the complexity of the biological systems involved. The latter approach is also named mechanistic approach and it conceptualizes the physical and biological processes. It has many advantages, first of all the fact that the relationships are of a more comprehensive nature and they are frequently more reliable than the empirical models; secondly it includes a better approximation to reality. The scientifically based models ensure

more reliability in utilization outside the confines in which the model has been developed, because of their concept based nature.

In the plant several different types of mechanisms are combined, whereby this leads to a quite complex description. The various links and interactions between the diverse compounds and processes are described and the quantities (process rates and stoichiometry relationships) are defined through the mathematical formulation of a model.

Any model needs to be verified and rigorously calibrated on experience bases. Therefore, the latter approach should better be named science-based deterministic approach, because the mathematical quantitative description of the involved mechanisms and the parameters can be modified to match the real world only by induction. The mathematical model will most likely not include all the processes of the mechanical model, but only those relevant for the accomplishing of the aim of the simulation.

Often there is no need to consider every single process: The art of create a model consists in understanding which processes are allowed to be disregarded. A simpler model is frequently adequate to fulfil the objectives of the simulation. For example in modelling biological behaviour it is not necessary to describe every single species of bacteria. Usually micro-organism species that carry out a peculiar function are processed as a single surrogate organism, which is assigned a series of characteristics, so that it reflects the behaviour of the entire group of bacteria. This approach has mainly one great advantage: Less information are required for the model set up and for its calibration.

1.2 Definition of dynamic model

A model is defined as a representation or description, often simplified, of a system of interest (Wentzel *et al.*, 1997).
A model does not describe every detail of the treated process, but only the pertinent parts, that are relevant to understand, to interpret and to deal with.

The most important aspects of modelling are the time and the scale (Henze *et al.*, 2008). From the perspective of time processes can be separated in those characterized by frozen, steady and dynamical state. The latter are

usually described by models and in in these simulations variations occur as functions of time. Frozen state of the process means that the process will change in time, but not in the relevant interval, for example the processes that take place in the digester in the sludge line. In addition to these types of processes there are ones that are so rapid, that the speed of change surpasses the dynamics that are interesting for the modeller, for example changes in the ammonium concentration.

Therefore, one of the first operations in making a model is to select which process are of interest, considering the relevant time frame, the modeller has to select the interesting processes that have the dynamics in the order of time constants and those that do not (frozen or steady state).

The second issue to consider, in trying simplifying the reality, is the space resolution and it basically depends on the purpose of the model: Which systems are relevant to be described and which processes are interesting to be investigated and which are not.

The third point in modelling is the decision of the right level of detail of a microbial model. Traditional plant design bases on a black-box approach, which means focus on the influent and effluent characteristic and not on the inner processes. This method is based on food to microorganism ratio (F/M), which is the sludge loading rate (Fujimoto, 1963), but nothing is known about the processes inside the plant.

It is possible to move towards grey-box approach, refining the level of understanding what is happening inside the plant: For instance in the Activated Sludge Model NO. 1 (ASM NO.1, Henze *et al.*, 2000a) the sludge is split up into relevant fraction (organic matter; heterotrophic, nitrifying, denitrifying and phosphate removing bacteria).

Moreover, it is possible to consider the metabolism of the organisms and, as a result, a more complicated model is obtained, also defined glass-box approach. This is often not useful to increase the quality of the outputs of the model except for some categories of organism, for example the phosphate removing bacteria.

Ultimately, the needed level of complexity of the model depends on the purpose of what should be described. Often there is no need for the model to perfectly describe the reality: The primary aim of a model is that its inputs and outputs fit the real ones, or at least to match real process trends

and this depends on the purpose of the study. If the point is predicting the process performance, the accuracy of parameters is fundamental. On the contrary, if just an idea about a compound effluent concentration is needed, in order to select one model out of many to incorporate in the simulation, first of all the reality best-fitting one should be chosen.

1.2.1 Advantages of dynamic modelling of wastewater treatment

The reasons why modelling is useful and important are described by Henze *et al.* (2008).

In wastewater treatment the most salient advantages of the use of models are:

- Deeply understand plant performance
- Evaluate possible scenarios for upgrading and evaluate new plant design
- Support management decisions
- Develop new control schemes
- Supply operator training
- Save time and money

Qualitative comparisons are often not useful and of subjective nature; in mathematical simulations it is needed to use quantitative inputs *e.g.* sizes, rates. Hence the approach of the modellers has become quantitative and objective.

A model should contain everything which is considered relevant. Mathematical simulations drive to structured and more extensive data collection, enhancing good plant monitoring practices. Getting insight the plant performance (mass balances and data reconciliation) is often a much more fundamental practice than modelling itself.

By modelling money and time in technology and/or process selection can be saved: Decision making is easier and faster because the model itself compares systems performances in a quantitative instead of a qualitative way. Furthermore, calibrated models make possible to avoid expensive full scale wastewater treatment plant tests.

Evaluating upgrading scenarios, it is more functional to compare trends while small gaps are not important in the usual wastewater treatment engineering design horizon. Therefore it is not useful to have a fine tuned model and the same is valid for evaluating new plant design, because of uncertainty of the loading incoming to the plant over the next ten or twenty years. Usually static models are applied for primary plant design, whereas dynamic models are employed for design optimization and sensitivity analysis. Statistical methods are applied to the occurrence of worst case scenario, therefore meaning savings are made possible and the effluent quality standard are achieved for about 95% of the time (Henze *et al.*, 2008).

Another reason for using numerical simulations is the possibility of diminishing the minimizing risk: It is possible to analyse what-if scenarios and to find up-front measures to mitigate or control risks. Besides, models are useful for plant operator for training: For instance through modelling the consequence of taking a certain action at a treatment plant can be analysed, avoiding upsetting the operation of the plant.

1.3 Activated Sludge Model NO.1

Activated Sludge Model NO.1 (ASM NO.1, Henze *et al.*, 2000a) is a mathematical model to represent the biological processes that appear in the activated sludge stage of a wastewater treatment plant. The model was developed by the task group of the International Water Association (IWA, former IAWPRC) and it is a advantageous tool for the design, optimisation and operation of a wastewater treatment plant. The first purpose of the modellers was to incorporate carbon oxidation, nitrification and denitrification in the model, setting out a reliable standardisation of biological wastewater treatment plant design.

The first task in developing a mathematical model is the selection of the appropriate equations (kinetics and stoichiometry) and depth of detail of the model to depict the real process. The more close to reality and detailed the equations are, the more complicated the solutions are likely to be. Eight processes were selected as the best compromise between the need of a good description of the phenomena and the demand of minimisation of the computational effort. In fact the first requires a a certain degree of complexity, while the second the minimized one.

The primary aim of the task was to accurately predict activated sludge concentration of solids in the basins and the electron acceptor requirements, since large differences from plant to plant occur. Whereas the effluent concentration was not one of the main aspect in the model, since it usually does not vary significantly from plant to plant. Consequently stoichiometric equations and rate equation were picked out to better define respectively the activated sludge concentration and the electron acceptor requirements.

1.3.1 State variables and model parameters

Thirteen variables are incorporated in the model, including carbon-based, nitrogen-based pollutants, biomass, oxygen and alkalinity.

Chemical Oxygen Demand (COD) was selected as the superior measurement unit between the ones related with carbon removal. It alone supplies a link between electron equivalents in organic substrate, biomass and the oxygen consumption. Furthermore, it allows practical mass balances in terms of COD units, provided consistent units have been used for every state variable and each coefficient. Carbonaceus and nitrogenous matter are subdivided into several fractions in the model, according to Marais and Ekama (1976) and Dold *et al.* (1980).

The total COD (COD_t) is subdivided into six fractions according to two principles: Physical state (denoted S, soluble or X, particulate) and biodegradability (subscripted $_s$, biodegradable or $_i$, inert, non biodegradable). The division between the different fractions is essential as many of the steps in the treatment plant are only effective against one or more of these.

The COD_t fractionation is illustrated by the equation 1.1:

$$COD_t = S_s + S_i + X_s + X_i + X_{bh} + X_{ba} + X_p \tag{1.1}$$

where Ss means soluble (or dissolved) easily biodegradable organic matter, S_i is dissolved biological inert organic matter, X_s means suspended (or particulate) slowly biodegradable organic matter, X_i is the suspended inert organic matter, X_{bh} and X_{ba} means respectively heterotrophic and autotrophic biomass and X_p is the particulate result of biomass decay.
The sum of the particulate X fractions constitutes the volatile solids.

Regarding biodegradable carbon fractions, for merely modelling purpose it

is convenient to assume readily biodegradable carbon as entirely dissolved and slowly biodegradable carbon as all particulate. Nevertheless it is a well known fact that some of the soluble carbon could contain slowly biodegradable carbon.

To facilitate the understanding the COD fractionation layout is presented in Fig. 1.1.

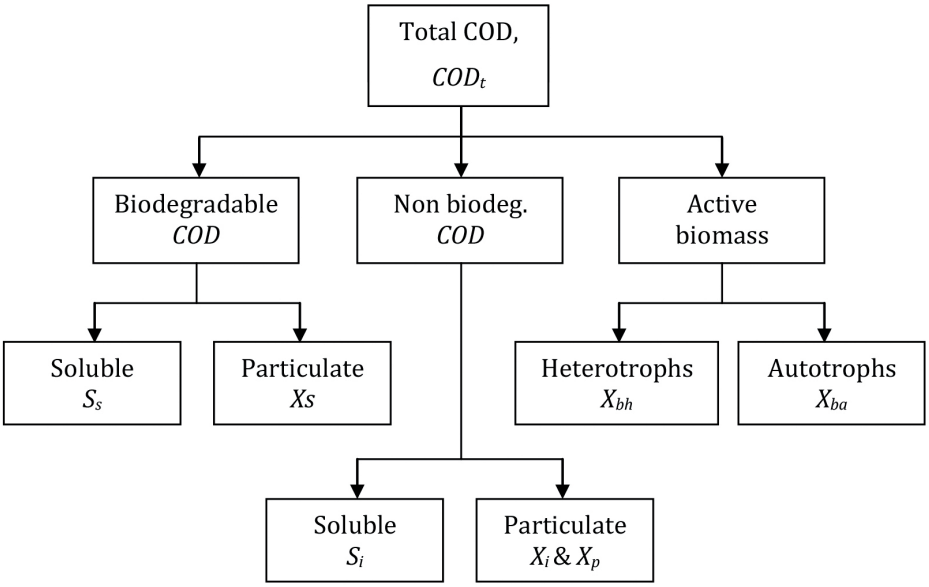

Figure 1.1: COD fractionation in ASM NO.1 (modified from Jeppson, 1996, with kind permission)

The COD fractions according to Henze *et al.* (2000a) are described below:

- *Readily biodegradable substrate, S_s:* It consists in rather simple molecules and it is considered to be the only substrate utilised by heterotrophic bacteria for growth; it is introduced in the plant through the influent wastewater, but most of it is the result of hydrolysis of X_s enmeshed in the bioflocs.
- *Slowly biodegradable substrate, X_s:* It is assumed to be captured outright in the bioflocs, then it is transformed in S_s by hydrolysis.
- *Soluble inert organic matter, S_i:* It is presumed to leave the system at the same concentration that it enters, therefore it strongly contributes to the effluent COD concentration.

- *Particulate inert organic matter, X_i:* It becomes entrapped in the sludge and leaves the activated system through the excess sludge.

- *Active heterotrophic biomass, X_{bh}:* Its growth occurs under either aerobic or anoxic conditions and it is assumed to be destroyed by decay.

- *Active autotrophic biomass, X_{ba}:* It grows only under aerobic condition and it is destroyed by decay, too.

- *Particulate products arising from biomass decay, X_p:* It is an inert particulate, product of both heterotrophic and autotrophic bacteria decay, along with X_s. Whereas X_s reenters the cycle of hydrolysis, X_p is inert to further biological transformation and it accumulates in the system.

Nitrogenous matter is assumed to be fractionated into several fractions, in the same way as carbon matter. The Total Nitrogen (TN) is the sum of the Total Kjeldahl Nitrogen (TKN), nitrate and nitrite nitrogen:

$$TN = TKN + S_{no} \tag{1.2}$$

where S_{no} is nitrate nitrogen fraction.

The Total Kjeldahl Nitrogen may be divided into a number of fractions, as described in the equation 1.3:

$$TKN = S_{nh} + S_{nd} + X_{nd} + S_{ni} + X_{ni} + N_{bh} + N_{ba} \tag{1.3}$$

where S_{nh} is ammonium and ammonia nitrogen, S_{nd} is dissolved degradable organic nitrogen, X_{nd} is suspended easily degradable organic nitrogen, S_{ni} is dissolved inert organic nitrogen, X_{ni} is suspended inert organic nitrogen, N_{bh} is the heterotrophic biomass and N_{ba} is the autotrophic nitrifying biomass.

However biomass fractions of nitrogen and S_{ni} are not incorporated in the model.

To facilitate the understanding the TN fractionation layout is presented in Figure 1.2; the grey boxes are neglected in the Activated Sludge Model NO.1.

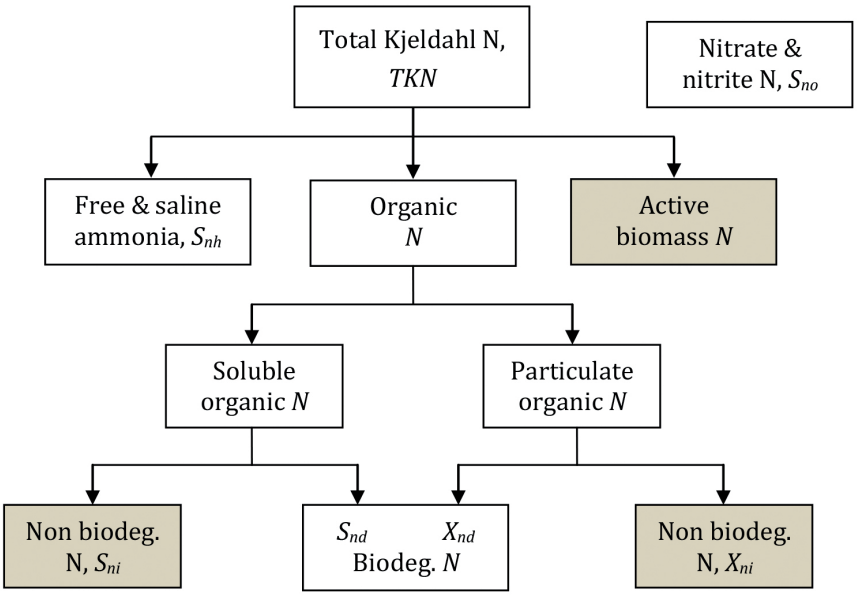

Figure 1.2: Total Nitrogen fractionation in ASM NO.1 (modified from Jeppson, 1996, with kind permission)

As reported by Henze *et al.* (2000a), the TN fractions that are considered in the model are described below:

- *Nitrite and nitrate nitrogen, S_{no}:* It substitutes oxygen as the primary electron acceptor for heterotrophic bacteria under anoxic conditions. It is the result of autotrophic bacteria growth under aerobic conditions and it is consumed by facultative heterotrophic bacteria for growth, returning nitrogen gas. For simplicity, the conversion of ammonia nitrogen to nitrate nitrogen is assumed to be a single aerobic mechanism.

- *Ammonium and ammonia nitrogen, S_{nh}:* It is the result of ammonification of S_{nd}. It is utilised for synthesis by both autotrophic and heterotrophic biomass and also used for energy by growth of autotrophic nitrifying bacteria.

- *Soluble biodegradable organic nitrogen, S_{nd}:* It is the result of the hydrolysis of particulate organic nitrogen, then it is converted to ammonia nitrogen by heterotrophic bacteria (ammonification process).

- *Particulate biodegradable organic nitrogen, X_{nd}:* It is hydrolysed together with slowly biodegradable nitrogen to soluble organic nitrogen (S_{nd}).

According to Henze *et al.* (2000a) the remaining variables are the following:

- Dissolved oxygen, S_o: It is consumed by aerobic growth of bacteria and it is the primary electron acceptor. The biological processes included in the model only act to remove oxygen from the system. The main aim of the oxygen term is to switch on/off the aerobic/anaerobic growth of biomass when its concentration is high/low. Oxygen is considered to be negative COD.
- Total alkalinity, S_{alk}: Its inclusion in the model may be helpful to predict pH variations. The model consider several processes that affect the alkalinity, that is processes involving switching of protons: Conversion of ammonia nitrogen to amino acids, nitrification (largest impact in consuming alkalinity) and denitrification (increasing alkalinity).

1.3.2 Mathematical model and processes

In this section dynamic processes and mathematical formulation are described.
The model equations describing processes are in matrix format described as Petersen matrix and presented in appendices (see Table 6.1). This format was selected by Henze *et al.* (2000a) to trace all the interaction between the model components in a relatively easy way. The columns of the matrix are as many as the relevant components (13 for ASM NO.1), while the rows are the same number as the involved processes (8 for ASM NO.1: Biochemical reactions and degradation).

Four types of processes are considered in this model: Growth and decay of biomass, ammonification of organic nitrogen and hydrolysis of particulate carbon. Considering the different type of bacteria involved in wastewater treatment and the different environmental conditions, eight equations are the minimum amount to describe a system where carbon removal, nitrification and denitrification are performed.

The equations need to account the environmental conditions, therefore the effect of each component is modelled with a saturation function, which acts as switching function to turn on/off a certain process when it is appropriate. All the equations presented in this section are displayed with kind permission of Mogens Henze *et al.* (2000a). Three kinds of growth of biomass are treated in ASM NO.1 and the kinetic expression are of the type: $\frac{dX}{dt} = \mu \cdot X$, where X is a generic biomass and μ is the specific growth rate. The yeld coefficient Y_h and Y_a are used to describe the relationships between biomass and readily biodegradable substrate: $\frac{dX}{dt} = -Y_h \cdot \frac{dS}{dt}$, respectively for heterotrophs and autotrophs.

Microbial growth process equations (p_i, i=1,2,3) are described as:

- *Growth of heterotrophs under aerobic conditions*

$$p_1 = \Big(-\frac{1}{Y_h} S_s + X_{bh} - \frac{1-Y_h}{Y_h} S_o - i_{xb} S_{nh} - \frac{i_{xb}}{14} S_{alk} \Big) \cdot \cdot \hat{\mu}_h \Big(\frac{S_s}{K_s + S_s} \Big) \Big(\frac{S_o}{K_{oh} + S_o} \Big) X_{bh} \tag{1.4}$$

  where $\hat{\mu}_h$ represents the maximum growth rate for heterotrophic biomass, K_s is the half-saturation coefficient for S_s, K_{oh} is the half-saturation coefficient for oxygen and i_{xb} the fraction of S_{nh} incorporated in the new cells.

  The equation shows that only S_s is consumed during heterotrophic growth, supplying energy and carbon source and in parallel oxygen consumption occurs. As a result X_{bh} increases. Two limitations of the growth are considered: Presence of S_s and S_{no}; when S_{no} has a low value, the growth stops, due to the low value of K_{oh}.

- *Growth of heterotrophs under anoxic conditions*

$$p_2 = \Big(-\frac{1}{Y_h} S_s + X_{bh} - \frac{1-Y_h}{2.86 Y_h} S_{no} - i_{xb} S_{nh} + \frac{1-Y_h}{14 \cdot 2.86 - \frac{i_{xb}}{14}} S_{alk} \Big) \cdot \cdot \hat{\mu}_h \Big(\frac{S_s}{K_s + S_s} \Big) \Big(\frac{K_{oh}}{K_{oh} + S_o} \Big) \Big(\frac{S_{no}}{K_{no} + S_{no}} \Big) \eta_g X_{bh} \tag{1.5}$$

  where K_{no} is the half-saturation coefficient for S_{no} and η_g is a correc-

tion factor for the anoxic growth of heterotrophs, to take into account the lower rate in substrate removal.

The process needs S_s as a carbon source and S_{no} as a electron acceptor, resulting in growth of X_{bh}. A fraction of S_{nh} is merged in the new cells. The limiting factors of growth are oxygen, nitrate and readily biodegradable substrate concentration. An increase of alkalinity occurs during denitrification process, however the net balance with nitrification is negative.

- *Growth of autotrophs under aerobic conditions*

$$p_3 = \left[X_{ba} - \frac{4.57 - Y_a}{2.86 Y_h} S_o + \frac{1}{Y_a} S_{no} - \left(i_{xb} + \frac{1}{Y_a} \right) S_{nh} + \right. \\ \left. - \left(\frac{i_{xb}}{14} + \frac{1}{7 Y_a} \right) S_{alk} \right] \cdot \hat{\mu}_a \left(\frac{S_{nh}}{K_{nh} + S_{nh}} \right) \left(\frac{S_o}{K_{oa} + S_{nh}} \right) X_{ba} \tag{1.6}$$

$\hat{\mu}_a$ represents the maximum growth rate for autotrophic biomass. The process utilises S_{nh} as an energy source for growth; however a small fraction of the amount of ammonia is incorporated in the new cell mass. An amount of oxygen proportional to the bulk of ammonia is utilised.

The limiting factors are both oxygen and ammonia nitrogen concentration and the dependence is expressed as a saturation function. Being both K_{oa} and K_{nh} small, the latter are switching functions. The dependence upon pH is replaced by the dependence upon alkalinity and the process reduces alkalinity.

The decay of both autotrophic and heterotrophic bacteria is modelled in accordance with death-regeneration concept (Dold *et al.*, 1980). This approach makes the assumption that biomass is converted into two fractions during decay: Inert particulate (X_p) and slowly biodegradable substrate (X_s). Only the latter re-enters the cycle of hydrolysis, becoming again available S_s for biomass growth. The hypothesis of the model is that the decay rate does not depend upon the environmental conditions, *i.e.* type of electron acceptor or its concentration.
This theory mimics well the loss of biomass occurring in activated sludge vessel, however it was adopted only for pragmatic reasons since it does not reflect the real mechanisms occurring (Henze *et al.*, 2008).

Decay expressions for heterotrophs and autotrophic biomass are included in ASM NO.1:

- *Decay of heterotrophs*

$$p_4 = ((1 - f_p)X_s - X_{bh} + f_p X_p + (i_{xb} - f_p i_{xp})X_{nd})b_h X_{bh} \tag{1.7}$$

  The process converts heterotrophic biomass (X_{bh}) into a combination of slowly biodegradable substrate (X_b) and inert particulate (X_p). The process involves the release of particulate organic nitrogen, that is then converted into soluble organic nitrogen by hydrolysis and hence available for ammonification. The decay coefficient for heterotrophs b_h is higher than the usually experienced, since the recycling of carbon substrate occurs.

- *Decay of autotrophs*

$$p_5 = ((1 - f_p)X_s - X_{ba} + f_p X_p + (i_{xb} - f_p i_{xp})X_{nd}) \cdot b_a X_{ba} \tag{1.8}$$

  The rate expression is analogue to the one for the heterotrophic biomass, but the decay coefficient b_a is lower.

The last three important processes considered in the model are ammonification of soluble organic nitrogen, hydrolysis of slowly biodegradable substrate and hydrolysis of particulate organic nitrogen.

- *Ammonification of soluble organic nitrogen*

$$p_6 = \left(S_{nh} - S_{nd} + \frac{1}{14}S_{alk}\right) \cdot k_a S_{nd} X_{bh} \tag{1.9}$$

  where k_a is the kinetic parameter for ammonification. The process generates a mass of ammonia directly proportional to the amount of biodegradable soluble organic nitrogen.

- Hydrolysis of slowly biodegradable substrate

$$\begin{aligned} p_7 =& (S_s - X_s) \cdot k_h \frac{X_s/X_{bh}}{K_x + (X_s/X_{bh})} \left[\left(\frac{S_o}{K_{oh} + S_o}\right) + \right. \\ &\left. + \eta_h \left(\frac{K_{oh}}{K_{oh} + S_o}\right)\left(\frac{S_{no}}{K_{no} + S_{no}}\right)\right] X_{bh} \end{aligned} \tag{1.10}$$

where k_h is the kinetic parameter for hydrolysis, K_x is the half-saturation coefficient for hydrolysis and η_h is the correction factor for anoxic hydrolysis lower than one, because this occurs at a lower rate in comparison with aerobic hydrolysis.

Modelling of slowly biodegradable matter degradation is fundamental to realistic depict the activated sludge inner processes and it is described by the presented equation illustrating the surface reaction. The breaking down of organic matter occurs extracellularly and S_s becomes available for biomass growth. The process is assumed to lower under anoxic condition, compared with aerobic condition. The growth rate stops to increase with the biomass amount as the amount of X_s becomes large with respect to X_{bh}.

- *Hydrolysis of particulate organic nitrogen*

$$p_8 = (S_{nd} - X_{nd}) \cdot \rho_7 \frac{X_{nd}}{X_s} \tag{1.11}$$

where $\rho_7 = k_h \frac{X_s/X_{bh}}{K_x+(X_s/X_{bh})} \left[\left(\frac{S_o}{K_{oh}+S_o} \right) + \eta_h \left(\frac{K_{oh}}{K_{oh}+S_o} \right) \left(\frac{S_{no}}{K_{no}+S_{no}} \right) \right] X_{bh}$ is the process rate for hydrolysis of entrapped organics.

Particulate organic nitrogen is converted to soluble organic nitrogen.

1.4 Activated sludge model NO.2d: Focus on the chemical precipitation

Since the ASM NO.1 does not include treatment of phosphorus, but only carbon oxidation, nitrification and denitrification, ASM2 NO.2d was used instead for this purpose. This section focuses on the mathematical modelling of chemical precipitation of phosphorus.

Therefore two models were used: while primary settlers, biological treatment units, secondary settlers were simulated in ASM NO.1, chemical dosage, flocculation basins, post-precipitation and the polishing stage were modelled using ASM NO.2d. Outputs from the former model were provided as inputs for the latter.

The existing plant layout is presented in chapter 2.

The outputs from ASM NO.1 were provided as inputs to ASM NO.2d.

The ASM NO.2d includes phosphorus as inorganic soluble phosphorus (S_{PO_4}); in order to balance the electrical charges, it assumes that S_{PO_4} consists 50% of $H_2PO_4^-$ and 50% of HPO_4^{2-}, regardless of pH (Henze *et al.*, 2000b).

X_{MeOH} represents the metal hydroxides and stands for the phosphorus binding capacity of some metal-hydroxides, which may be in the wastewater and/or added to the system in order to precipitate the S_{PO_4}. In the commercial ASM NO.2d, the active metal hydroxide ($MeOH$) used in stoichiometry calculations is $Fe(OH)_3$, that is ferric hydroxide (DHI, 2014b).

X_{MeP} is the metal-phosphate $MePO_4$, resulting from binding phophorus to the metal-hydroxides. With respect to stoichiometric computations, this component is assumed to consist of $FePO_4$.

The model describes the addition of $Fe(OH)_3$ for the simultaneous precipitation of phosphorus.

The model assumes that a solution of pure iron hydroxide is dosed; the solution is characterised by its flowrate and by the concentration of the active species.

The flux of the metal hydroxide is computed as described in equation 1.12:

$$Q(X_{Fe(OH)_3}) = Q_{dose} \cdot C_{dose} \cdot E_p \tag{1.12}$$

where the unit of Q_{dose} is the flowrate of the solution (m^3/d), C_{dose} is the concentration of the solution (g/m^3) and E_P is the molar equivalence to phosphorus (mol/mol of P).

The output variables of this model are $Q(X_{Fe(OH)_3})$, that is the outgoing flow for all components (g/d), $M_{Fe(OH)_3}$ and $Q_{Fe(OH)_3}$, that are the sensors for the amount and the flow rate of chemical dosed, respectively.

Chemical precipitation model makes the assumption that precipitation and redissolution of S_{PO} are reverse process, that at steady state are ruled by equation 1.13:

$$X_{Fe(OH)_3} + S_{PO_4} \longleftrightarrow X_{FePO_4} \tag{1.13}$$

The process rates of precipitation and redissolution are respectively modelled by the equation 1.14 and 1.15:

$$\rho_{PRE} = k_{PRE} \cdot S_{PO_4} \cdot X_{Fe(OH)_3} \tag{1.14}$$

$$\rho_{RED} = k_{RED} \cdot X_{FePO_4} \tag{1.15}$$

If both processes are in equilibrium, which means that the equation $\nu_{PRE,i} \cdot \rho_{PRE} = \nu_{RED,i} \cdot \rho_{RED}$ is satisfied, then the equilibrium constant is derived as described in equation 1.16 (Henze *et al.*, 2000b):

$$K_{eq} = \frac{\nu_{RED,i} \cdot k_{RED}}{\nu_{PRE,i} \cdot k_{PRE}} = \frac{S_{PO_4} \cdot X_{Fe(OH)_3}}{X_{FePO_4}} \tag{1.16}$$

The resulting stoichiometry is presented in Table 1.1.

Table 1.1: Stoichiometry of the processes describing the simultaneous precipitation of phosphorus (Henze *et al.*, 2000b, with kind permission).

Process	S_{PO_4}	S_{alk}	X_{MeOH}	X_{MeP}	X_{TSS}
Precipitation	-1	$\nu_{PRE,alk}$	-3.45	4.87	1.42
Redissolution	1	$\nu_{RED,alk}$	3.45	-4.87	-1.42

1.5 Model calibration, verification and estimation

During the calibration step, first it is necessary to make sure that the layout and settings of the model represent the existing plant in all the needed units. Then in order to utilize a model it is recommended to ascertain the proper parameters that fit the problem in mind (Henze *et al.*, 2002). This procedure is commonly applied for example to determine fractions of the incoming wastewater *e.g.* proportions between inert vs. organic and/or soluble vs. particulate fractions of COD and stoichiometric parameters (growth rate, decay coefficients and half-saturation coefficients, etc.).

1.5.1 Calibration

Calibration is a reverse process to regression: An explanatory variable is predicted using a known observation of the corresponding dependent variable (Upton *et al.*, 2008). It is the most commonly used method to make a model fit to the problem in question.

Calibration of dynamic wastewater treatment model is often based on two time series: the first with measured loadings of the plant and the second with

concentrations from the outlet of the treatment plant. The model should mimic the conversion of the wastewater in a way as similar as possible to the existing plant, in order to get comparable results.

Some appropriate parameters depending on the model adequacy are changed in order that the best fit of the effluent measurements is obtained. The best set of parameter is achieved commonly on trial and error basis: the aim is to attain the set of parameters that gives the minimum of the standard deviation between outputs of the model and available measurements.

1.5.2 Verification

The statistical method named verification or validation is accomplished in order to determine whether a model fits the problem in question with the parameters achieved after the calibration step. It may involve the analysis of the goodness of the fit of the model *e.g.* R-squared coefficient.

Another time series of loading and concentrations in the outlet of the plant is used to test the quality of the model.

The adjustment of the outputs of the model to the measured data from the effluent is compared, without modifying the parameters achieved with the calibration.

Commonly half of a time series is used for calibration and half for verification.

Interpretation of the results could be problematic for the following reasons:

- The best set of parameters is not uniquely determined by this method; there may exist another set that could achieve a similar fit.
- Some parameters may not be defined relying on the information contained in the available measurements.
- If the data series used for calibration and validation are characterized by the same statistical features, then they fit to the data in the same way, except for the standard deviation; then it is possible to use standard deviation to measure the goodness of fit of the model.
- If the two series do not have the same statistics, then the procedure is false and the results could be described as a poor fit, but the reason may be a poor set of parameters.

Therefore sometimes it is careful to use the entire data series to calibrate the model, since the more the data contain variations, the wider range of information are available and thus a better calibration is expected. Also depending on the quality of the data series, it is common practise to assume some parameters from a-priori knowledge set.
As reported by Weijers (2003), the art of the procedure consist of selecting the right parameters to be calibrated *e.g.* growth and decay rate and these that are assumed by a priori knowledge *e.g.* yield coefficients. This depends both on the type of observed problems with respect to goodness of fit and on the available loadings/measurements from the outlet.
There is also a risk inherent this procedure, called overparametrisation. This occurs when informations from data series are too poor to calibrate a large number of parameters. It may be possible to obtain a good fit by calibration, but this is likely to fail in validation.

1.5.3 Parameter estimation

Parameter estimations are a statistical methods to estimate the best parameter values satisfying certain statistical criteria.
Uncertainty with which these factor have been determined is also incorporated in the results, and thus if the procedure is appropriate to identify the parameter. Information on the adequateness of the model and the standard deviation of the fit.

1.5.4 Model uncertainty

Any prediction provided by a model is characterized by an inherited uncertainty and forecasting as to be considered an approximation of the real operation of the plant. Any prediction should better be meant as a predicted mean performance and an estimated uncertainty.
The following tools are relevant for estimation of model uncertainty:

- Sensitivity analysis, in which the importance of each parameters is a regarding the final result of performance.
- Error propagation, in which an uncertainty is assigned to each parameter and the input data, based on a priory knowledge; these informations are then combined with the uncertainty in the model as it alter the model predictions (Henze *et al.*, 2002).

Chapter 2

The Källby wastewater treatment plant

2.1 General informations about Källby wastewater treatment plant

The Källby wastewater treatment plant is situated in Lund (Sweden) and treats an average of ca 28000 m^3/d of wastewater. It treats both domestic and industrial wastewater for a total capacity of 120000 population equivalents. The wastewater is received from central Lund and the boroughs Dalby, Värpinge, Vallkärra, Stångby, Genarp and Björnstorp. Approximately 80000 residents are connected to the plant, which was started to be built and operated in the 1930s (VA SYD, 2009).

The older areas of central Lund are served by combined sewers, which conduct both sewage and stormwater to the wastewater treatment plant in the same pipes (10% of the entire sewer system). The residual 90% of the sewer system is a duplicate system with separate pipes for sewage and stormwater. In the future the Källby wastewater treatment system will also receive wastewater from the boroughs of Veberöd through Dalby. From there a transmission sewer is conducted to the Källby wastewater treatment plant.

As a consequence the load on the plant will increase and optimisation of the treatment process is likely to be required.

The main task of the Källby wastewater treatment system is to treat wastewater in compliance with the existing wastewater treatment regulations,

which are local discharge limits consistent with Swedish legislation (SNFS 1994:7) that incorporates European Union directive (91/271/EC).

To ensure that the process units work well and that the effluent requirements are met, a computerised control system is monitoring and adjusting the treatment process. The monitoring is effectuated by meters that continuously measure parameters such as water flow, loadings and other important parameters for the process control in the inlet, in the outlet and in the different units of the treatment plant *e.g.* temperature, dissolved oxygen, suspended solids, etc.

The parameters from the on-line control system are used to monitor the relations and the changes in the processes. The results received from the laboratory are accredited and therefore more reliable than those from the meters, and used for report of the effluent discharges. In fact the on-line sensors are more sensitive to failure and often require maintenance, as stated by the plant operators.

The focus on protecting the environment has increased in the last years and higher standards for environmental compatibility can be expected (Foladori *et al.*, 2015). Källby wastewater treatment management contributes to the common current endeavour to make use of the resources in the best possible way *e.g.* by aiming at an optimal use of the energy content in wastewater.

2.2 The Källby wastewater treatment process

Wastewater treatment line

The aim of the wastewater treatment lines is to recover the incoming raw water achieving a good efficiency in removal of pollutants and obtaining a environmentally safe effluent.

The treatment stages in the wastewater treatment lines of the Källby wastewater treatment system are the following:

- Mechanical
- Biological
- Chemical
- Polishing step

The plant scheme is presented in Figure 2.1.

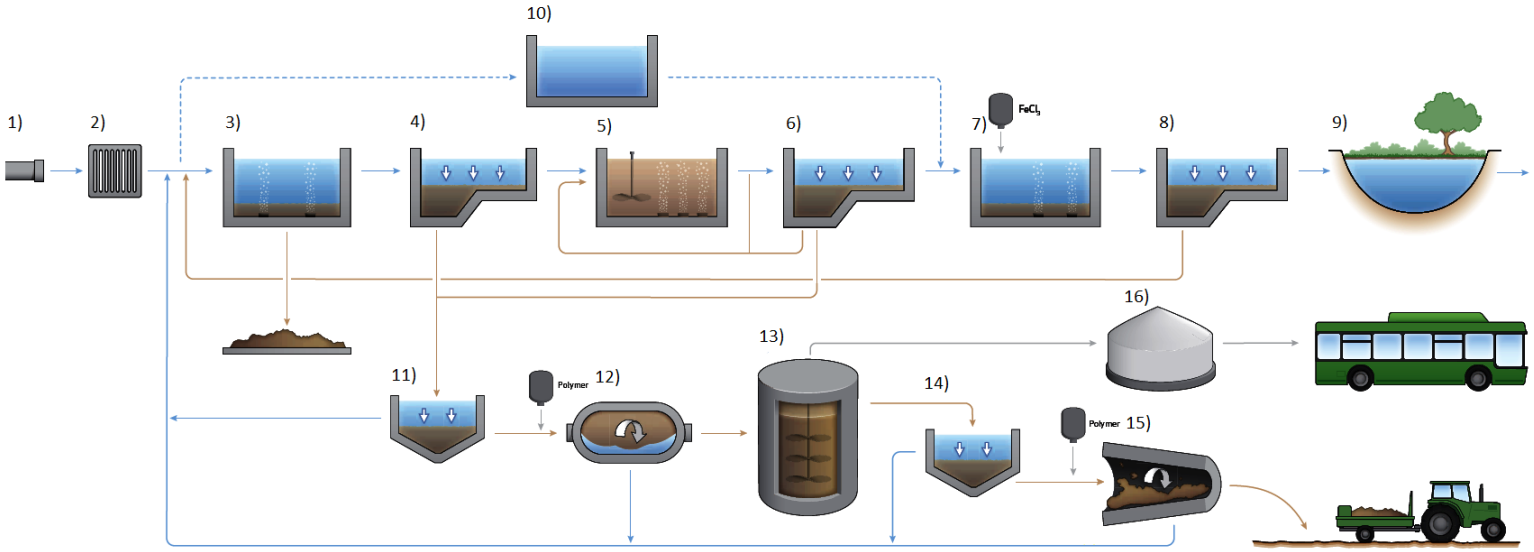

Figure 2.1: Scheme of Källby wastewater treatment layout (VA SYD, 2009).
1) Incoming raw wastewater 2) Screen 3) Aerated grit removal 4) Primary settler 5) Activated sludge stage 6) Secondary clarifier 7) Chemical dosing unit 8) Post precipitation 9) Pond 10) Overflow basin 11) Sludge thickening 12) Mechanical thickener 13) Anaerobic digester 14) Digested sludge thickening 15) Sludge dewatering 16) Gas-holder

Mechanical treatment

Screenings separation

The wastewater is conducted into the Källby wastewater treatment plant by gravity and is passed through screens, 6 mm hole-plate frames. The screenings amount depends on the weather and the incoming flowrate. Then the debris are transported to the screening washing and further to a combustion facility.

During heavy rain, the influent flow to the plant is sometimes higher than the capacity for biological treatment in the activated sludge basins. The wastewater is then directed to overflow basins for storage. From there the wastewater is either returned to the plant inlet or transported to the chemical stage for post-precipitation if the flowrate exceed the storage for biological treatment.

Aerated grit removal and treatment

Grit is removed in aerated basins. The velocity of the incoming sewage is adjusted in order to allow settling of sand, grit, stones and broken glass. Aeration contributes to a correct flow field and prevents the settling of the lighter organic matter, which is then treated biologically. The removed grit is pumped to a grit washer and then mixed with the sludge treated in the sludge treatment lines (VA SYD, 2009).

Primary clarification

In the primary clarifiers, particles with density greater than water sink to the bottom and are described as primary sludge. The sludge is scraped into hoppers from which it is pumped into the sludge treatment plant. Sludge from the following treatment steps is transported to the primary clarifiers. From there it is pumped on as mixed sludge for thickening before digestion.

Biological treatment

Activated sludge stage

In the activated sludge (AS) stage microorganisms remove nitrogen and degrade the organic material in the presence of oxygen to carbon dioxide and water. Nitrogen is removed by two biological processes: Nitrification and denitrification. In the first process, ammonium is converted into nitrate and then, in the second process, the nitrate is converted into nitrogen gas that is then discharged in the atmosphere. Nitrification occurs in aerobic

conditions, that is in presence of oxygen. Therefore the appropriate basins to perform this are aerated by air diffusers.

The air flow is regulated by oxygen concentration in the basins and ammonium concentration meters from the outlet of AS units. Contrariwise denitrification is performed in anoxic conditions, which occurs in presence of carbon and absence of oxygen and this is the reason why the denitrification sections are non-aerated.

The activated sludge stage at Källby WWTP is divided into four parallel lines.

Secondary clarification

In the secondary clarifiers the activated sludge is removed from the wastewater after the activated sludge units through settling. Most of the sludge removed is transferred back to the activated sludge basins as the return sludge. The purpose of this transfer is to maintain an adequate sludge content in the aeration basins. The leftover sludge, surplus (or wastage) sludge, is transferred through the primary clarifiers to the sludge treatment plant.

Chemical treatment

Post precipitation

In the chemical stage, ferric chloride ($FeCl_3$) is added to the biologically treated wastewater to precipitate phosphorus mainly.

Final clarification

In the final clarifiers the particles formed in the chemical stage will sink to the bottom. This sludge is called chemical sludge and is first transported to the primary clarifiers and then further to the sludge treatment.

Polishing stage

Ponds

Following the wastewater treatment plant there is a series of six connected ponds. The ponds have a polishing effect, which means that they aim to remove the residual phosphorus and nitrogen, even if during some periods they release these compounds. The wastewater is passing through the ponds by gravity to the outlet in the stream Höje Å. The sampling point for the outgoing treated wastewater is placed after the last pond.

Sludge treatment line

The sludge treatment lines aim to attain two main purposes: Dewater the sludge and reduce the fraction of biodegradable matter from sludge bulking. The first is implemented in order to diminish expenses for treated sludge disposal, whereas sludge stabilisation aims to reduce and/or eliminate pathogens, offensive smells and putrefaction potential. The second process leads to the production of biogas.

The treatment processes mixed sludge, *i.e.* a comprehensive term for the primary sludge from the primary clarifiers, the surplus sludge from the secondary clarifiers and the chemical sludge from the post-precipitation.

The treatment stages in the sludge lines of the Källby wastewater treatment system are the following:

- Gravity thickening
- Mechanical thickening
- Anaerobic digestion and biogas production
- Digested sludge thickening
- Sludge dewatering

Sludge thickening

The water content of the mixed sludge is reduced by gravity thickeners as solid particles sink to the bottom. Then it is pumped to a mechanical thickener and the water phase is returned to the inlet of the plant.

Mechanical thickening

In order to further reduce the water content the raw sludge is thickened in a drum thickener. Polymer is added to the sludge which is then transported to a rotating drum. The water is passed through the screen cloth and returned to the inlet of the plant, while the sludge is screwed through the drum.

Digestion and biogas production

The thickened sludge is directed to the digesters where part of the organic material is degraded under anaerobic conditions (van Haandel *et al.*, 2012). The digestion is a microbiologically complex process carried out by many different types of microorganisms. They are all very sensitive to oxygen so it is important to keep the digestion system airtight.

From the organic material mainly carbon dioxide (CO_2) and methane (CH_4) are formed. The energy-rich methane gas can be used for many different

purposes, for example vehicle fuel. The digestion at the Källby wastewater treatment plant takes place in two digesters at a temperature of approximately 37°C (mesophilic digestion). The retention time in the digesters is 20-30 days.

The obtained biogas is collected and stored in a gas-holder to even out any variations in the amount of produced biogas.

The biogas is purified (upgraded) by removing carbon dioxide, water and hydrogen sulphide, if any, so that the gas mainly consists of methane. Then the biogas is delivered to the natural gas network and is mainly used as vehicle fuel.

Digested sludge thickening

The digested sludge is tapped off from the digesters at regular intervals and transported to the sludge thickener for storage.

Sludge dewatering

The digested sludge is dewatered in centrifuges. A polymer is added before the centrifuges for better separation of water and sludge, which results in higher dry-solids content of the sludge after the centrifuges. The dry-solids content at the inlet of the centrifuges is approximately 5 % and approximately 25 % at the outlet. The formed water phase reject water (rich in ammonium) is returned to the inlet of the plant.

The dewatered sludge is certified which means that the quality is accepted to be used as fertilizer on farm land.

In Figure 2.2 an aerial photos of the Källby wastewater treatment plant is shown. The sludge treatment lines are in the upper left corner, while the wastewater treatment lines occupy the center/center-right part of the figure.

Figure 2.2: Aerial photo of Källby wastewater treatment plant (VA SYD, 2009).

Chapter 3

Dynamical modelling of Källby wastewater treatment plant

3.1 Introducing the dynamic modelling and simulation environment

For this study WEST® was chosen as the modelling platform. It is designed for engineers, researchers and operators interested in studying physical, biological or chemical processes in wastewater treatment plants, sewer systems and rivers (DHI, 2014e).

Dynamic modelling of activated sludge processes can be performed to study real wastewater treatment plants (WWTPs). This software can be used during the design, operation and optimisation in wastewater treatment systems (Vanhooren *et al.*, 2003).

In the graphical environment, the physical layout of the real plant can be rebuilt and the proper parameter for each unit can be set-up.

The user can experience different features of the software, which allow simulations, optimisations of the design of the plant's layout, development and test of improved control strategies and new configurations.

In Sections 6.2 and 3.1.2 the set-up of the model and the parameters included in the simulation are explained step by step.

3.1.1 Plant layout and simulations set-up

First geometric data are required by the model to define volumes and areas of tanks in the activated sludge stage and settlers. In this section primary settler, activated sludge step and secondary settler are considered. Simulation of the pre-treatment and sludge processing was not included in the overall WWTP model, due to the lack of some relevant data.

Furthermore, it should be emphasised that the inclusion of those treatment facilities would increase the model's complexity significantly and could return unreliable simulation outputs.

For the set-up of the model, only routine operational data from Källby WWTP were used, without additional measurements campaigns.

The studied period is from 23rd July 2013 to 15th September 2014, for a total amount of 420 days. The average incoming flowrate within this terms is 29160 m^3/d.

Input block

First block to be included is the input block (see Figure 3.1) and it allows to import experimental data including the measured concentration data incoming to the plant, to set up and revise the fractionation model. The latter allows the calculation of the model state variables and the generation of the dynamic input file from the available measured data series (further explained in Section 4.2). Thus with this tool it is possible to characterise the influent.

Bypass

The bypass for the high rain flows was required to be simulated and in the model it leads the water directly to the chemical stage. Its operation is explained in subsection 3.1.2.

Primary clarifier

In the existing plant the number of primary settlers is twelve with a total area of 1600 m^2 and a volume of 3100 m^3, with an average depth of 1.94 m (calculated as the ratio between volume and area).

The model for the primary clarifier is the one-dimensional Takács primary clarifier (Takács *et al.*, 1991). The Takács model was chosen because it was proved to be the most reliable model, faithfully reproducing experimental data set either in steady-state or dynamic conditions (Grijspeerdt *et al.*,

1995). The software needs the area and the height of the settler as input data. The underflow from the primary settler was set proportional to the incoming flowrate with a ratio of 0.0148 in order to get an average flowrate equal to the real average value (5 L/s) during the studied period.

In the model the twelve primary settlers were represented by one primary settler. It was characterised by an area equal to the total area and an underflow equal to the total underflow.

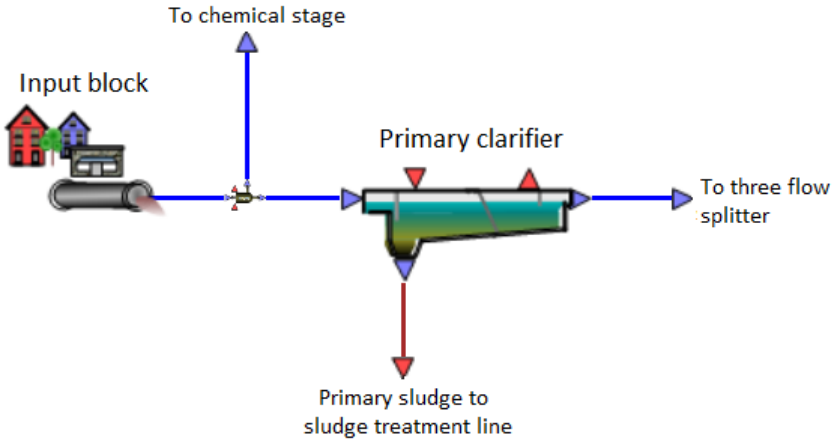

Figure 3.1: First two blocks included in the model. All displayed items in this figure are excerpted from the WEST® template (DHI, 2014d).

Splitting wastewater between biological lines

Next to the primary clarifier the flow is subdivided into three fractions by a three flow splitter. The first two portions go to first and second biological lines, while the third is then further split between the third and the fourth. To a better comprehension see Figure 3.2.

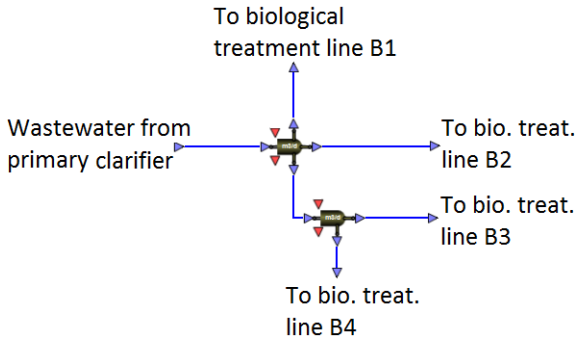

Figure 3.2: Three and two flow splitter operation. All displayed items in this figure are excerpted from the WEST® template (DHI, 2014d).

Biological step

The used model for the biological treatment is Activated Sludge Model NO.1 (ASM NO.1, Henze *et al.*, 2000a).

The biological step at the Källby WWTP consists of four biological lines (B1, B2, B3 and B4). Lines B1 and B2 have the same physical features, likewise lines B3 and B4. The first two lines treat 40% of the flow load, equally subdivided, while the latter two lines treat 60% of the flow load (30% B3 and 30% B4).

As can be seen in appendices, each biological line is subdivided in ten sections (1-10). The incoming flow enters the second section, while the first receives the nitrate recycle flow. Each section of each line of the biological step is represented as an activated sludge tank implementing ASM NO.1 in a Continuous Stirred Tank Reactor (CSTR), with constant mixing and uniform concentration within its confines (Schmidt, 2005).

The dimensions of the tanks of the activated sludge stage are shown in Table 3.1.

Table 3.1: Volumes of the activated sludge tanks.

	Section				
n.	1	2	3	4	5
Unit	m^3	m^3	m^3	m^3	m^3
Lines B1 and B2	410.3	420.5	420.5	420.5	420.5
Lines B3 and B4	603.9	648.3	644.6	648.8	668.8
	Section				
n.	6	7	8	9	10
Unit	m^3	m^3	m^3	m^3	m^3
Lines B1 and B2	417	507.3	514.4	514.4	83.2
Lines B3 and B4	636.3	715.1	723.1	715.1	284.8

In Figure 3.3 the biological stage included in the model is represented. Section 2 and 3 are displayed as a single anoxic tank and sections 4-9 by a single aerated tank. Sections 1 and 10 are both depicted as a tank each. Return flows are also shown.

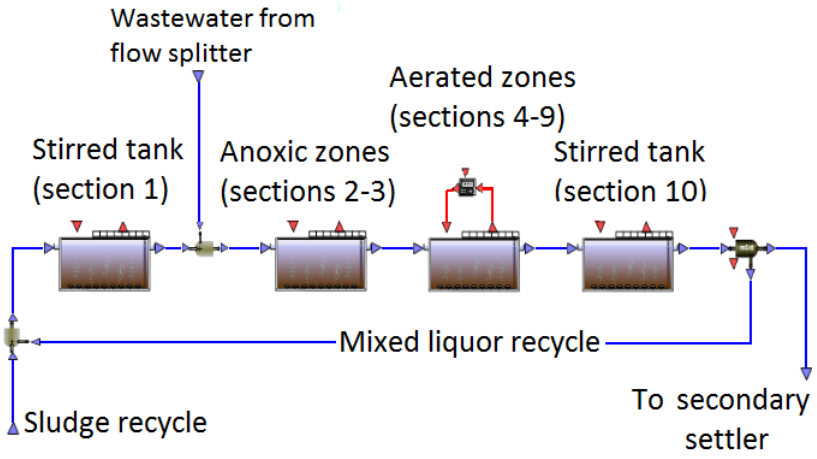

Figure 3.3: Activated sludge units. All displayed items in this figure are excerpted from the WEST® template (DHI, 2014d).

Secondary settler

The model for the secondary settler is a Tackas SVI secondary clarifier. The secondary settler has a total volume of 3420 m^3 and an area of 9040 m^2. In order to manage to define the recycles more properly, the total area has been subdivided into the 4 biological lines, proportionally according to the flowrate percentage of each line. The model needs also the height of the secondary settler as input data: The average value of height has been used.

In Figure 3.4 the layout of secondary clarifier in the model is shown.

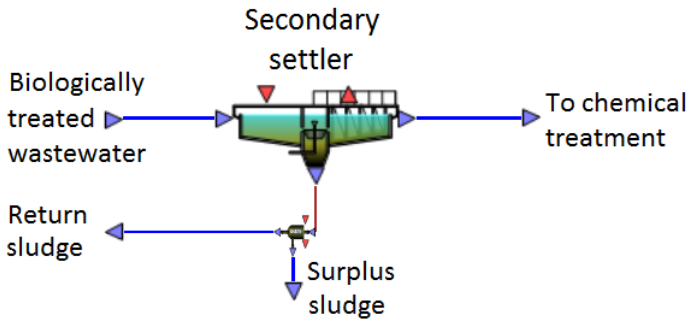

Figure 3.4: Secondary settler. All displayed items in this figure are excerpted from the WEST® template (DHI, 2014d).

In Table 3.2 the dimensions of the secondary settlers set up in the model are reported.

Table 3.2: Dimensions of the secondary clarifiers.

	Area	**Height**
Unit	m^2	m
Lines B1 and B2	684	2.64
Lines B3 and B4	1026	2.64

The recycle of nitrate and the underflow of the secondary settler was set in the model as proportional to the incoming flowrate, in each line, using a proportional controller with constant ratio.

Both recycle flowrates enter the first section, in each biological line. In the recycle pipes it was necessary to insert blocks of type loop breaker in order to allow the simulation to occur, avoiding numerical errors.

After dragging and dropping all the proper units, the layout with the considered treatment plant was built. It is shown in appendices.

3.1.2 Process parameters and settings

In this section process parameters and settings of the required controller and blocks are described:

- Bypass
- Splitting wastewater between biological lines
- Nitrate recycle, sludge recycle, total suspended solids (TSS) in the activated sludge units and wastage sludge extraction amount
- Aeration controller
- Temperature and sludge volume index (SVI)
- Restarting a biological treatment plant

Bypass

In this paragraph bypass operation is presented.

Considering the hourly average incoming flowrates, they are higher than the maximum flow that the biological stage can manage to treat (95040 m^3/d) during 16 days. The hours in which the flowrate was higher than the maximum admissible flowrate were calculated for each day in which there was overflow. Then the average overflow during this hours was calculated and rearranged on 24 hours of the corresponding day (see Table 3.3).

Table 3.3: Overflows values during days in which bypass appeared.

	Day (no.)							
	22	377	138	82	341	110	404	50
Overflow (m^3/d)	13590	7471	6237	5225	4135	3830	2094	1959

	Day (no.)							
	292	413	170	382	356	288	90	112
Overflow (m^3/d)	831	587	497	245	208	106	97	12

Splitting wastewater between biological lines

Measurement of total incoming flowrate and inflow of lines B1 and B2 were available. Thus it was possible to calculate the sum of the inflow of lines B3 and B4. The flowrates exiting the three flow splitter block were then defined as time series containing the measurements and the calculated sum. The third outflow of the block was containing the total amount of incoming flowrate of lines B3 and B4 and was then split by a two fractions splitter (see Figure 3.2).

Regarding TSS concentration in the biological lines (see Figure 3.5), some remarks about the proper way to split the water need to be done.

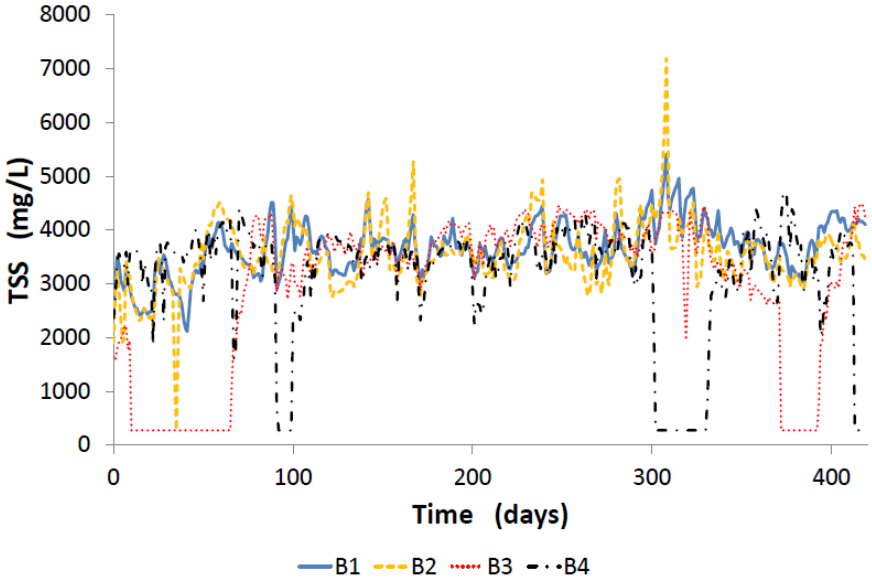

Figure 3.5: TSS measurements in the four biological lines.

It is immediately apparent that lines B1 and B2 are always turned on (except line 2 at day 35, but this was disregarded in the model). Contrariwise lines B3 and B4 are sometimes out of service, due to maintenance.
In fact when TSS concentration is low the line is turned off. In particular, in the existing plant line B3 is turned off during two time intervals (from day 10 to day 65 and from day 372 to day 393), although line B4 in three intervals (from day 91 to day 99, from day 302 to day 331 and from day 413 to day 419). To better understand, see Figure 3.5.

Therefore a time series fix the quotes of the flow from exit three directed to line B3 and line B4: When both lines are turned on the fractions are 50% to line B3 and 50% to line B4.

When line B3 is shut down, line B4 is running and receives 100% of the water from exit three of the splitter and and vice versa.
The operation of the splitter is shown in Table 3.4.

Table 3.4: Percentages of wastewater from the third exit of the splitter.

Lines	**Term**	(d)	0-9	10-65	66-90	91-99	100-300
	B1 and B2	(%)	50	0	50	100	50
	B3 and B4	(%)	50	100	50	0	50

Lines	**Term**	(d)	301-332	333-371	372-393	394-414	415-419
	B1 and B2	(%)	100	50	0	50	100
	B3 and B4	(%)	0	50	100	50	0

Control of nitrate, sludge recycle, TSS in the activated sludge units and waste sludge amount

Since measurement of recycled flowrates were only available for the first biological line, it was not possible to use measurements to define recycle in all lines.
It is not possible to use measurement from line B1 to define also the flowrates of the recycled mixed liquor and of the return sludge in lines B3 and B4. In fact, they are expected to differ a lot with respect to line B1, being the treated wastewater approximately 50% higher in these two lines.
Therefore the recycle of nitrate (RNO) and the underflow of the secondary settler (SSTU) was set in the model as proportional to the incoming

flowrate, in each line, using a ratio controller. The constant multiplying factor (constant ratio) was chosen in order to get recycle flowrate (RNO and return sludge or RAS) comparable to the real ones (see Table 3.5).

Table 3.5: Recycles in reality and in the model.

		RNO	
	Ratio	**Computed max**	**Measured max**
Unit	-	m^3/d	m^3/d
Lines B1 and B2	2.5	30462	31190
Lines B3 and B4	2.1	34727	36288

		RAS	
	Ratio	**Computed max**	**Measured max**
Unit	-	m^3/d	m^3/d
Lines B1 and B2	1.3	15732	16800
Lines B3 and B4	1.2	21852	23328

The underflow from the secondary settler is split in two streams: The wastage sludge and the return sludge. The amount of the wastage sludge is controlled by a proportional controller, which keeps the TSS concentration in the last activated sludge tank controlled.

The wastage valve discharge the surplus sludge when the TSS measured in the last activated sludge section exceeds the threshold. The set point of the TSS concentration is variable in time and is given by a time series that includes the real measurements from the plant.

The TSS measurement have been included in the model creating a top-level interface variable and using an Data input block, that was then linked to the block controlling the wastage sludge. A top-level interface variable is a variable defined at the level of the overall plant. Every time series added in the model was included using an input block.

This generates an input file readable by the model and links it to the previously created top-level interface variables. The maximum amount of wastage sludge extracted from the biological compartment was controlled and set as the real maximum measured value (720 m^3/d), while the minimum was set to 20 m^3/d for lines B1 and B2 and to 30 m^3/d for the other lines.

The set point for the steady state simulation for the four biological lines are different and presented in Table 3.6.

Table 3.6: TSS set point of the controllers for the biological stage.

	Line			
	B1	B2	B3	B4
Unit	g/m^3	g/m^3	g/m^3	g/m^3
TSS set point	3662	3551	3350	3560

Aeration control

The first three sections in each line are non aerated (anoxic conditions) in order to accomplish denitrification and partial carbon removal without the need of oxygen. This configuration is called Modified Ludzack-Ettinger layout (Wang *et al.*, 2009).

The pre-denitrification step is followed by six compartments (4-9) in which aeration is turned on alternatively so as to perform nitrification and carbon removal combined with denitrification.

In the model the aeration in these six sections is controlled by a time series containing measurement in the biological tanks.

The dissolved oxygen in the alternatively aerated tank is controlled by a proportional-integral (PI) controller that manipulates the K_{La} (oxygen transfer coefficient).

The last tank in each line has the purpose to stir the liquor before it reaches the secondary settler, in order to minimise the recycle of oxygen via the nitrate recycle, avoiding inhibition of denitrification (Oh *et al.*, 1999).

Temperature and sludge volume index control

The measured data of wastewater temperature and sludge volume index (SVI) were included in the model as time series using input blocks to better mimic the actual dynamic behaviour of the plant.

Temperature effects the biological and chemical reactions, while SVI measures the sludge settleability (Dick *et al.*, 1969).

The procedure was the same used to enter the TSS as set point in the model, but in this case the input block containing the top level interface variables were linked to the activated sludge tanks and to the secondary settlers, respectively.

The average value of temperature, used for the steady state simulation and to initialise the dynamic simulation was 12.9 °C.
In Table 3.7 the average values of SVI calculated during the studied period in the four biological lines, used for the steady state simulation, are presented.

Table 3.7: SVI in the secondary settler in the steady state simulation.

	Line			
	B1	B2	B3	B4
Unit	g/m3	g/m3	g/m3	g/m3
SVI	213.9	182.9	200.8	190.1

Restarting a biological treatment plant

The restart of a biological treatment line needs active biomass in order to faster restart the biological processes within the activated sludge units. This happens when a line is shut down for a period due to maintenance or malfunctioning and then is restarted.
When *e.g.* line B3 is restarted, surplus sludge from line B4 is pumped to the tanks of line B3 and vice versa. This happens in order to have enough amount of TSS and active biomass to accomplish the biological treatment. In the model this was simulated by pumping all the surplus sludge from biological treatment line B4 to line B3 for 8 days after the restart of line B3 and from line B3 to line B4 after the restart of line B4.

3.2 Modelling chemical precipitation

In order to simulate the chemical post precipitation, the model for precipitation built in ASM NO.2d was used (Henze *et al.*, 2000b), since phosphorus is not included in ASM NO.1.
In fact, chemical post-precipitation with iron dosage was not available in ASM NO.1 of WEST®.
Therefore two models were used: while primary settlers, biological treatment units, secondary settlers were simulated in ASM NO.1, chemical dosage, flocculation basins, post-precipitation and the polishing stage were modelled using ASM NO.2d. The existing plant layout is presented in chapter 2.
Input data to define the state variables of the latter are mainly the outputs of the model in ASM NO.1 of WEST®.

These are Flowrate, COD, TSS, COD_s, COD_b (obtained from BOD_∞, which has been approximated with BOD_{20} in the outlet of biological treatment), S_i, Alk, NH_4 and NO_3.

Instead S_{po} (soluble orthophosphate) has been obtained using the influent TP and the measured TP and S_{po} after the biological treatment. Since just a limited number of measurements was available after the activated sludge step (169 data for TP and 17 data for S_{po}), linear regression has been used to recover the missing data, with an analogous procedure as presented in subsection 3.3.2.

The layout of chemical post-precipitation and polishing step is shown in Figure 3.6.

The pond as polishing step has also been included in the plant layout.

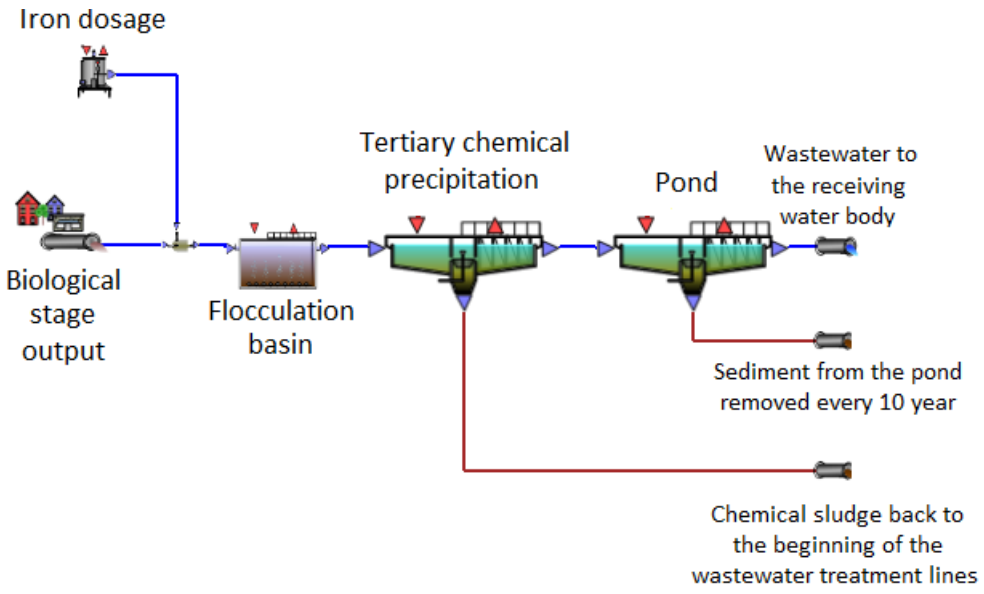

Figure 3.6: Post-precipitation and pond model layout. All displayed items in this figure are an excerpt from the WEST® template (DHI, 2013).

An AS tank without biology was used as flocculation basin and the volume was set to 1040 m^3, the total volume of the six existing flocculation basins. The twelve chemical clarifiers were merged and simulated by one Takács SVI secondary clarifier. This was characterised by the total volume equal to 4320 m^3 and the height was set equal to the average height (2 m), which was calculated by dividing the total volume by the total area (2160 m^2).

The six biological ponds were simulated by a Takács SVI secondary clarifier characterised by the total area (111250 m^2) and average height (1.1 m).
The underflow from the chemical settler and from the pond were set proportional to the incoming flowrate with a constant ratio, respectively equal to 1% and 0.1%, in order to have a reasonably correct underflow.
In the existing plant the sediments formed in the pond are removed every ten years, while the chemical sludge from the post-precipitation is sent back to the beginning of the wastewater treatment lines.
The measured time series of S_{PO} from the outlet of Källby wastewater treatment plant was included in the model to define the set point of the controller of the iron hydroxide dosing unit: $Fe(OH)_3$ is dosed when the measured S_{PO} after the chemical precipitation is higher than the threshold. The concentration of the solution was set equal to the density of the one used in the existing plant (1420 kg/m^3).

3.3 Influent characterisation

A detailed characterisation of the influent wastewater needs to be performed, before proceeding with the proper simulation using the dynamic model. This characterisation aims to translate the incoming water measurements available in the plant to data useful for modelling that are the state variables of the models.
A precise description of the loading is one of the dominant factor of the quality of dynamic model outputs and predictions (Roeleveld *et al.*, 2002). Moreover the achievement of a model strongly depends on the availability of measurements describing the variability at the plant inlet, in terms of concentrations, flowrates, temperatures and other relevant measurement (Flores-Alsina *et al.*, 2014).
Therefore, on the chance that many data are missing, a reliable data treatment is a key factor for the success of the model.

3.3.1 Available data

Sampling and analysis of most of the compounds are performed often at Källby wastewater treatment plant. Data used for the present study were collected from 23rd July 2013 to 15th September 2014, for a total number of 420 days.

As can be seen in Table 3.8, analysed compounds were total Chemical Oxygen Demand (COD_t), soluble (or filtered) COD (COD_s), total Biochemical Oxygen Demand (BOD_t), soluble BOD (BOD_s), Total Suspended Solids (TSS), Total Nitrogen (TN), Ammonium Nitrogen (NH_4-N), Total Phosphorus (TP), Total Organic Carbon (TOC_t), soluble TOC (TOC_s) and hydrogen carbonate (HCO_3). Moreover, the inlet wastewater flow rate (Q_{in}) and the temperature were measured.
Unfortunately, many of the data were lost in database or were not evaluated concurrently, resulting in a different number of measurements for the diverse compounds (n), as shown in Table 3.8. Moreover, the number of measurement was limited for almost all compounds (except TN and NH_4-N). The loss of measurements affects especially COD and BOD data; the acronym BOD refers to BOD_7 in this thesis.

Table 3.8: Number of measurements, mean and standard deviations from the inlet of the plant.

	Mean	**Std dev**	**Unit**	**Measurements in 420 days**		**Dilution** (*)
				n	%	
Q_{in}	29141	7520	$m^3 \cdot d^{-1}$	420	100%	-
COD_t	402.7	127.5	$gO_2 \cdot m^{-3}$	49	11.7%	M-D
COD_s	126.6	34.1	$gO_2 \cdot m^{-3}$	46	11.0%	D
BOD_t	179.0	80.5	$gO_2 \cdot m^{-3}$	30	7.1%	D
BOD_s	53.4	13.1	$gO_2 \cdot m^{-3}$	30	7.1%	-
TSS	190.0	93.3	$gSS \cdot m^{-3}$	217	51.7%	D
TN	42.9	9.1	$gN \cdot m^{-3}$	386	91.9%	M-D
NH_4-N	31.9	6.6	$gN \cdot m^{-3}$	391	93.1%	M
TP	6.0	1.8	$gP \cdot m^{-3}$	388	92.4%	D
TOC_t	100.8	34.1	$gTOC \cdot m^{-3}$	53	12.6%	D
TOC_s	39.2	11.4	$gTOC \cdot m^{-3}$	70	16.7%	-
HCO_3	294.3	28.1	$gHCO_3 \cdot m^{-3}$	49	11.7%	-
Temperature	12.9	2.4	°C	420	100%	-

(*) characterisation according to Henze *et al.* (2002):
M=moderately diluted wastewater, D=diluted wastewater
and M-D=moderately diluted-diluted wastewater

According to Henze *et al.* (2002), considering the average value of total BOD, COD, TN and TP, the inlet wastewater of Källby was classified

as a diluted wastewater wastewater (3.8), which means that it does not include only municipal wastewater, instead also industrial wastewater and stormwater, as it is known.

3.3.2 Data treatment

A literature search was necessary to characterize the inlet municipal wastewater and complete the missing data, detecting any possible correlation between the measured compounds.
As reported by Henze *et al.* (2002) the wastewater components show up in typical ratio in raw wastewater (see Table 3.9).
Considering the literature ranges according to Henze *et. al* (2002, 2008), half of the measured ratios between compounds in raw wastewater are contained in them.
Regarding the ratios concerning COD_t, COD_t/TN and COD_t/VSS are respectively in the typical and high range, whereas COD_t/BOD_t, COD_t/TP and COD_t/TOC_t are just slightly higher than the upper limit of the highest literature range.

Table 3.9: Comparison of raw ratios and literature ratio between compounds in wastewater.

Compounds	**Pairs**	**Computed ratio**	**Henze et al. (2002, 2008)**		
			Low	Typical	High
COD_t/BOD_t	24	3.6	1.5-2.0	2.0-2.5	2.5-3.5
COD_t/TN	47	9.1	6-8	8-12	12-16
COD_t/TP	48	66.9	20-35	35-45	45-60
BOD_t/TN	28	4.0	3-4	4-6	6-8
BOD_t/TP	30	28.7	10-15	15-20	20-30
COD_t/VSS	48	1.7 *	1.2-1.4	1.4-1.6	1.6-2.0
COD_t/TOC_t	40	4.3	2-2.5	2.5-3.0	3-3.5
NH_4-N/TN	386	0.7		0.7	

* This value was calculated from COD_t/TSS ratio using the typical literature ratio VSS/TSS=0.8 (Henze *et al.*, 2008) to calculate VSS

According to Table 3.9 the analysed wastewater presents a high COD_t/BOD_t ratio. This denotes the presence of industrial wastewater in the incoming

sewage; this perception is confirmed by the high values of the other ratios pertaining COD.

The model requires intensive input data to properly perform a long-term simulation (420 days) with 24 h time step. Therefore the data treatment step was required.

First, linear regression was implemented to estimate some of the missing values and fill some gaps in the incomplete data set (Hey *et al.*, 2012).

The procedure described below was applied to these couples of compounds:

- COD_t - TSS
- $NH_4 - N$ - TN
- COD_s - BOD_s

The COD_t and TSS couple is chosen as example to explain the data treatment. First data measured in the same day were selected *e.g.* for COD_t - TSS the number of pairs was 48 (see Figures 3.7 and 3.8).

Secondly it is necessary to calculate and compare the ratios between the compounds of each couple to the literature ratio.

Then the linear regression between each couple of compounds is calculated. During days in which one data of the couple was available, the other one was determined via the calculated linear regression.

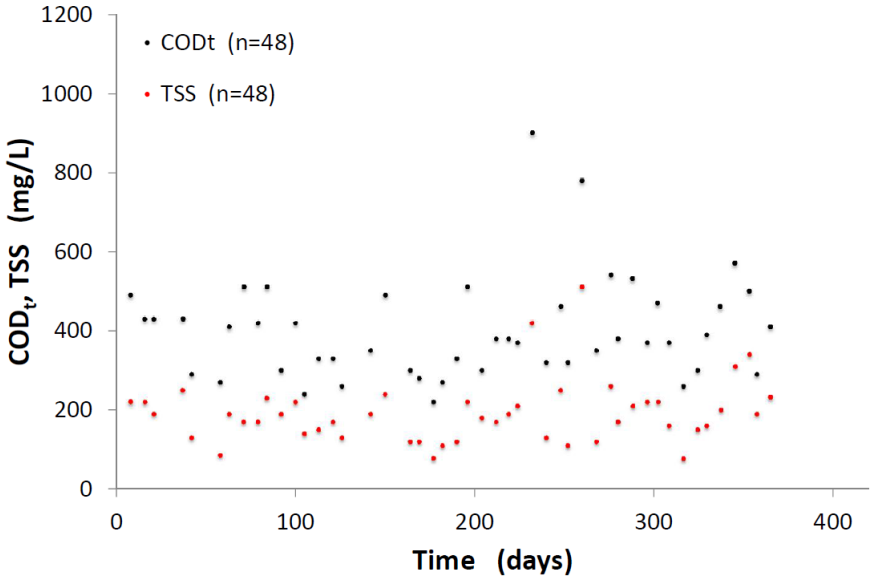

Figure 3.7: Time series of COD_t and TSS pairs (available measured data).

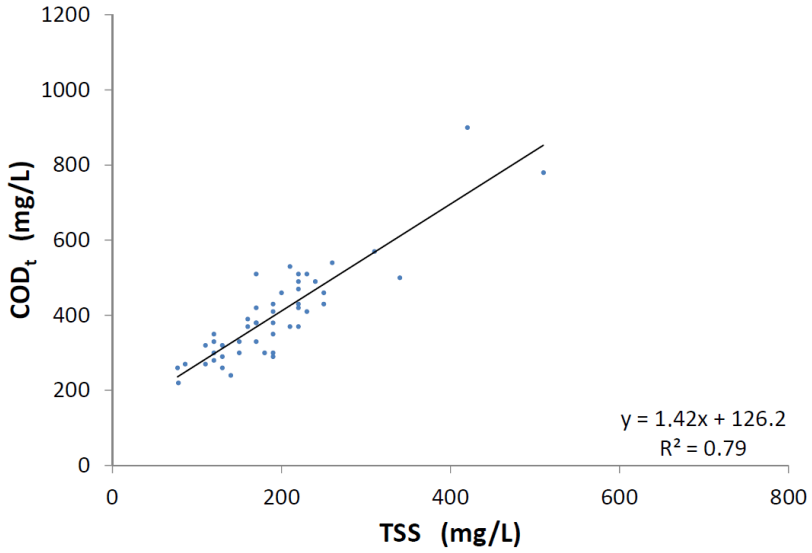

Figure 3.8: Scatter plot of COD_t and TSS with the best fit line (available measured data).

Afterwards, the remaining values of COD_t and TSS concentration, that were not measured on the corresponding day, were calculated using the linear equation: Respectively 169 and 1 values. In Figures 3.9 and 3.10 the values calculated by the usage of linear regression between COD_t and TSS are included.

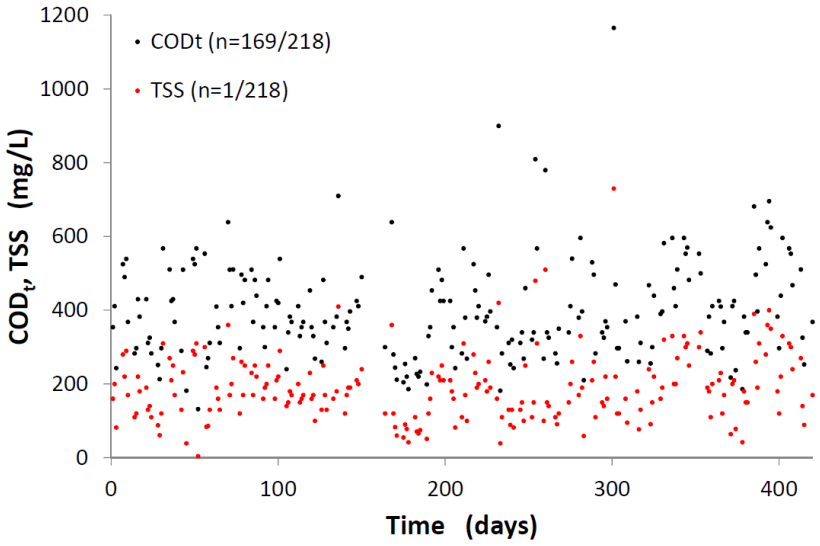

Figure 3.9: Time series (top) including all the COD_t and TSS calculated and measured values.

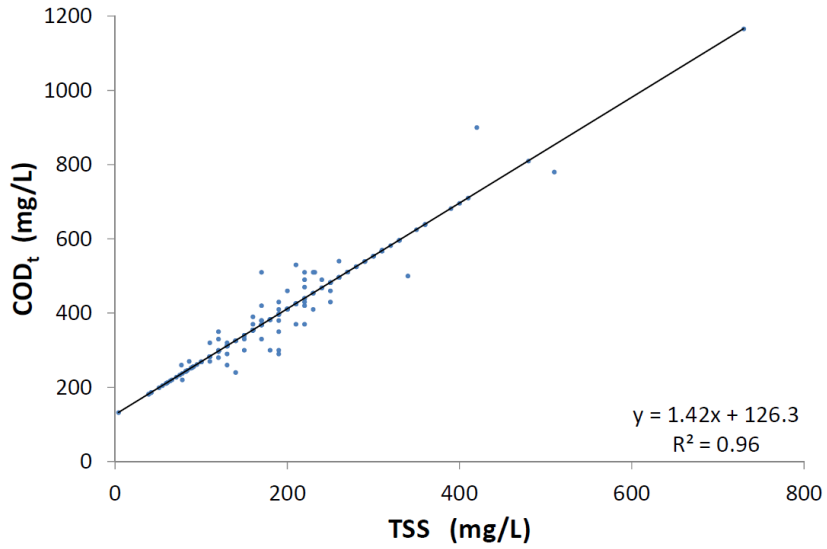

Figure 3.10: Scatter plot (bottom) with the best fit line including all the COD_t and TSS calculated and measured values.

Finally, to complete the data series, the complete series means, monthly means and weekly means values were used to fill the gaps. In Figures 3.11 and 3.12 the complete series average values were used. Using the mean of the complete data set to fill a large number of gaps reduced the actual variation and smoothed the dynamic fluctuations of the real system.

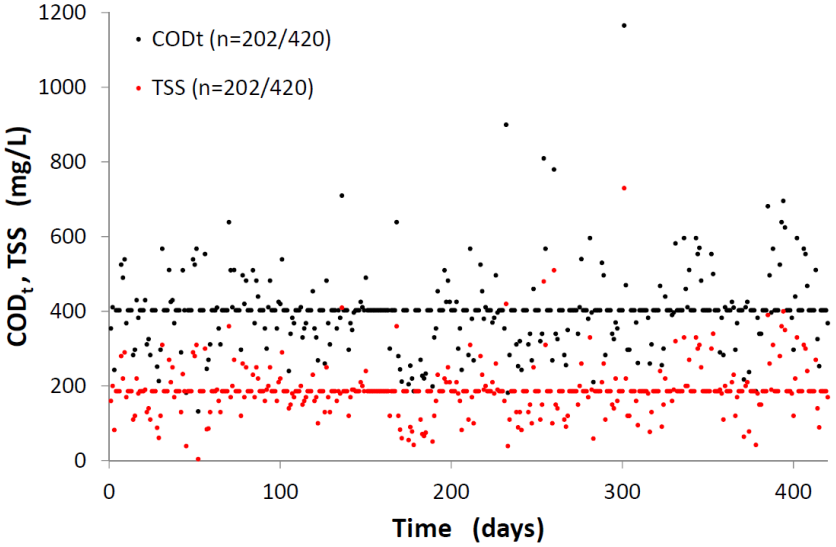

Figure 3.11: Complete (420 days) time serie of COD_t and TSS values, including measured data, data obtained from linear regression and averages calculated from the complete series of the measurement.

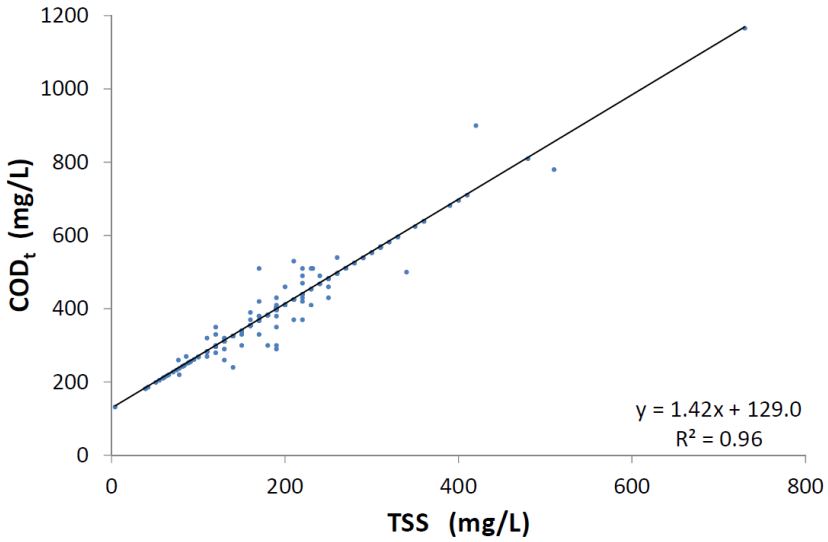

Figure 3.12: Complete (420 days) scatter plot of COD_t and TSS values, including measured data, data obtained from linear regression and averages calculated from the complete series of the measurement.

Figures 3.13 and 3.14 show the complete data series, filled out using monthly mean values. Using the monthly average values reflected more likely the seasonal variability of the influent concentration, in comparison of the data obtained filling the gaps with means of the complete data series.

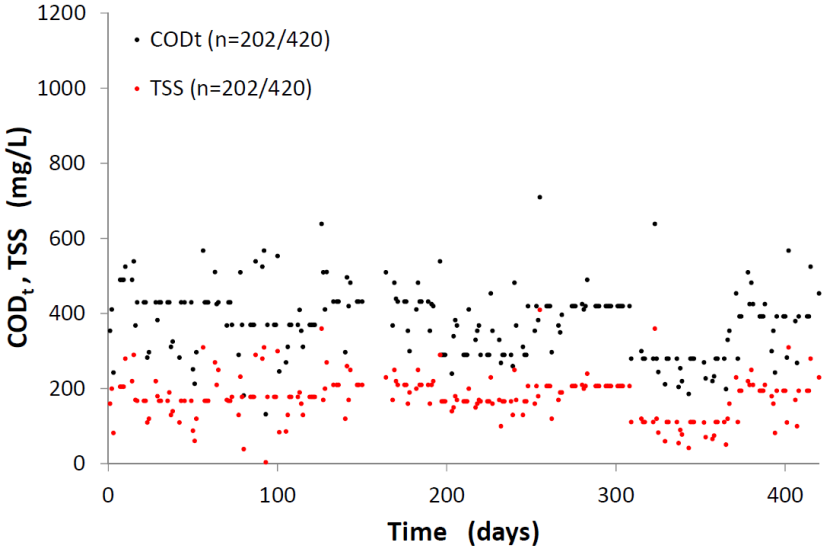

Figure 3.13: Complete (420 days) data set of COD_t and TSS values, including measured data, data obtained from linear regression and averages calculated monthly from the measured data.

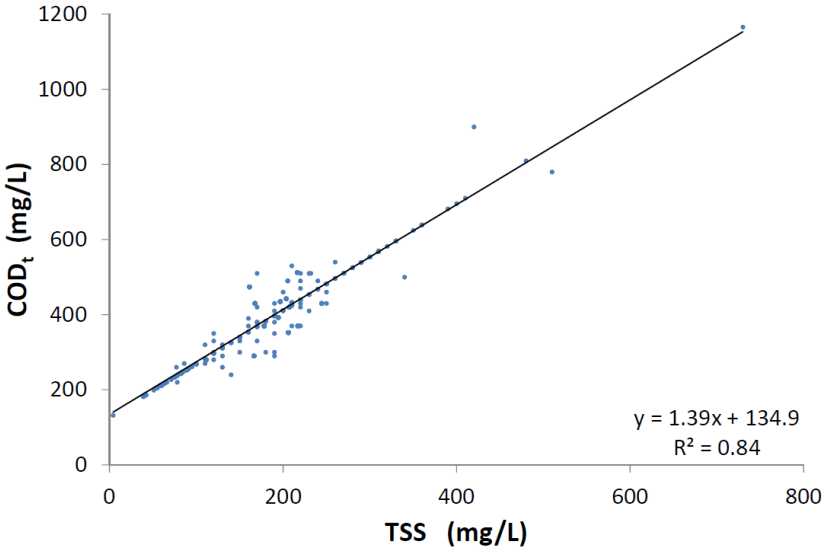

Figure 3.14: Complete (420 days) scatter plot of COD_t and TSS values, including measured data, data obtained from linear regression and averages calculated monthly from the measured data.

Figures 3.15 and 3.16 show the complete data series, filled out using weekly mean values.

The usage of weekly average data seemed to depict better the dynamic behaviour of the influent: The data are more scattered.

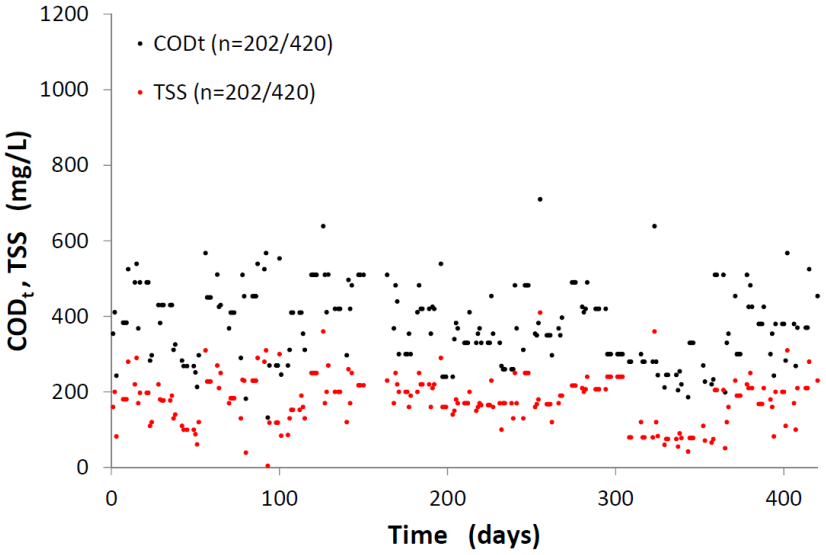

Figure 3.15: Complete (420 days) data set of COD_t and TSS values, including measured data, data obtained from linear regression and averages calculated weekly from the measured data.

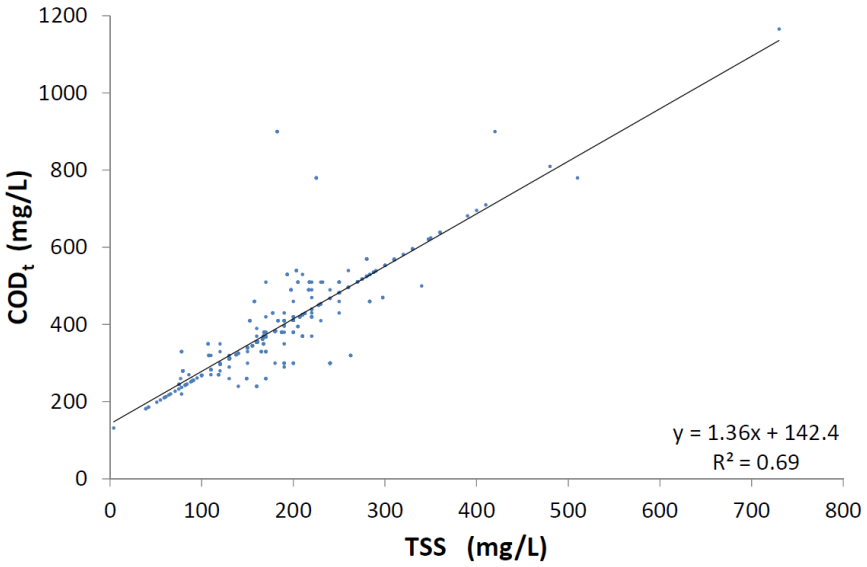

Figure 3.16: Complete (420 days) data set of COD_t and TSS values, including measured data, data obtained from linear regression and averages calculated weekly from the measured data.

When one data of a couple was missing for entire weeks or months, this was recovered using the linear equations presented in the graphics previously. If both data of a couple were missing for entire weeks or months, data of the same week/month of the previous/next year were used instead.

The same data treatment was applied to the couples NH_4-$N - TN$, $COD_t - BOD_t$ and $COD_s - BOD_s$. The remaining data treatment is shown in appendices.

Recovering data from an initial low amount was characterised by a considerable workload. Data are affected by the scarcity of the number of the measurements.

However, weekly series mean values were selected to fill the gaps, since they mimic better the dynamic behaviour of the plant, and the R squared are admissible (see Table 3.10).

Last component useful for the simulation was the TP. Being most of the measurements available in the considered period (388 data), gaps in the series were filled with weekly mean values in order to have a complete input string.

Table 3.10: Comparison of ratio (r) and R square coefficient between raw and processed data.

		Raw data	**Linear regression**	**Complete average**		
				Complete average	Monthly average	Weekly average
COD_t/TSS	n	48	218	420	420	420
	R^2	0.789	0.958	0.957	0.843	0.690
	r	1.7	1.9	1.8	1.8	1.9
NH_4-N/TN	n	386	391	420	420	420
	R^2	0.728	0.730	0.730	0.737	0.742
	r	0.8	0.8	0.8	0.8	0.8
COD_t/BOD_t	n	24	54	420	420	420
	R^2	0.404	0.565	0.543	0.157	0.428
	r	3.6	3.0	2.5	2.5	2.8
COD_s/BOD_s	n	22	54	420	420	420
	R^2	0.607	0.727	0.614	0.218	0.664
	r	2.1	3.6	2.5	2.5	3.1

Chapter 4

Results and Discussion

In this chapter mostly the graphics from line B1, the first biological line, are shown in order to summarize the results of the biological treatment. Model outputs are compared with real measurements and interpretations are attempted.
The results from the remaining biological lines are presented in appendices.

4.1 Fractionation model

The default ASM NO.1 fractionation of WEST® is presented in Fig. 4.1.
The fractionation model requires the following data recovered with the data treatment step as inputs:

- Water
- COD
- TSS
- TKN

The fractionation calculates the input file for the dynamic model from these data.
The outputs are the 12 state variables explained in Section 1.3.1 plus the H_2O variable containing the flow. Most of the 13 fractions (blocks with right pointed arrow) are calculated as portion of those measured input (blocks with left pointed arrow), see Figure 4.1.

The fractions calculated from the blocks containing the number 1 are fixed to constant concentrations.

The default values of the conversion factors to generate the state variables and the default fixed concentrations are presented in Table 4.1.

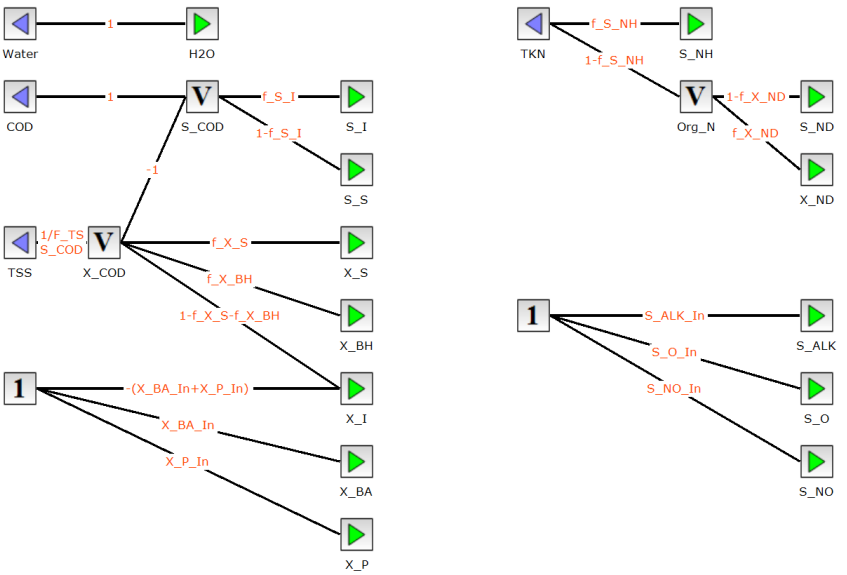

Figure 4.1: Standard ASMTemp1 (version of ASM NO.1 in WEST®) fractionation model. This figure is excerpted from the WEST® template (DHI, 2014d).

Table 4.1: Default parameters in the fractionation layout. (DHI, 2014d).

Parameter	**Description**	**Value**	**Unit**
$F_{TSS/COD}$	Conversion factor TSS/COD	0.75	-
f_{S_i}	S_i fraction of COD_s	0.25	-
f_{X_s}	X_s fraction of COD_x	0.75	-
$f_{X_{bh}}$	X_{bh} fraction of COD_x	0.1	-
$f_{S_{nh}}$	S_i fraction of COD_s	0.65	-
$f_{X_{nd}}$	X_{nd} fraction of biodeg. organic nitrogen	0.6	-
$X_{ba,in}$	Autotrophic biomass	0.01	g/m^3
$X_{p,in}$	X_p	0.01	g/m^3
$S_{alk,in}$	Alkalinity	30	g/m^3
$S_{O,in}$	Oxygen	0.01	g/m^3
$S_{no,in}$	Nitrate	0.01	g/m^3

As an example the X_i fraction is calculated as follow: First the particulate COD (X_{COD} in Figure 4.1) is obtained, which is determined by: $X_{COD} = \frac{TSS}{F_{TSS/COD}}$. Then the X_i is calculated with the formula 4.1:

$$X_i = (1 - f_{X_s} - f_{X_{bh}})X_{COD} - X_{ba,in} - X_{p,in} \tag{4.1}$$

The standard Activated Sludge No.1 fractionation model was then adapted to include also the following type of data as inputs:

- COD_s (soluble COD)
- COD_b (biodegradable COD)
- S_i
- TN
- NH_4-N
- Alkalinity

The measured values of these variables were included directly, instead of calculating them as rates of total COD and TKN. In the modified fractionation model the TN measurements were included, since they were the only available data regarding the overall nitrogen amount. Furthermore, measured values of alkalinity were included (see Figure 4.2), while measured values of TSS were excluded since in the default fractionation layout they are used to obtain particulate fractions of COD.

COD, TSS, COD_s, TN and NH_4-N were directly available in the measured data set.

Källby being a wastewater treatment plant receiving medium low diluted sewage, full S_s removal efficiency in the plant is expected. Furthermore the inert soluble COD production, which occurs in reality, is not simulated by the model , therefore it is possible to simply set S_i equal to the measured data of COD_s in the effluent.
The available measurements about soluble COD in the effluent were telling the modeller only that COD_s was always lower than 30 mgCOD/l. Hence it was assumed that the S_i was 3% of measured COD_t in the inlet, in order to have an influent S_i always lower than 30 mg/l, as reported by Roeleveld *et al.* (2002).

Then S_s was calculated as the difference between COD_s and S_i in the fractionation model.

COD_b was calculated through the use of BOD_7 measured data, as illustrated by Weijers (1999) and Roeleveld and van Loosdrecht (2002). First the calculation of ultimate BOD (BOD_∞) was needed. In fact, BOD_7 represents approximately 80% of the biodegradable matter, because the biodegradable organic matter is oxidised just partially after 7 days BOD test.

The formula used to determine the BOD_∞ is shown in equation 4.2:

$$BOD_\infty = \frac{BOD_7}{1 - e^{-7 \cdot k_{BOD}}} \tag{4.2}$$

where the k_{BOD} was assumed equal to the typical value of 0.23 d^{-1} (Metcalf & Eddy Inc. *et al.*, 2003).

Therefore the following conversion was obtained:
$BOD_\infty = \frac{BOD_7}{1-e^{-7 \cdot k_{COD}}} = \frac{BOD_7}{0.8} = 1.25\ BOD_7$.

Afterwards a conversion to COD_b was performed as illustrated in the formula 4.3:

$$COD_b = \frac{BOD_\infty}{1 - f_{BOD}} \tag{4.3}$$

where the correction factor f_{BOD} was set equal to 0.15 (in middle of the typical range 0.1 - 0.2) and it represents the particulate products arising from biomass decay during the BOD test (Roeleveld and van Loosdrecht, 2002).

Therefore $COD_b = 1.18\ BOD_\infty$ and the complete conversion was obtained: $COD_b = 1.47\ BOD_7$.

Once COD_b was known, the biodegradable particulate COD was calculated as follow: $X_{COD} = COD_b - S_s$ in the fractionation model.

Finally the remaining COD fraction contains X_i, X_p and the active biomass fractions. X_p and X_{ba} were kept unchanged from the default and both set to 0.01 g/m^3. X_{bh} was also set to 0.01 g/m^3, unlike in the default ASMTemp1 (commercial version of ASM NO.1) fractionation model, where it was set proportional to the particulate COD. In fact, according to Wentzel and Ekama (2006) the heterotrophic biomass can be considered negligible. Then

the X_i was determined subtracting from the remaining COD fraction, the sum of X_{ba}, X_p and X_{bh}.

Regarding the nitrogen modified fractionation, the TN was included in the model instead of the TKN, since it was the only available measurement. The standard calculated nitrite and nitrate fraction (S_{no}) was then subtracted to obtain TKN, even if it is almost negligible (0.01 mg/l).

Furthermore ammonium was directly included in the model and also subtracted from the TKN to obtain organic nitrogen, since the active nitrogen biomass is neglected in the nitrogen fractionation.

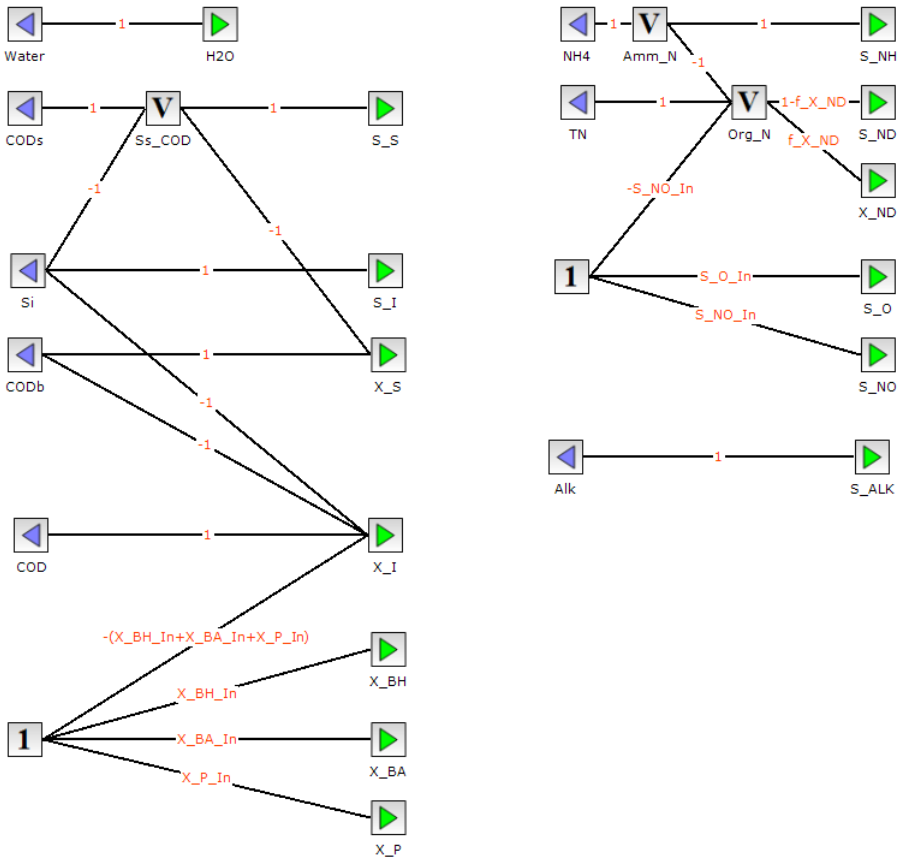

Figure 4.2: Modified ASMTemp1 fractionation model. This figure is excerpted from the WEST® template (DHI, 2014d).

In Table 4.2 parameters to fractionate the incoming raw wastewater are shown. The table emphasises the parameters that were used or not with

respect to the default; the table also shows the changed parameter related to the heterotrophic biomass in the influent (highlighted).

Table 4.2: Parameters in the modified fractionation layout (N = nitrogen).

Parameter	**Description**	**Value**	**Unit**	**Used**
$F_{TSS/COD}$	Conversion factor TSS/COD	0.75	-	✗
f_{S_i}	S_i fraction of COD_s	0.25	-	✓
f_{X_s}	X_s fraction of COD_x	0.75	-	✗
$f_{X_{bh}}$	X_{bh} fraction of COD_x	0.1	-	✗
$f_{S_{nh}}$	S_i fraction of COD_s	0.65	-	✗
$f_{X_{nd}}$	X_{nd} fraction of biodegradable organic N	0.6	-	✓
$X_{bh,in}$	Heterotrophic biomass	0.01	g/m^3	changed
$X_{ba,in}$	Autotrophic biomass	0.01	g/m^3	✓
$X_{p,in}$	X_p	0.01	g/m^3	✓
$S_{alk,in}$	Alkalinity	30	g/m^3	✗
$S_{O,in}$	Oxygen	0.01	g/m^3	✓
$S_{no,in}$	Nitrate	0.01	g/m^3	✓

In order to perform the dynamic simulation, first it is necessary to perform a steady state simulation to reach a stationary condition in the plant, especially with respect to the amount of TSS in the activated sludge and the amount of autotrophic biomass, which requires a certain time for growth and resettling in the biological stage.

The input for the steady state is calculated by the software and is presented in Table 4.3

Table 4.3: Input data of the steady state simulation.

Parameter	Water	COD_t	COD_b	COD_s	S_i
Unit	m^3/d	g/m^3	g/m^3	g/m^3	g/m^3
Value	29132	396.5	240.4	125.3	11.9

Parameter	TN	NH_4-N	TSS	Alk
Unit	g/m^3	g/m^3	g/m^3	g/m^3
Value	41.7	30.9	187.8	297.5

Given the fractionation layout and the input data for the steady state, the state variables are presented in Table 4.4.

Table 4.4: Input state variables in the default (Def. frac.) and modified fractionation (Mod. frac.) layout.

Parameter	S_s	S_i	X_s	X_i	X_{bh}	X_{ba}	X_p
Unit	g/m^3	g/m^3	g/m^3	g/m_3	g/m^3	g/m^3	g/m^3
Def. frac.	109.5	36.5	187.8	37.5	25.0	0.01	0.01
Mod. frac	113.4	11.9	127.0	144.2	0.01	0.01	0.01
Diff. (%)	+3.6	-67.4	-32.4	+284.5	-99.9	=	=

Parameter	S_{nh}	S_{nd}	X_{nd}	S_{no}	S_o	S_{Alk}
Unit	g/m_3	g/m^3	g/m^3	g/m^3	g/m^3	g/m^3
Def. frac.	27.1	5.8	8.7	0.01	0.01	30
Mod. frac	30.9	4.3	6.4	0.01	0.01	297.5
Diff. (%)	14.0	-25.9	-26.4	=	=	891.7

As shown in Figure 4.3, in order to reach a stable concentration of TSS in the activated sludge, about 20-days steady simulation is required. The concentration achieved is equal to the set point of the controller of wastage sludge for the steady state.

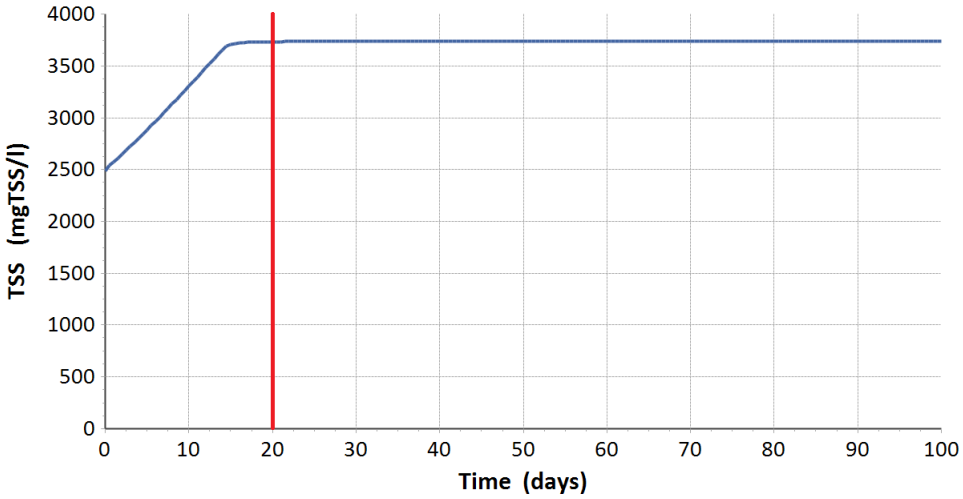

Figure 4.3: Growth of TSS in the last section of activated sludge tank line B1.

The growth of autotrophic and heterotrophic biomass and the concentrations of ammonium and nitrate during the steady state simulation are presented in Figure 4.4.

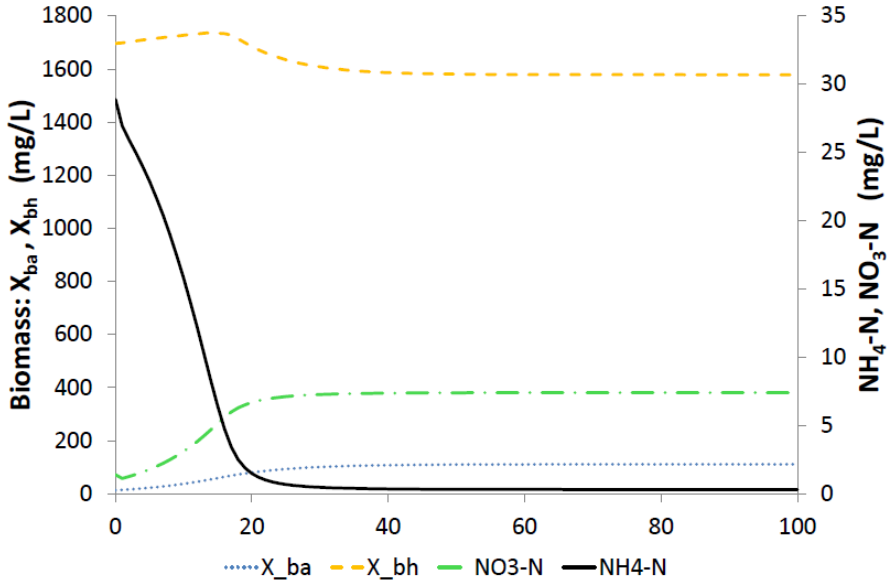

Figure 4.4: Biomass growth and substrate consumption in the last section of activated sludge tank in line B1.

As can be seen, autotrophs consume ammonium and are subjected to a fast growth within the first 25 days, when a large amount of ammonium is available. Therefore when this turns to be a limiting factor, their fast growth stops. The amount of nitrate increases as long as ammonium and oxygen are available for nitrification and NH_4 is consumed at the same time.
The lowering in concentration of heterotrophs is faster when the denitrification process starts to balance the production of nitrate due to nitrification and the increase of the nitrate slows (around day 20). Another limiting factor is availability of easily biodegradable carbon: Its lack may stop and/or inhibit the process.
After the steady state is finished, the first dynamic simulation is performed. In WEST® the derived state variables of the steady state are used as initial conditions for the first dynamic simulation. After that, it is possible to initialize the dynamic simulation via the previous dynamic simulation.

4.2 Reference scenario results

In this section outputs from line B1 are shown as example, representing the results of the model (ASM1Temp in WEST®) also in the remaining biological lines. The data are compared with real measurement from Källby

wastewater treatment plant and an exhaustive interpretation of the results is then attempted.

The remaining outputs from the other biological lines are presented in appendices. Lines B3 and B4 are presented combined, since the available data were measured in an output combining the two lines.
The following data are presented below:

- TSS
- TN
- $NO_3 - N$
- $NH_4 - N$

First data to be presented is the TSS, since this is the first one to be adjusted as similar as possible as the real values, in order to have a realistic response of the model and in order to have biological processes in the activated sludge tanks.

The model data are from the last section of the biological line B1 as well as the measurements (see Figure 4.5). Results regarding the TSS concentration in the activated sludge units of lines B2, B3 and B4 are shown respectively in Figures 6.18, 6.22 and 6.23 in Appendices.

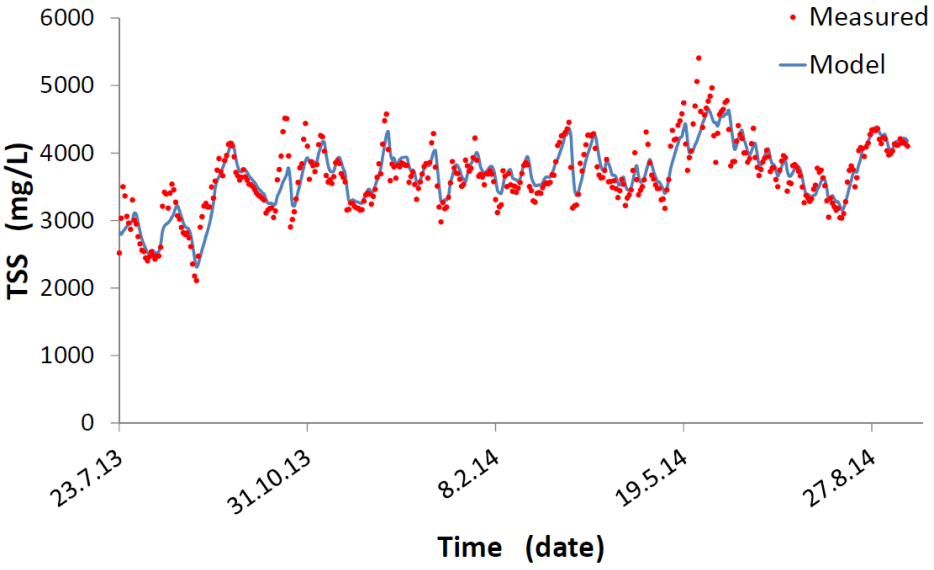

Figure 4.5: Comparison between model output (blue line) and measurements of TSS (dots) from line B1.

The model fits almost completely with the measurements, since the measured data were used as set-point to control the concentration of the suspended solids in the activated sludge units. Afterwards a check needs to be done: The amount of surplus sludge should be almost the same amount as the one in the reality, in order to have a reasonably comparable sludge retention time.

Although the model get slightly worse when the variations are faster than usual, for instance around 31/10/2014 and after 19/05/2014 (see Figure 4.5).

Secondly, in Figures 4.6, 4.7 and 4.8 results regarding nitrogen are presented. As can be seen in figures 4.6, 4.7 and 4.8, results are basically included in the range of the real measurements.

Regarding the total nitrogen and the nitrate, the model shows a trend of overestimation with respect to the measured values (see Figures 4.6 and 4.7). Instead the ammonium fits quite well with the measurements at least considering lines B1 and B2 (see Figures 6.19, 6.20 and 6.21 in Appendices), while lines B3 and B4 are not well represented (see Figures 6.24, 6.25 and 6.26 in Appendices).

Considering that the gap is even larger with regard to NO_3 concentration (see Figure 4.7), it can be concluded that the model perform a full nitrification, but the denitrification process is not performing well.

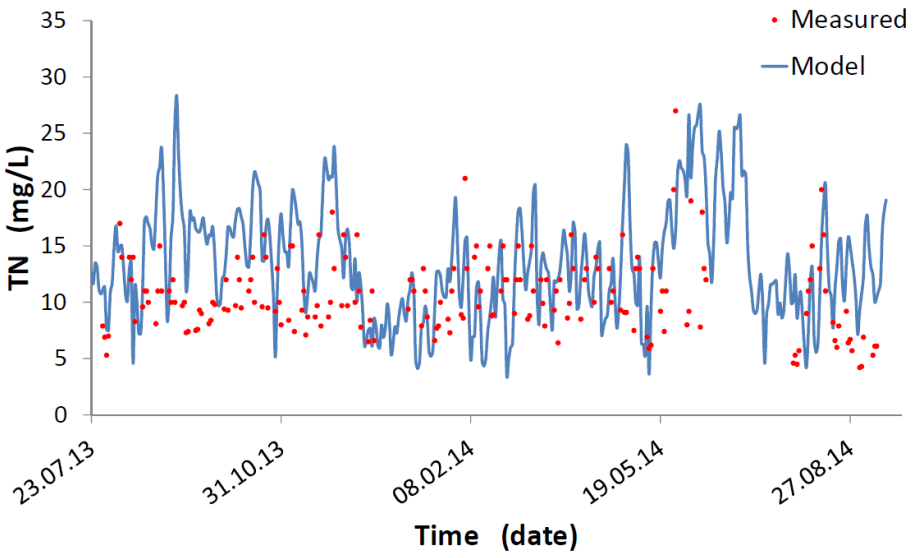

Figure 4.6: Comparison between model output (blue line) and measurements (dots) of TN from line B1.

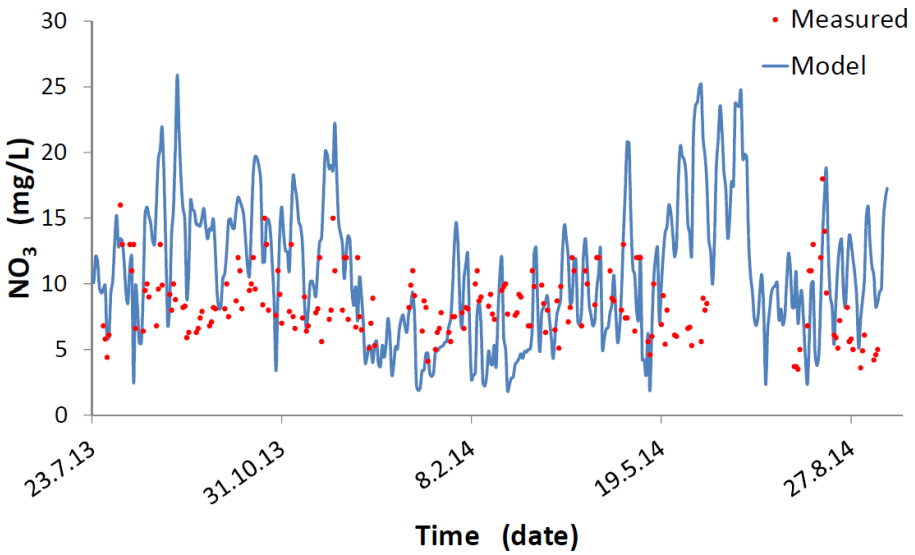

Figure 4.7: Comparison between model output (blue line) and measurements (dots) of NO_3-N from line B1.

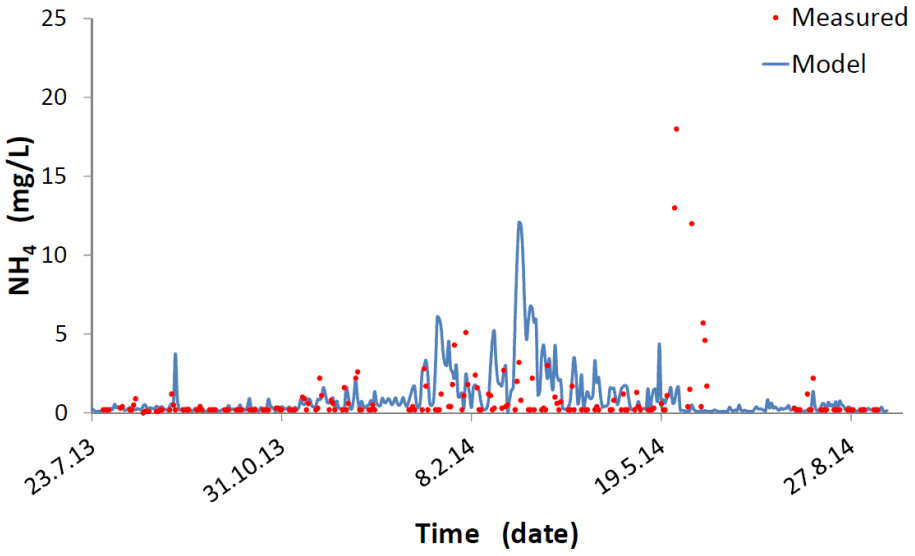

Figure 4.8: Comparison between model output (blue line) and measurements (dots) of NH_4-N from line B1.

It might also be the case that the nitrification process is performing too well. In fact, as can be seen in the outputs from lines B3 and B4 combined presented in appendices, a tendency of underestimation of ammonium with respect to the measurement is shown by the model. That means that even though the trend is broadly correctly mimicked, the variations are represented by the model, but the peaks are not of the right magnitude and the average value is lower in the model.

In Figure 4.8 the results regarding the ammonium concentration are shown; the $NH_4 - N$ concentration in the model is different from the measured one.

The real measurements are for most of the year around 0.2 mgNH_4-N/l but some peaks appear in mid-autumn and especially in winter. This is probably related to the lower temperatures, that cause a lowering in bacteria activity, according to Arrhenius (1889a and 1989b).

Other peaks are probably due to changes in operation: For instance those around 19/05/2014 (see the Figure 4.8). In fact on this day biological line B3 is shut down and its flowrate and loading is entirely deflected to line B4 for a period about 30 days.

The model simulates quite well these peaks in lines B3 and B4 (see Figures 6.24 in Appendices), while these are not shown by lines B1 and B2.
This may be due to a power failure that would led to the turning off of the blowers providing air in the activated sludge tanks and thus to the inhibition/interruption of the aerobic processes. Another possible cause might be the fact that during some periods in which *e.g.* B3 is turned off its flowrate is entirely deviated to the activated sludge units of line B4 but after them it is split to all running secondary settlers and not just to the secondary settler after line B4, and vice versa. This would get an impact on the outputs from lines B1 and B2 during these periods.

In Table 4.5 a comparison between the mean values obtained at the end of the dynamic simulation and from real measurement is shown. It highlights the fact that the model overestimate the total nitrogen and the gap is mostly due to the difference between modelled and measured NO_3 and NH_4.

The outputs of the model from lines B3 and B4 are compared jointly with measurements, since the available data were measured in an outlet combining the treated water from both lines. The average values reported for

lines B3 and B4 for TN, NO and NH were calculated as average values from the outputs from lines B3 and B4, when both were working (since they treat the same flowrate). Whenever one line was out of operation, the combined outputs from lines B3 and B4 were set equal to the outputs of the running line.

The reasons for this general tendency of overestimation are further discussed in section 4.3.

Table 4.5: Comparison between modelled and measured average values for TN, NO_3 and NH_4 from the biological lines.

	Measurements			**Model**		
	TN	NO_3	NH_4	TN	NO_3	NH_4
Unit	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l
B1	10.6	8.4	0.8	13.5	10.8	1.0
B2	11.0	7.9	1.7	13.5	10.1	1.8
B3, B4	11.1	5.6	1.5	13.6	10.9	1.1

In Table 4.6, the mean values from the outlet of the secondary settler of the four biological lines are reported.

Table 4.6: BOD_5, COD and TSS simulated average values from the biological lines.

Parameter	BOD_5	COD	TSS
Unit	mg/l	mg/l	mg/l
B1	3.0	28.3	11.1
B2	3.0	27.8	10.8
B3	2.9	27.6	10.6
B4	2.9	27.9	10.9

Considering the BOD_5 and COD, results are in line with the few available measurements, even if the results are not so easy to be compared, being the measurement BOD_7 instead of BOD_5. The measurements report that BOD_7 was always lower than 3 mg/l.

In Figures 4.10 results regarding the post precipitation of phosphorus are shown.

As can be seen, the modelled S_{PO} fits the measurements after the tertiary settler, while the TP is underestimated after the pond by the simulation.

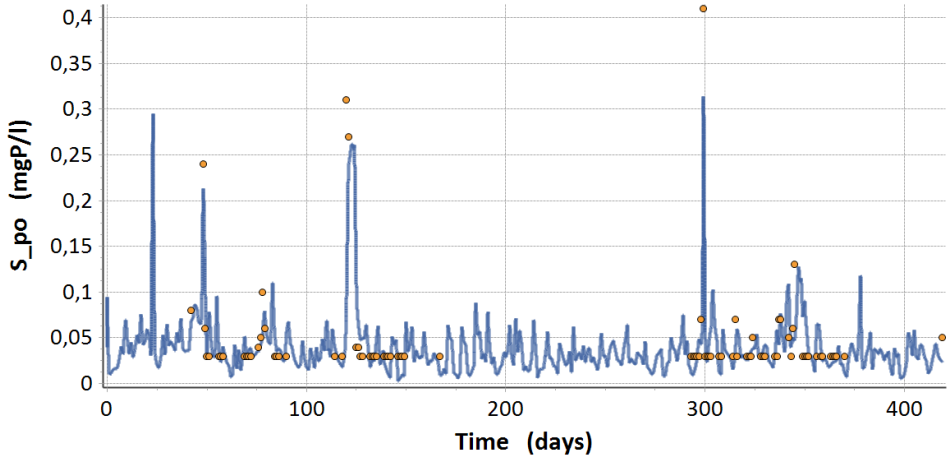

Figure 4.9: Comparison between model output (blue line) and measurements (dots) of S_{PO} from the tertiary chemical precipitation.

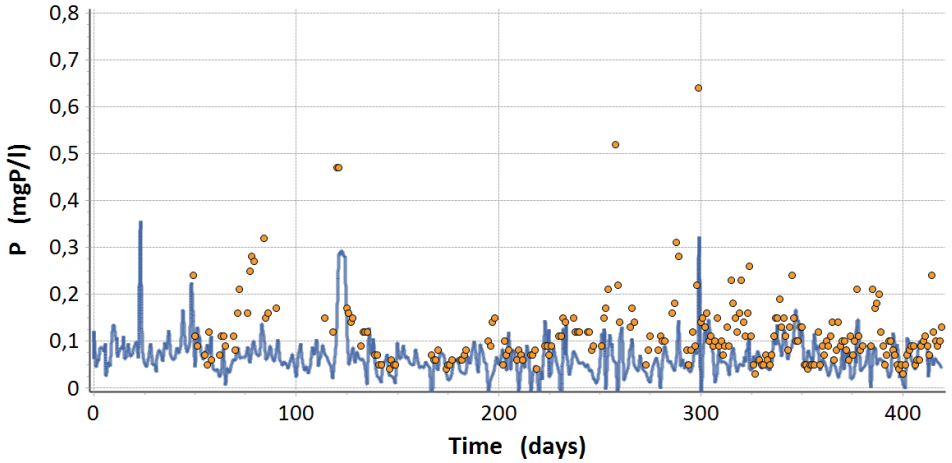

Figure 4.10: Comparison between model output (blue line) and measurements (dots) of TP from the outlet of the pond.

4.3 Results of calibration

During calibration the main mismatches of the model with respect to the measured data should be identified and the modeller should try to find solution in other to improve the simulation outputs.

Probably the main issue to be discussed and solved is the general trend of overestimation of nitrogen and nitrate and underestimation of ammonium. The primary reason might be the longer sludge age related to aerated zones

in the model, which could lead to a too well nitrification performance. In fact it is proved that sludge age is the fundamental parameter to design/model activated sludge treatment (van der Lubbe *et al.*, 2012).

According to Hammer *et al.* (2014) the definition of sludge age is given by the equation 4.4:

$$Sludge\ age = \frac{TSS_{AS}\ V_{ae}}{TSS_e\ Q_e + TSS_w\ Q_w} \tag{4.4}$$

where *Sludge age* is the mean cell residence time (days), TSS_{AS} is the mixed-liquor suspended solids concentration in the activated sludge units (mg/L), V_{ae} is the volume of aerated tanks (m^3), TSS_e is the concentration of TSS in the effluent, Q_e is the flowrate of the effluent (m^3/d), TSS_w is the concentration of TSS in the surplus (or wastage) sludge, Q_w is the flowrate of the wastage sludge (m^3/d).

The sludge ages of each biological treatment line achieved with the first set-up of the model is presented in Table 4.7. A threshold on the oxygen content equal to 0.5 gO_2/L has been considered at each 1 day-time step for each section, in order to decide whether to include the volume of a section in the calculus of aerated sludge age.

Table 4.7: Calculated sludge ages in the biological treatment lines

		Sludge age (days)			
	Line	B1	B2	B3	B4
Season	Summer 2013	26	34	19	43
	Autumn 2013	20	19	26	23
	Winter 2014	18	24	21	23
	Spring 2014	25	24	28	33
	Summer 2014	31	30	26	31
	Average	24	25	27	32

According to Table 4.7, sludge age appears to be too high. In fact, as stated by Marx *et al.* (2010), the sludge age is usually in the range 3-30 days, depending on the type of activated sludge treatment plant and surplus sludge extraction amount. Also the plant operators affirmed that the sludge age is much lower.

Moreover, being nitrification less performing in biological treatment lines B3

and B4, the sludge ages in these two lines are expected to be lower compared to lines B1 and B2. In fact, a significant performance of the nitrification process is achievable only if the sludge age is long enough (van Haandel *et al.*, 2012).

Regarding the values of the last two biological lines during summer 2013: On one hand the calculation of sludge age of line B3 takes into account just the first 10 days of the simulation, that is the period when this line is turned on. Thus it is not so meaningful. On the other hand the sludge age of line B4 is affected by the increased incoming flowrate when B3 is turned off.
Additionally, the sludge ages of summer 2013 are likely to be affected by the wrong initial condition. In fact the starting condition of the dynamical simulation is the last condition of the steady state simulation and thus the initial condition may be inaccurate.

Given the formula 4.4, the overestimation of sludge age might be due to one or more among the following reasons:

- Inaccurate fractionation of the incoming raw wastewater
- Overestimation of primary settler performance
- Overestimation of secondary settler performance
- Underestimation of surplus sludge extraction
- Overestimation of the effective aerated zones total volume.

In fact a imprecise fractionation, especially regarding a possible substantial underestimation of X_i fraction in the influent, causes an underestimation of sludge production. This leads to lower surplus sludge extraction and thus to overestimate the sludge age. Indeed the X_i fraction is included in the inactive sludge and in municipal wastewater it is in the order of 20-35% of the total sludge concentration concentration (Gerardi, 2002). Depending the sludge production (and thus the wastage sludge amount) on the TSS concentration in activated sludge units, this can affect the sludge age.
Overestimation of the primary clarifier efficacy generates a higher production of primary sludge, which contains X_i. This brings on the underestimation of TSS in the mixed liquor within activated sludge units, driving also to a too long sludge age.
Overestimation of the secondary settler performance causes lower TSS concentration in the effluent and hence to a high sludge age.

Underestimation of surplus sludge flowrate brings on a underestimation of the denominator of the right-hand side of equation 4.4 and thus to an overestimation of the left-hand side.

Regarding the effective aerated volume of activated sludge units, surprisingly it might be also overestimated by the model. Indeed, in the existing plant the aerated volume might be lower than the nominal total volume.

This may result from a non-perfect mixing within the overall volume in the aerated zones especially at the corners of the tanks or to the malfunctioning of some air diffusers. Contrariwise in the model the volume is perfectly stirred, as a result of the use of the continuous flow stirred-tank reactor model for the tanks in ASM NO.1. Regarding the existing lines B3 and B4, the rectangular shape of the tanks in these two lines may cause a considerably lower effective aerated volume compared to the model and thus to an overestimation of the sludge age in the simulation.

Another cause leading to a lower effective aerated volume might be the malfunctioning of some diffusers at the bottom of the basins.

The first assumption during the calibration step was assume that the X_i was correctly estimated by the modified fractionation explained in section 4.2, since the X_i 284% higher than the X_i obtained by applying the default layout (see Table 4.4).

After all the previous considerations, first the ratio TSS/COD in the primary settler was changed from the default value of 0.75 to 0.7, calculated from measurement from the inlet of the plant.

Furthermore, the suspended solids removal efficiency of the primary settler was corrected by adjusting the non-settleable fraction of suspended solids (f_{ns}) in the Takács primary clarifier model. This parameter was changed from the default value of 0.0024 to 0.19, in order to switch the average TSS removal efficiency from ca. 41% to ca. 35%. In fact the suspended solids removal efficiency in the existing primary settler is 30-40%, as stated by the plant operators. Furthermore 0.18 represents a more realistic fraction for non-settleable on total suspended solids and it is similar to the values set by Gernaey *et al.* (2001) and Coderre (1999).

Moreover, the f_{ns} of secondary settlers of lines B3 and B4 were changed from default value of 0.0028 to 0.005 since sometimes there are leaks of TSS from these two biological treatment lines, as stated by the plant operators.

Last, the minimum amount of surplus sludge extracted from biological treatment units was changed from 20 to 40 m^3/d in lines B1 and B2 and from 30 to 70 ^{3}/d in lines B3 and B4, in order to have a lower sludge age.

All the previous adjustments were based on trial error approach. Values of f_{ns} and minimum wastage sludge amount were modified taking into account the fact that the TSS concentration in the activated sludge model must match the measurements. Therefore the f_{ns} of the secondary settler and the minimum surplus sludge extraction cannot be further raised.

As a result, sludge ages lowered considerably in all treatment lines, as shown in Table 4.8.

Nevertheless sludge age of lines B3 and B4 is still higher than lines B1 and B2. However model outputs did not improve significantly their fit with measured data.

Table 4.8: Calculated sludge ages in the biological treatment lines after calibration.

		Sludge age (days)			
	Line	B1	B2	B3	B4
Season	Summer 2013	17	21	12	24
	Autumn 2013	14	14	16	16
	Winter 2014	13	17	15	16
	Spring 2014	17	16	18	20
	Summer 2014	20	21	17	18
	Average	16	18	18	19

Additionally, in order to get an impact on the processes concerning nitrogen (ammonification, nitrification and denitrification) within lines B3 and B4 some kinetic parameters were changed.

Maximum specific growth rate for heterotrophs ($\hat{\mu}_h$) from default value 6 to 6.6 d^{-1}, max. autotrophic growth rate ($\hat{\mu}_a$) from 0.8 to 0.72 d^{-1} and nitrate half-saturation constant for denitrifying heterotrophic biomass (K_{NO}) from 0.5 to 0.4 g NO_3-N/m^3.

In appendices in Table 6.2 default/changed stoichiometric and kinetic parameters used during the first model set-up/calibration are shown. Changed parameters are highlighted and their values are reported.

In Figures 4.11, 4.12 and 4.13 the comparison between first model set-up, results of the calibration and measurements from biological lines B3 and B4

combined after the secondary settlers can be seen. The representation of processes involving nitrogen slightly improved.

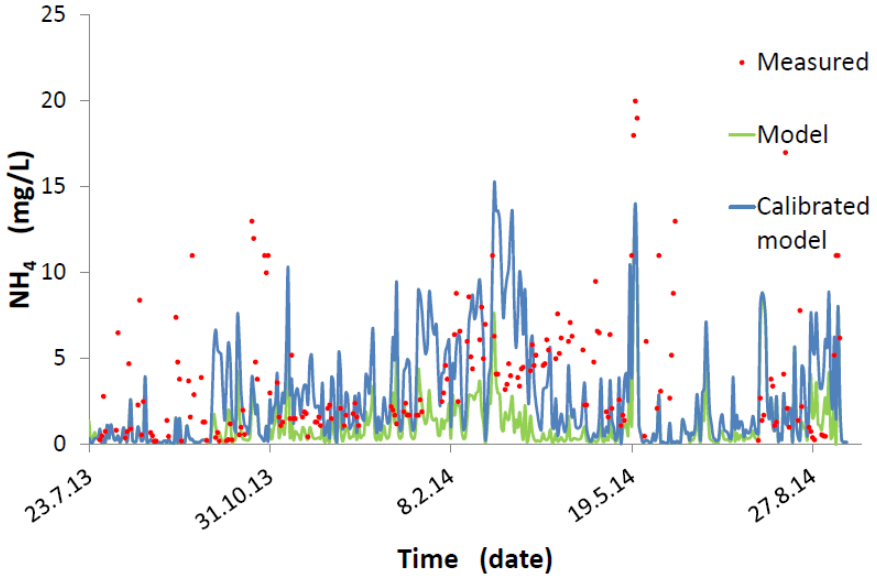

Figure 4.11: Comparison between calibrated model output (blue line), model after the first set-up (light green line) and measurements (dots) of NH_4-N from lines B3 and B4 combined.

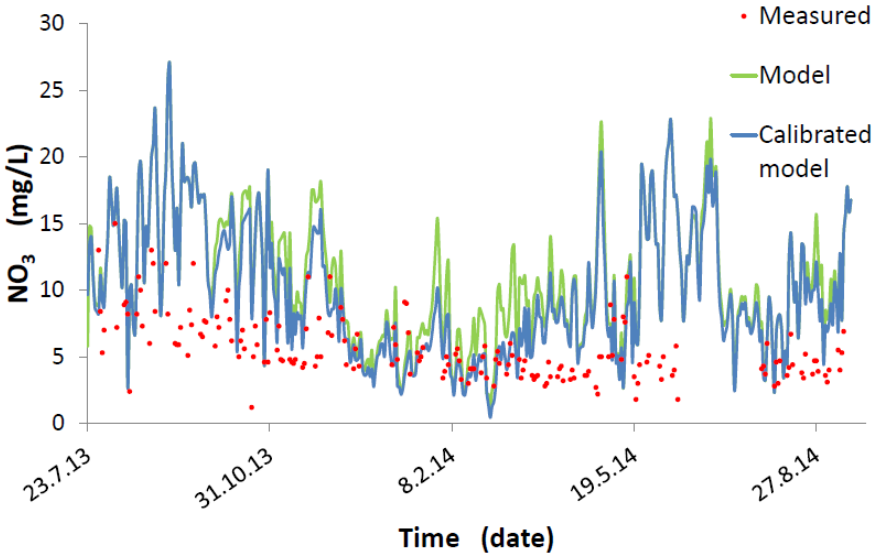

Figure 4.12: Comparison between calibrated model output (blue line), model after the first set-up (light green line) and measurements (dots) of NO_3-N from lines B3 and B4 combined.

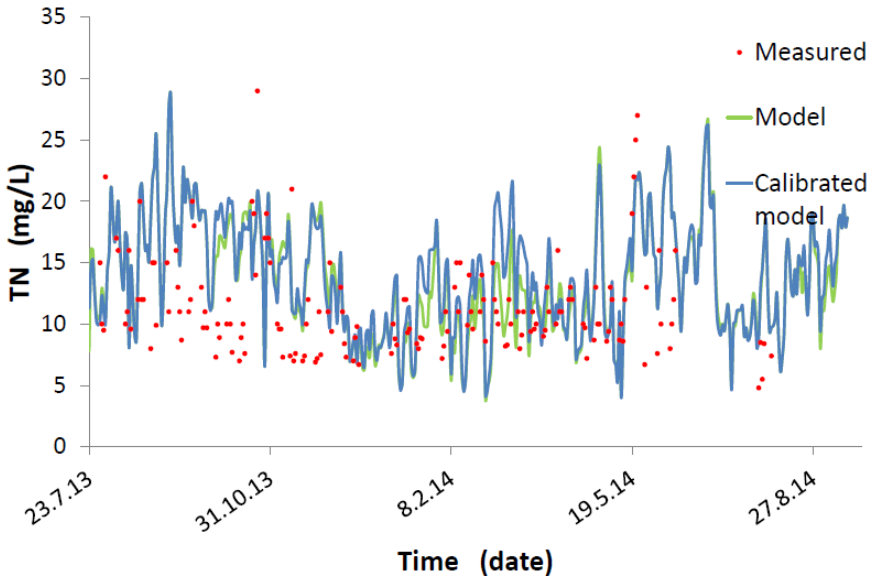

Figure 4.13: Comparison between calibrated model output (blue line), model after the first set-up (light green line) and measurements (dots) of TN from lines B3 and B4 combined.

Regarding the results of the calibration (see Figures 4.11, 4.12 and 4.13): On one hand the ammonium increased significantly and the nitrogen lowered considerably, especially in the middle of the studied period, the one that showed the main mismatches after the first model set-up. On the other hand total nitrogen was slightly affected by the calibration. Anyway the process did not correct remarkably the results.

The main reason why the calibration process was not very satisfying may be related to the poor influent data and/or to an inadequate fractionation at the beginning of the model set-up and/or to a poor representation of the primary settler behaviour.

The latter consideration brings to the following related reflections.

Only available measurements were used as inputs such as loadings and as boundary conditions for the model *e.g.* temperatures, dissolved oxygen and TSS measurements. No supplementary measuring campaigns were performed.

Nevertheless the first constraint of the model is the lack of relevant data, *e.g.* poor loading data, especially those regarding organic matter. Furthermore the time series regarding the mixed liquor and sludge recycle flowrates and

features for all four biological lines were missing and/or not reliable mainly due to the fouling of meters.

At this point a comment has to be done: If it is intended to model an existing plant there are two conflicting needs to be considered. In fact, the modeller would like to have the greatest number of data as possible, whereas the operator of the plant wants to minimize the number of required measurements to the amount needed to run the plant fulfilling the discharge requirements. Indeed, collection and measurement of data is not a cost to be neglected in running a wastewater treatment plant, in terms of time, money and employees.

In fact the main constraint of the model is the lack of some relevant data, *e.g.* poor loading data, especially those regarding organic matter. Furthermore the time series regarding the mixed liquor and sludge recycle flowrates and features for all four biological lines were missing and/or not reliable mainly due to the fouling of meters.

To solve the problem of missing data concerning the loading data, a rather large number of reasonable assumptions and hypotheses has been made, *e.g.* those regarding the influent characterisation during the fractionation, the settings of the recycled flowrates and the definition of the recycles and the surplus sludge extraction.

These are the main sources of uncertainty together with the unreliability of some measurements, especially those from the on-line meters.

Chapter 5

Conclusions

The main conclusions regarding the model results and calibration are presented in this section.

This study confirms the actual feasibility of setting up the Källby wastewater treatment plant in a mathematical model. Wastewater treatment lines were included in the model, while sludge treatment lines were excluded.

Only available measurements were used as inputs such as loadings and as boundary conditions for the model *e.g.* temperatures, dissolved oxygen and TSS measurements. No supplementary measuring campaigns were performed.

Focus of the work was the potential for nitrogen and phosphorus removal. Comparison of data regarding nitrogen and phosphorus fraction was allowed, since a large number of measurement regarding these compounds from the outlet of the secondary settler of the existing plant was available.

Regarding the available data provided by routine analysis, it can be stated that:

- They were in sufficient amount to achieve a satisfying model regarding nitrogen removal: The general trends of TN, NO_3-N and NH_4-N were replicated, especially considering outputs from biological lines B1 and B2; further measuring campaigns are needed to improve the representation of lines B3 and B4
- They were enough to simulate the phosphorus precipitation
- They were not in sufficient amount to simulate full scale Källby wastewater treatment lines including a satisfying representation of the primary settler

and/or the sludge treatment lines

- By linear regression and by using weekly averages it is possible to recover missing data and generate the needed input file containing the loadings in the inlet of the plant, but this is also a source of uncertainty
- By calibration of the ratio TSS/COD, the settling parameter f_{ns} in the primary settler, the surplus sludge extraction and f_{ns} of the secondary settler it was possible to lower the sludge age; Nevertheless an acceptable calibration of nitrogen removal in lines B3 and B4 was not achieved.

The result of this thesis is a deeper understanding of the actual behaviour of the plant and it has also an educational purpose of the dynamic behaviour of a WWTP. In the immediate future it is possible to use this model for the achievement of many goals:

- The knowledge achieved could be used by the plant operators to trouble-shoot some operational issues and/or to find some better control strategies *e.g.* evaluate whether the recycle of the mixed liquor is necessary or the recycle of sludge from the secondary settler is enough to respect the discharge limits regarding nitrogen; it can also be assessed if the recycled flowrate can be lowered
- Predict dynamic responses of the system to new scenarios *e.g.* influent variation (flow and/or concentration) and test possible solutions
- Forecast the effects of disturbances such as changing in temperature or failure of some compartments of the plant, in order to develop strategies and solutions to improve and optimise treatment plant operation
- Assess different operational settings with respect to energy efficiency and resource usage *e.g.* lower the aeration flowrate and evaluate whether the discharge limits are satisfied.

Chapter 6

Future works

The present work established a reference scenario for the actual behaviour of the plant. In this section some suggested further work are presented.

In order to have a fine-tuned model, further measurement campaigns and extra on-line meters are needed, especially regarding primary clarifier settling parameters, underflow from primary and secondary settlers, recycles flowrates in the activated sludge step and ammonium rich reject water from sludge treatment lines.

Since the currently available data were too poor to simulate the primary settler, one option for future simulations of the plant may be excluding the primary settler from the model and perform the measurements for the input loadings after the primary settler.

Therefore some suggested future works related to the modelling are listed below:

- Perform intensive measurement campaigns and/or install some new on-line meters in order to have a fine-tuned model *e.g.* use of tracers to understand the hydraulic behaviour of activated sludge units of lines B3 and B4 and improve their representation
- Simulate and evaluate different treatment strategies, such as treating wastewater only mechanically (micro-screening and membranes), to compare with the reference scenario; to achieve this using the present commercial software an experienced modeller is needed
- Extend the model also to the sludge treatment lines, to evaluate biogas production in the anaerobic digester and allow optimisation of the process.

Regarding the latter, during the present work, a quick look at the incorporation of sludge treatment lines in the model was done, but this was not further investigated, due to the time limitation to carry out the master thesis project and the lack of relevant data regarding the compartments included (see Figure 6.1).

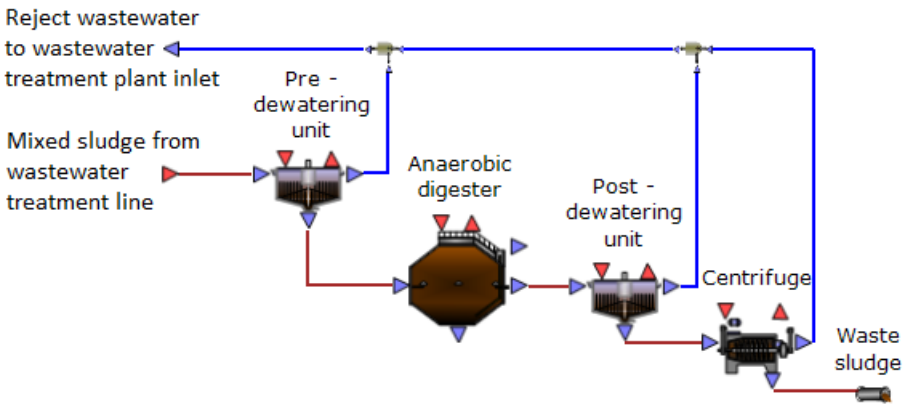

Figure 6.1: Sludge treatment lines layout. All displayed items in this figure are an excerpt from the WEST layout (DHI, 2014d).

It would be interesting to include in a single model biological and chemical wastewater treatment and sludge treatment.
On one hand ASM NO.1 includes anaerobic digestion, but the chemical sludge has to be disregarded because chemical treatment and precipitation of phosphorus is excluded from this model. On the other hand ASM NO.2d, besides nitrogen and carbon removal, allows the simulation of both biological and chemical phosphorus treatment, although it does not comprise anaerobic digester.

Thus one possible future work may be the modelling of the full scale Källby wastewater treatment plant, including sludge treatment, using the Plant Wide Model, which is also available in WEST® but has to be further developed before it can be profitably used.

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A wastewater treatment plant prediction in your computer

The Källby wastewater treatment plant was set-up in a mathematical model reflecting its actual behaviour.
Are the commonly available measurements good enough to perform a simulation? What kind of outcomes can we expect?

After you have read the heading and the introduction, I guess that two proper questions swirling around in your head might be: what is wastewater treatment and what is a model?

First wastewater treatment is the process that allows the return of sewerage and industrial wastewater to water cycle with minimal environmental impact and in accordance with existing discharge limits. There are three main reasons why this is performed: protect people from waterborne diseases that may be originated by contact with untreated wastewater, safeguard water environment from pollution that may arise from discharge of untreated wastewater and support of relevant life and economic systems.

Secondly I would answer that a model is the representation of a system of interest, that is something important to be studied. It often simplifies reality in order to describe only the relevant processes and makes use of software solutions to perform the required computations.

Modelling applied to wastewater treatment allows to simulate the actual physical, biological and chemical processes taking place in a wastewater treatment plant.

Now, why do we need to model a wastewater treatment plant?

Nowadays modelling is used as a design tool, instead of traditional design procedures. It is the most feasible and maybe less costly way to attain a process optimisation and it can also help the plant operators to test some corrective actions without expensive and environmentally risky full scale tests... wow!

Let's get to the point: The present work achieved to simulate the Källby wastewater treatment plant of Lund, Sweden. The work focused on the wastewater treatment lines, especially on carbon, nitrogen and phosphorus removal. The sludge treatment lines, necessary to dispose of sewage sludge produced during sewage treatment, were not included in the model.

Only available real data from the database of the company managing the plant were used to feed the model, without performing any additional measurement campaign.

A relevant part of the work regarded the data treatment concerning the influent concentration to generate the input file for the model. After that it was possible to perform the simulation.

At this point comparison between real measurements and model outputs was allowed. The reasons causing the main mismatches between the model outputs and real data were investigated and a troubleshooting step was performed in order to try to fix them.

Annual variations of nitrogen and phosphorus were shown by the model, meaning that, even with the limitation of poor data, modelling can still be a valuable tool to understand the behaviour of treatment plants and to predict the response of the plant to influent variations.

The result of this thesis is a deeper understanding of the actual behaviour of the plant. It also allows evaluations of new scenarios and possible future changes of the operation.

Knowledge achieved in this work could also be used by plant operator to troubleshoot or to find better control strategies.

Enjoy the reading!

Appendices

Dynamical modelling of wastewater treatment

Activated sludge model NO.1

Table 6.1: Process kinetics and stoichiometry for carbon oxidation, nitrification and denitrification (Henze *et al.* 2000a).

→ Component	i	1	2	3	4	5	6	7	8	9	10	11	12	13	Process Rate, ρ [M L-3 T-1]
j	Process ↓	S_i	S_s	X_s	X_s	X_{bh}	X_{ba}	X_p	So	S_{no}	S_{nh}	S_{nd}	X_{nd}	S_{alk}	
1	Aerobic growth of heterotrophs		$-\frac{1}{Y_h}$			1			$-\frac{1-Y_h}{Y_h}$		$-i_{xb}$			$-\frac{1}{14}$	$\hat{\mu}_h(\frac{S_s}{K_s+S_s})(\frac{S_o}{K_{oh}+S_o})X_{bh}$
2	Anoxic growth of heterotrophs		$-\frac{1}{Y_h}$			1				$-\frac{1}{2.86Y_h}$	$-i_{xb}$			$\frac{1-Y_h}{14\cdot 2.86Y_h-i_{xb}/14}$	$\hat{\mu}_h(\frac{S_s}{K_s+S_s})(\frac{K_{oh}}{K_{oh}+S_o})\cdot$ $\cdot\frac{S_{no}}{K_{no}+S_{no}}\eta_g X_{bh}$
3	Aerobic growth of autotrophs						1		$-\frac{4.57-Y_a}{Y_a}$	$\frac{1}{Y_a}$	$-i_{xb}-\frac{1}{Y_a}$			$-\frac{i_{xb}}{14}-\frac{1}{7Y_a}$	$\hat{\mu}_a(\frac{S_{nh}}{K_{nh}+S_{nh}})(\frac{S_o}{K_{oa}+S_o})X_{ba}$
4	Decay of heterotrophs				1-f_p	-1		f_p					$i_{xb}-f_p i_{xp}$		$b_h X_{bh}$
5	Decay of autotrophs				1-f_p		-1	f_p					$i_{xb}-f_p i_{xp}$		$b_a X_{ba}$
6	Ammonification of soluble organic nitrogen										1	-1		$\frac{1}{14}$	$k_a S_{nd} X_{bh}$
7	Hydrolysis of entrapped organics		1		-1										$k_h\frac{X_s/X_{bh}}{K_x+(X_s+X_{bh})}[(\frac{S_o}{K_{oh}+S_o})+$ $\eta_h(\frac{K_{oh}}{K_{oh}+S_o})(\frac{S_{no}}{K_{no}+S_{no}})]X_{bh}$
8	Hydrolysis of entrapped organic nitrogen											1	-1		$\rho_7(X_{nd}/X_s)$

Dynamical modelling of Källby wastewater treatment plant

Plant layout and simulations set-up

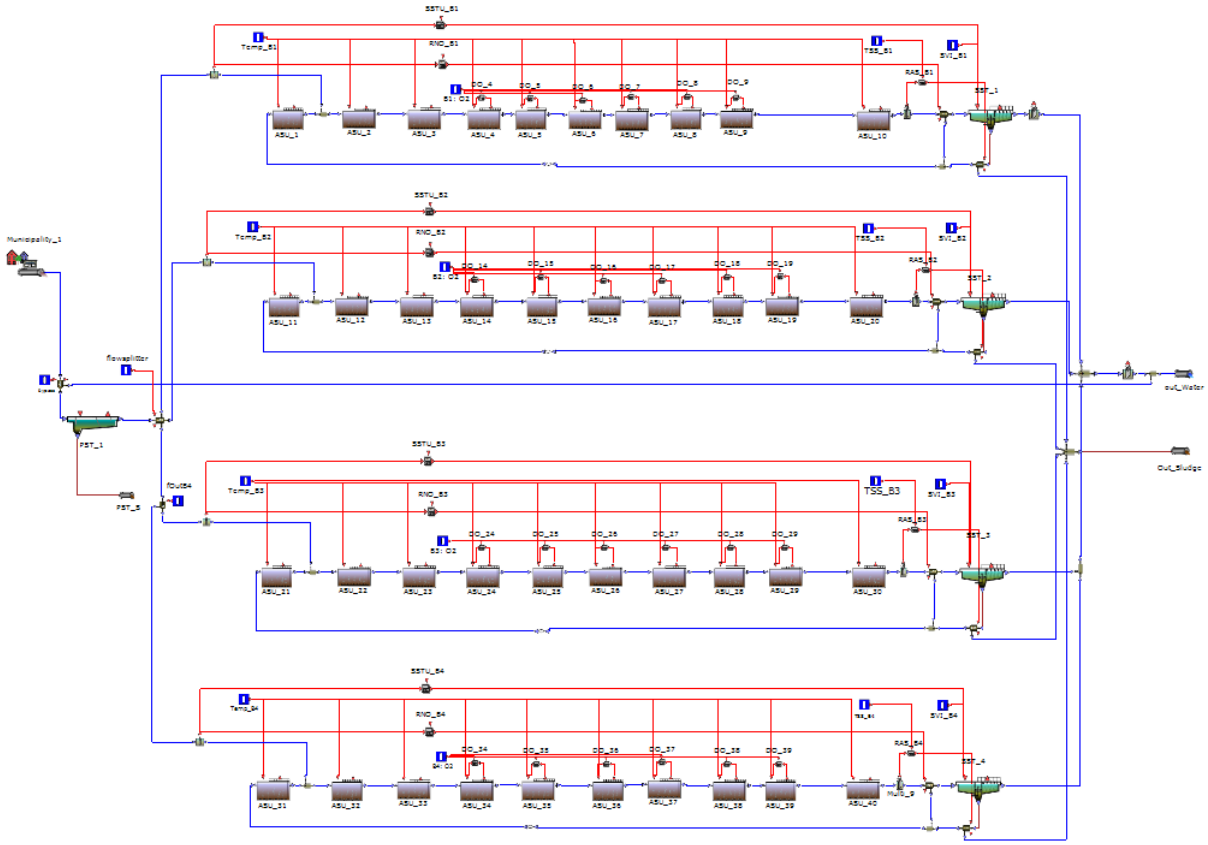


Figure 6.2: Layout of primary settler and secondary treatment step of Källby wastewater treatment plant's model. All displayed items in this figure are excerpted from the WEST® template (DHI, 2014d).

Data treatment

Nitrogen

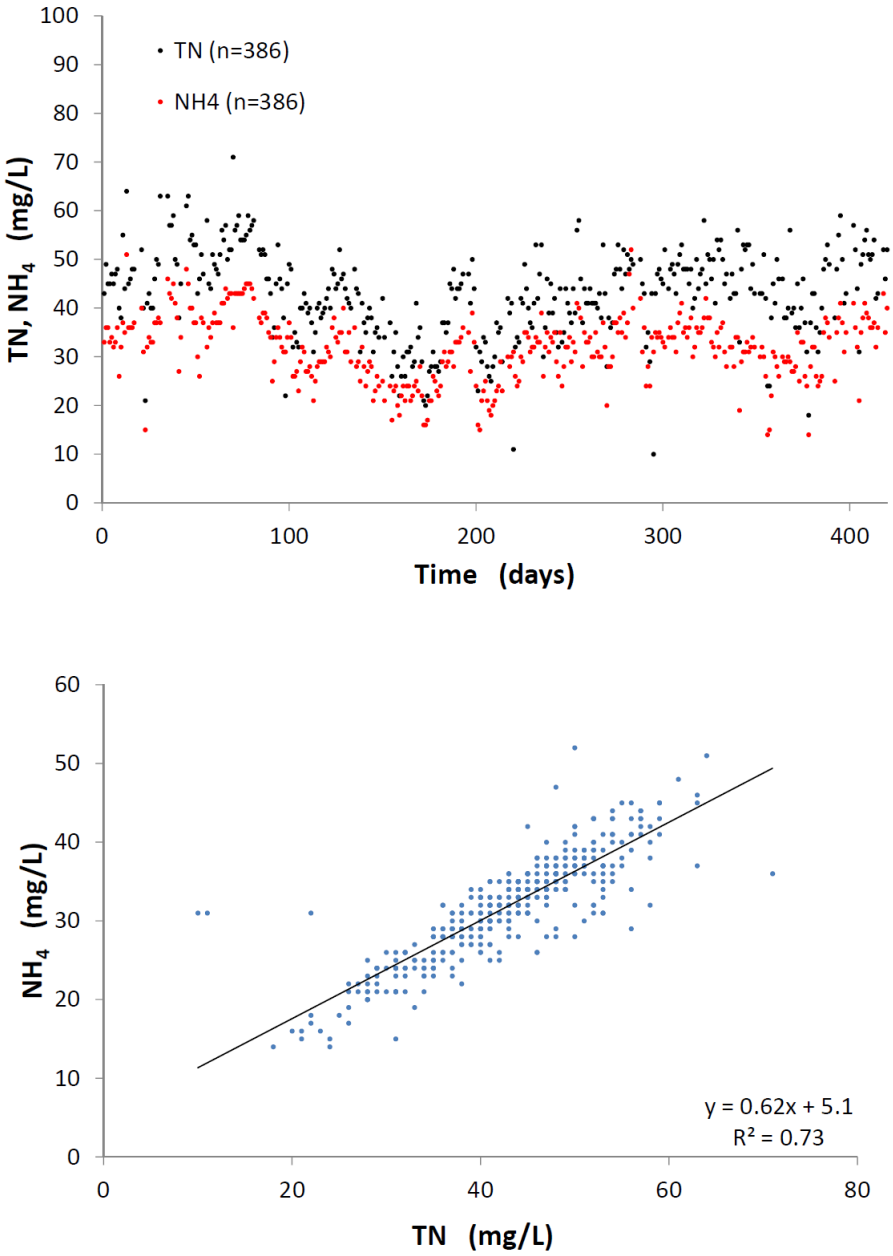


Figure 6.3: Initial available data set of total nitrogen and ammonia nitrogen; time plot (top) and scatter plot (with linear regression).

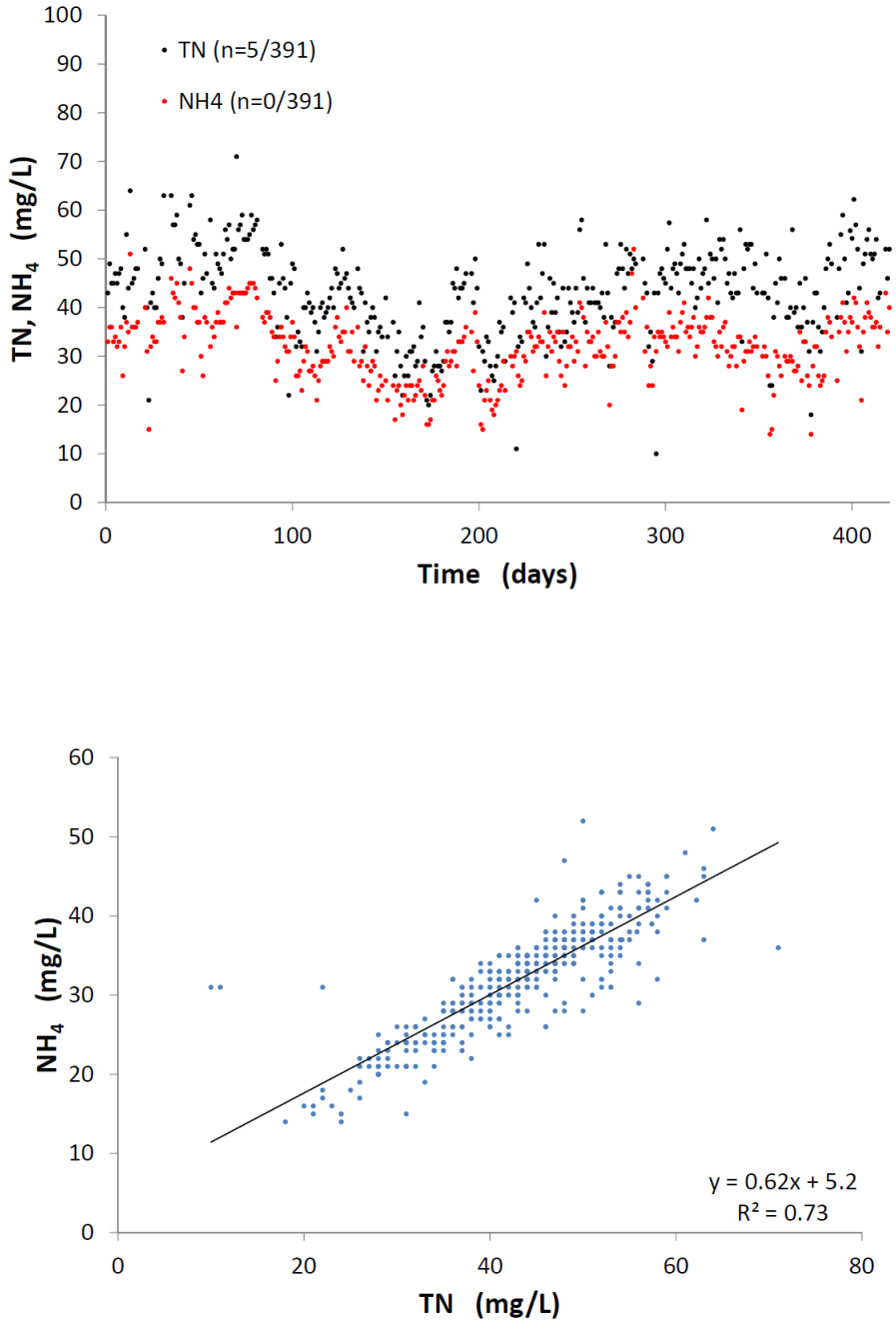


Figure 6.4: Time series (top) and scatter plot (bottom), including the total nitrogen and ammonia nitrogen measured and calculated (using linear regression) values.

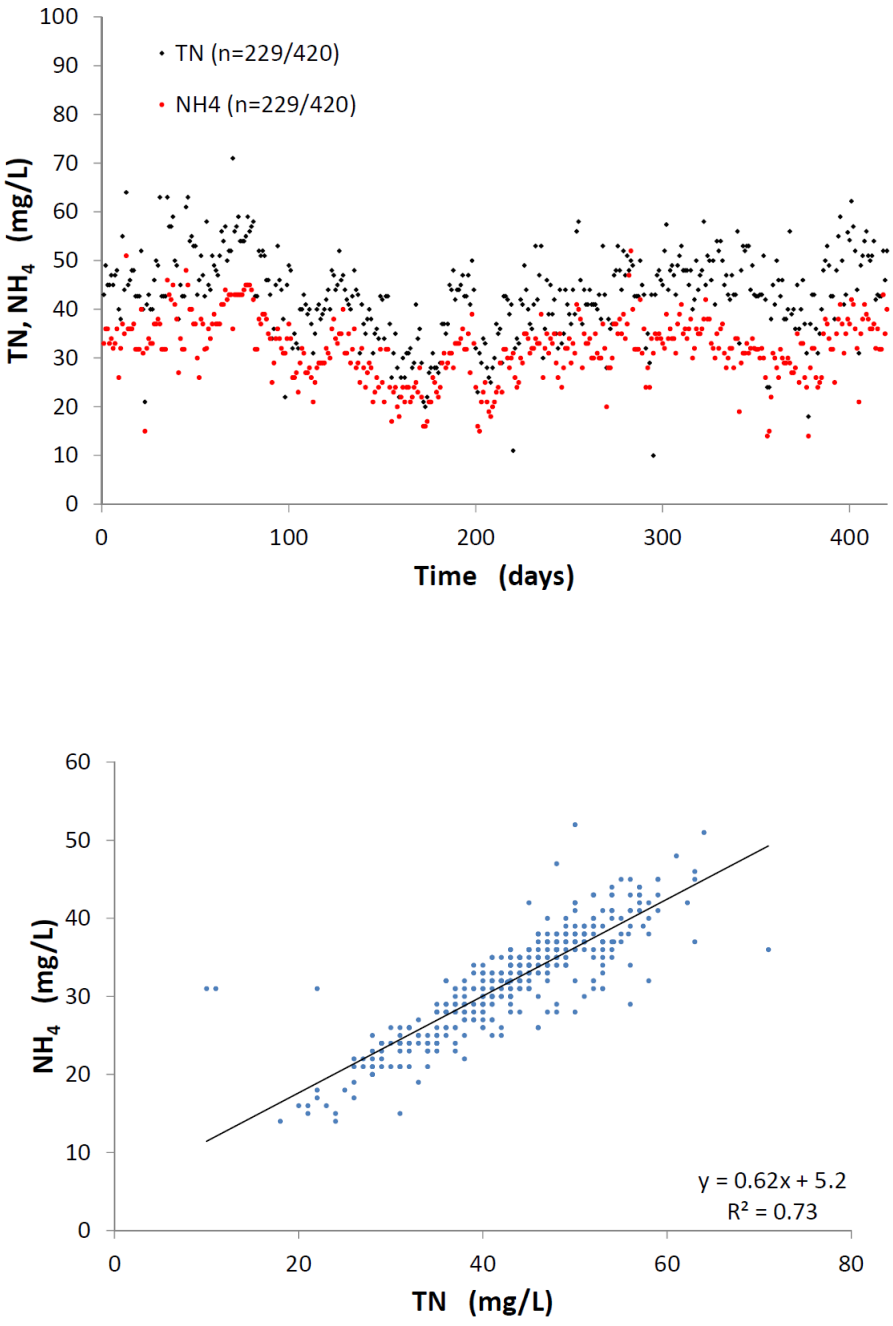


Figure 6.5: Complete (420 days) data set of the total nitrogen and ammonia values, including measured data, data obtained from linear regression and averages calculated from the complete series of the measured data.

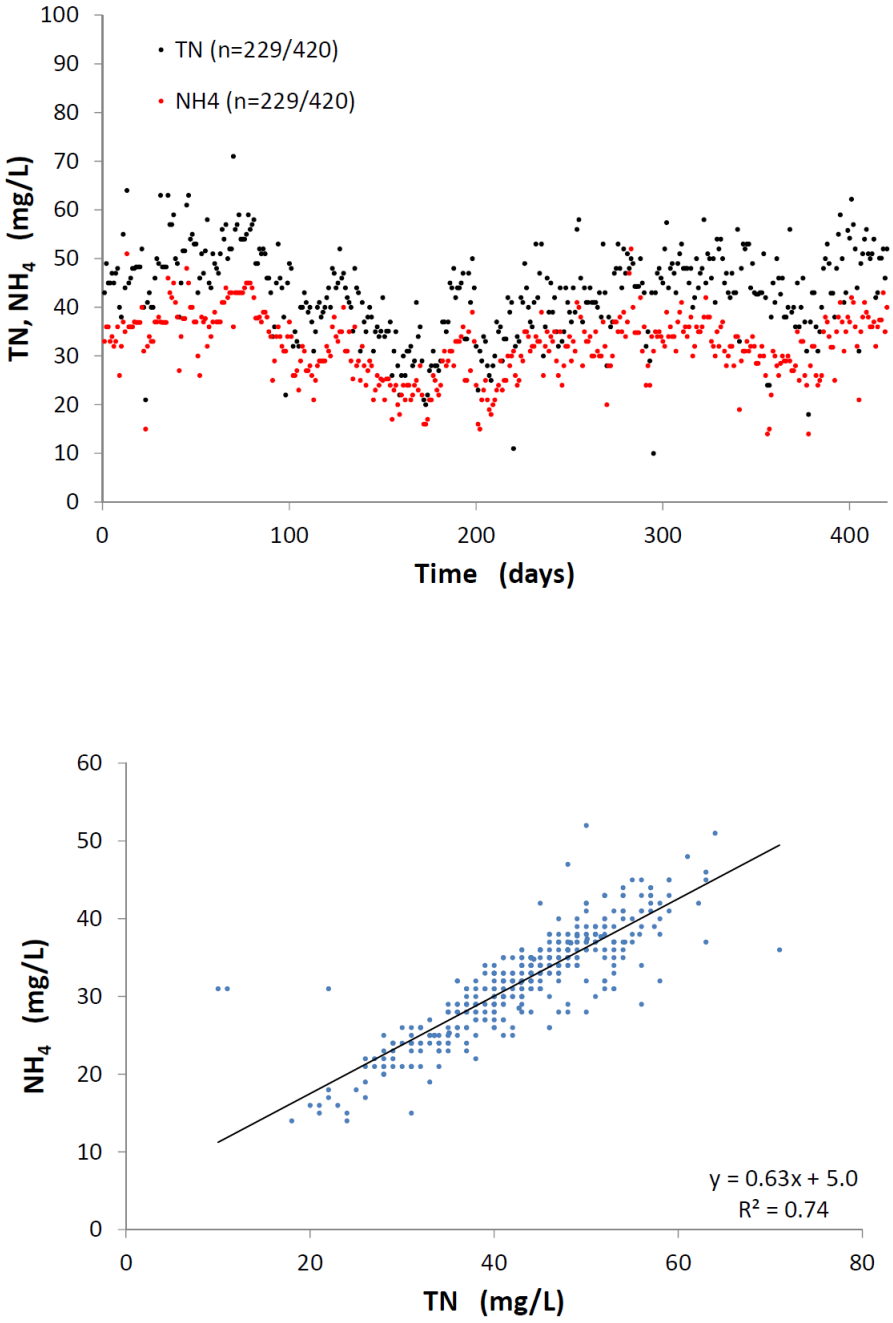


Figure 6.6: Complete (420 days) data set of the total nitrogen and ammonia values, including measured data, data obtained from linear regression and averages calculated monthly from the measured data.

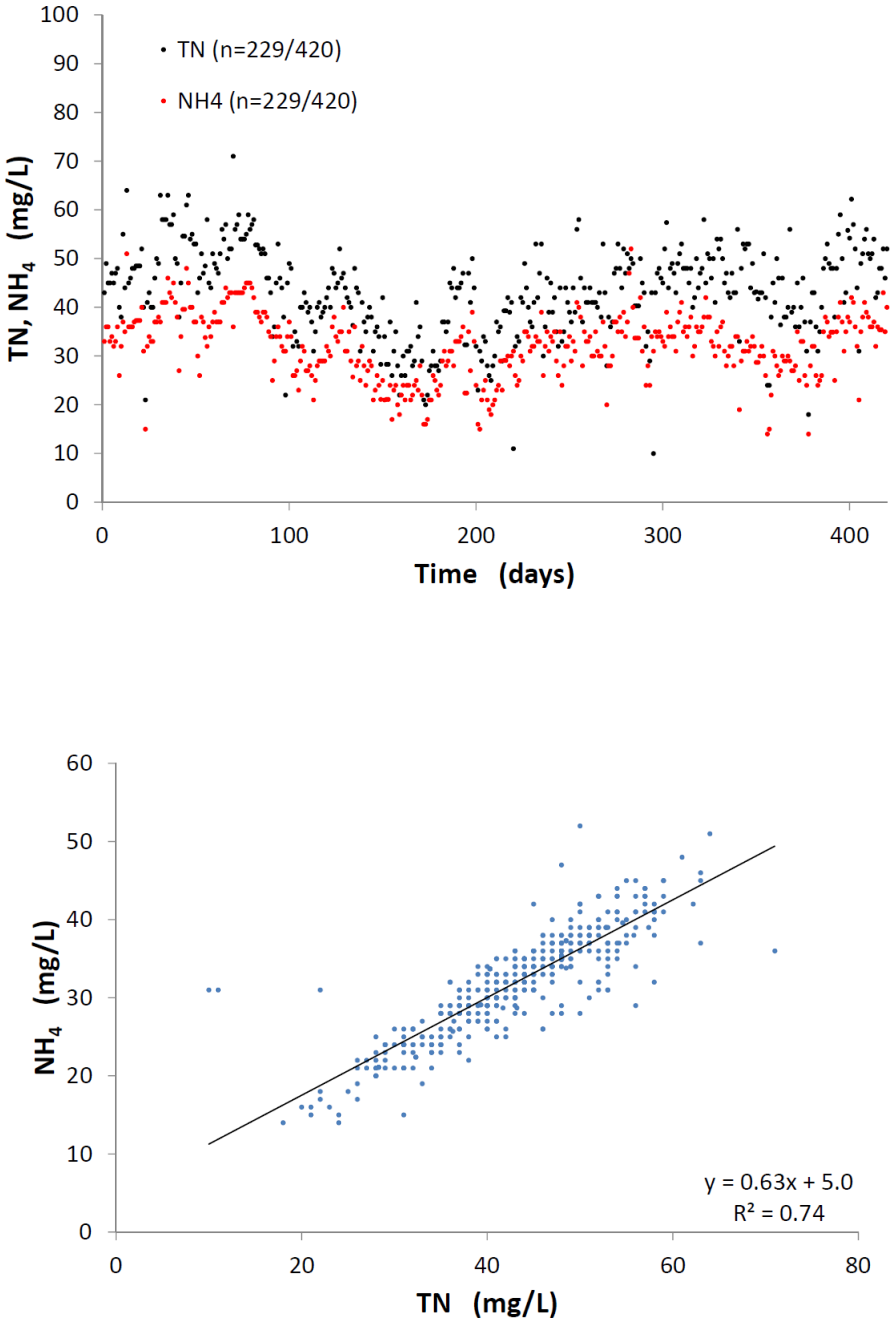


Figure 6.7: Complete (420 days) data set of the total nitrogen and ammonia values, including measured data, data obtained from linear regression and averages calculated weekly from the measured data.

Total organic matter

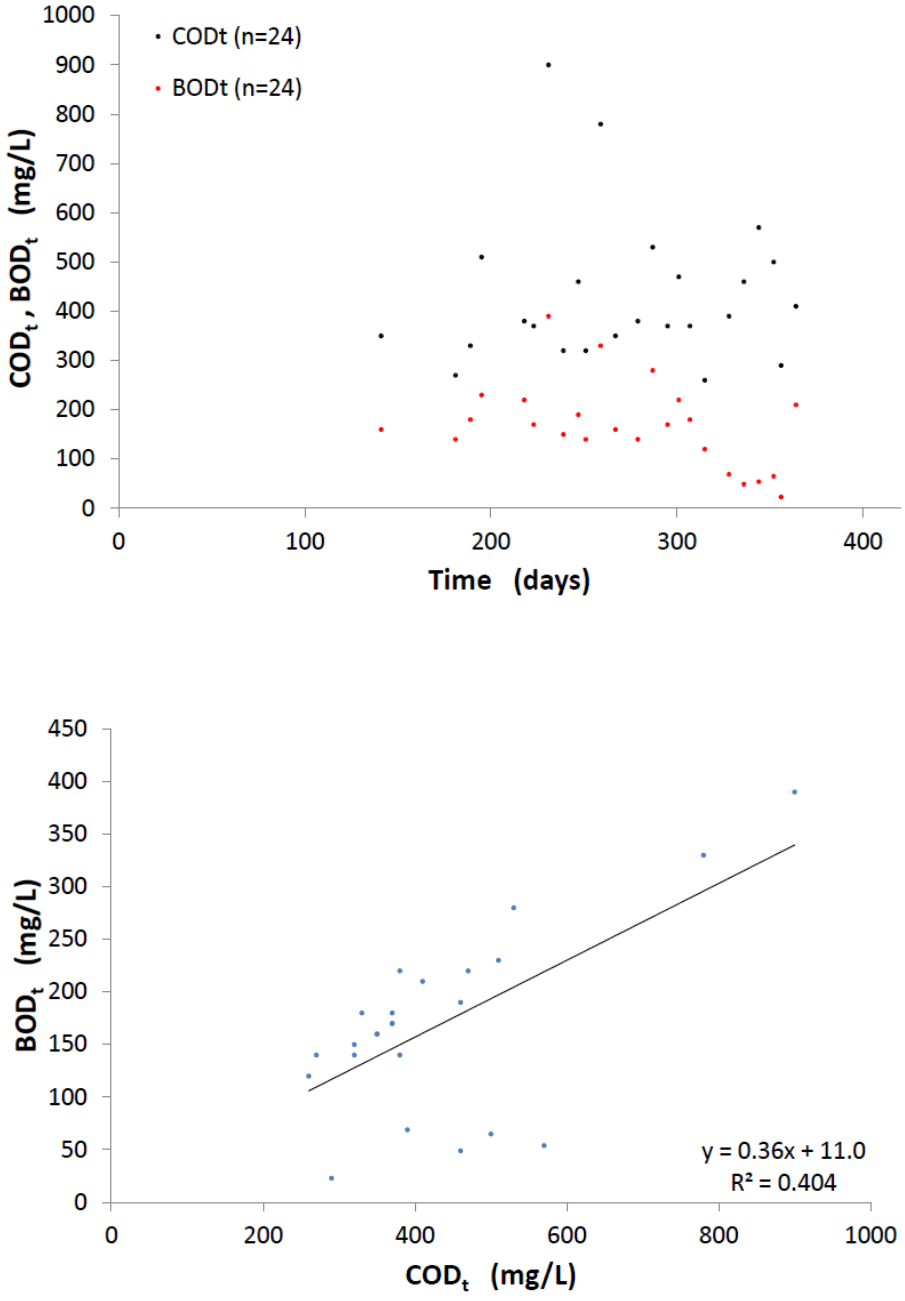


Figure 6.8: Initial available data set of total BOD and COD; time plot (top) and scatter plot (with linear regression).

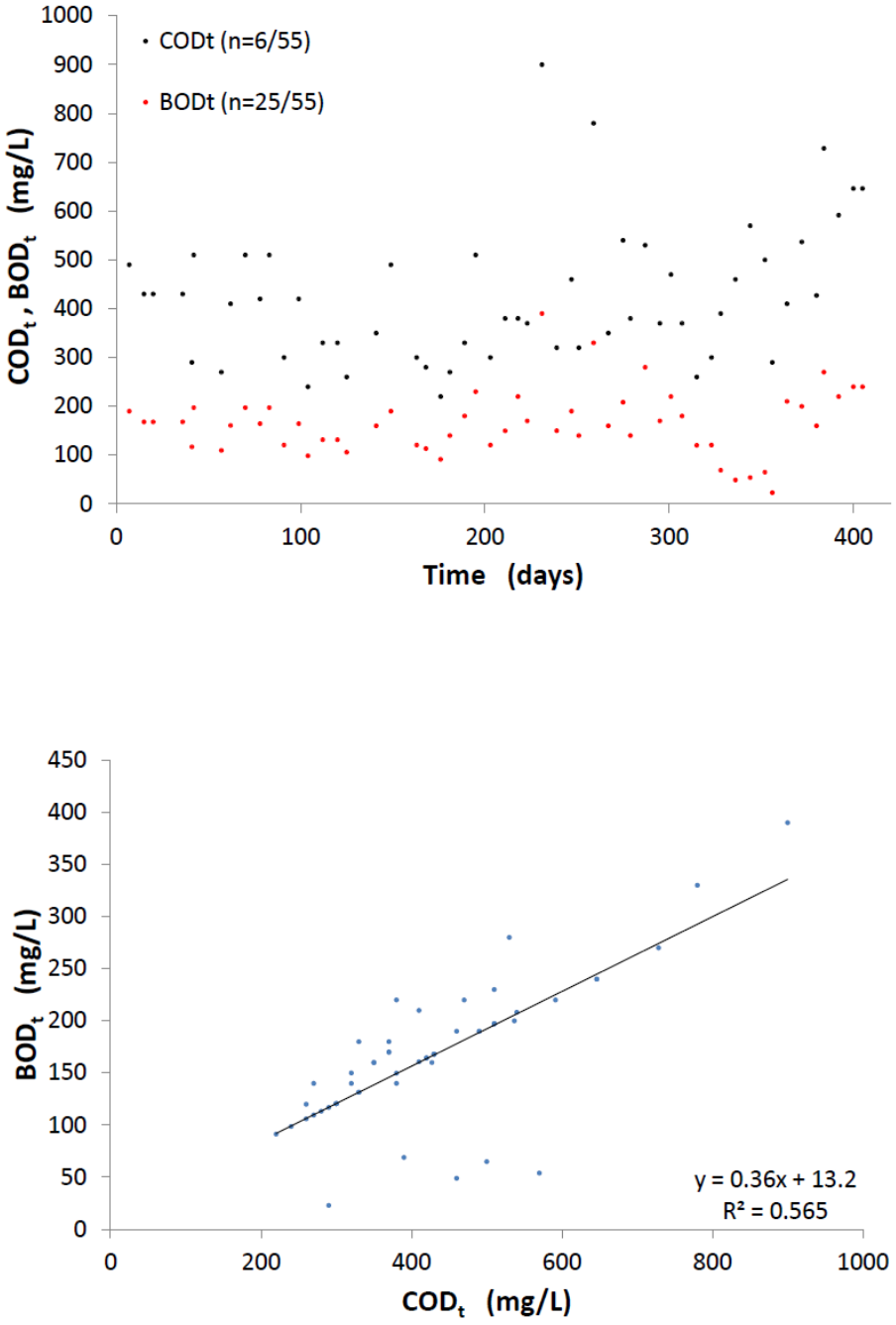
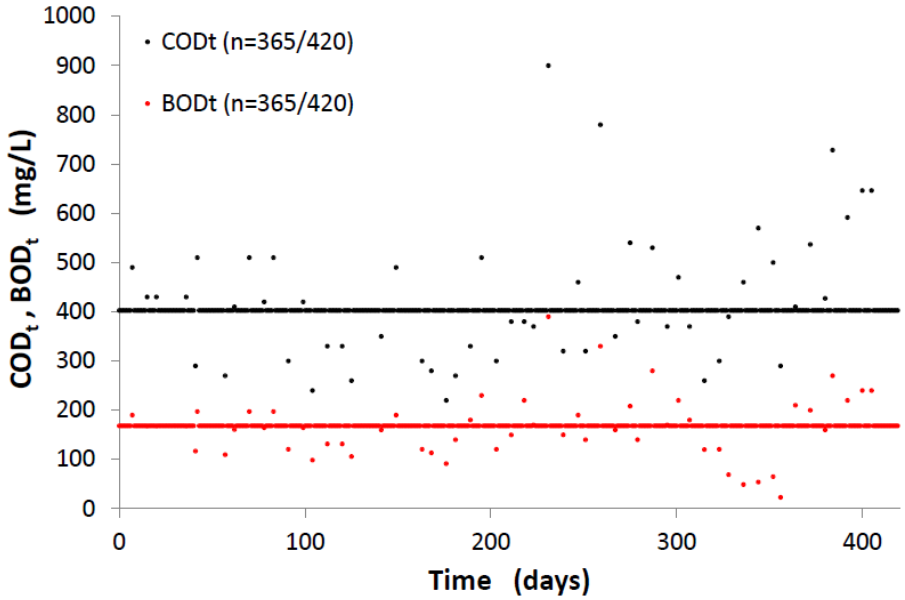


Figure 6.9: Time series (top) and scatter plot (bottom) with the best fit line including the BOD_t and COD_t measured and calculated (using linear regression) values.



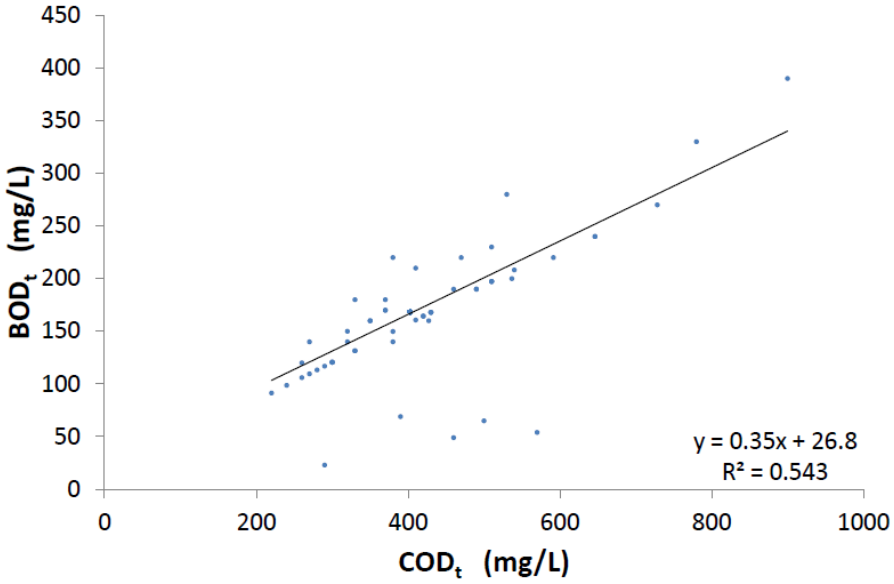


Figure 6.10: Complete (420 days) data set of BOD_t and COD_t values, including measured data, data obtained from linear regression and averages calculated from the complete series of the measured data.

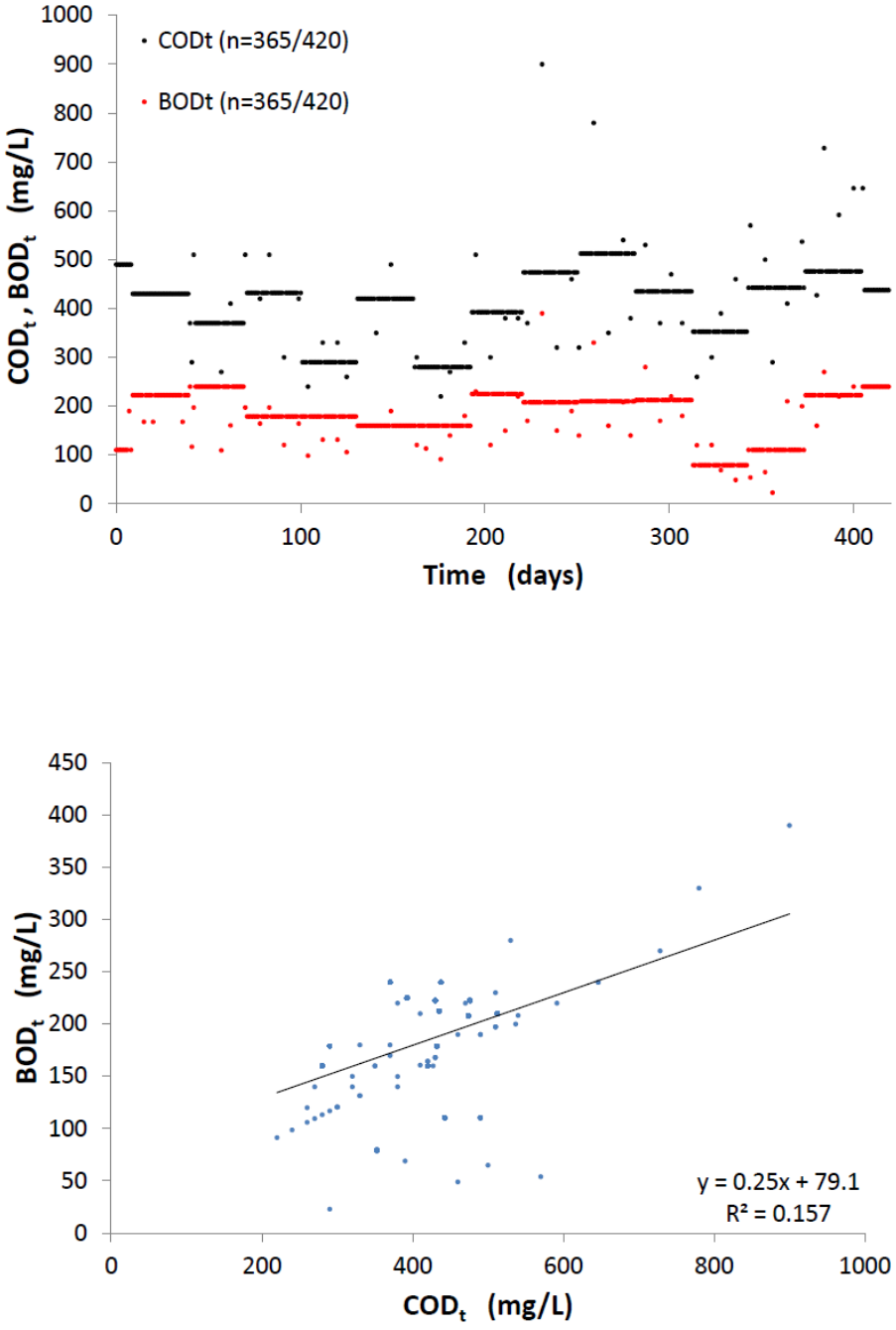


Figure 6.11: Complete (420 days) data set of BOD_t and COD_t values, including measured data, data obtained from linear regression and averages calculated monthly from the measured data.

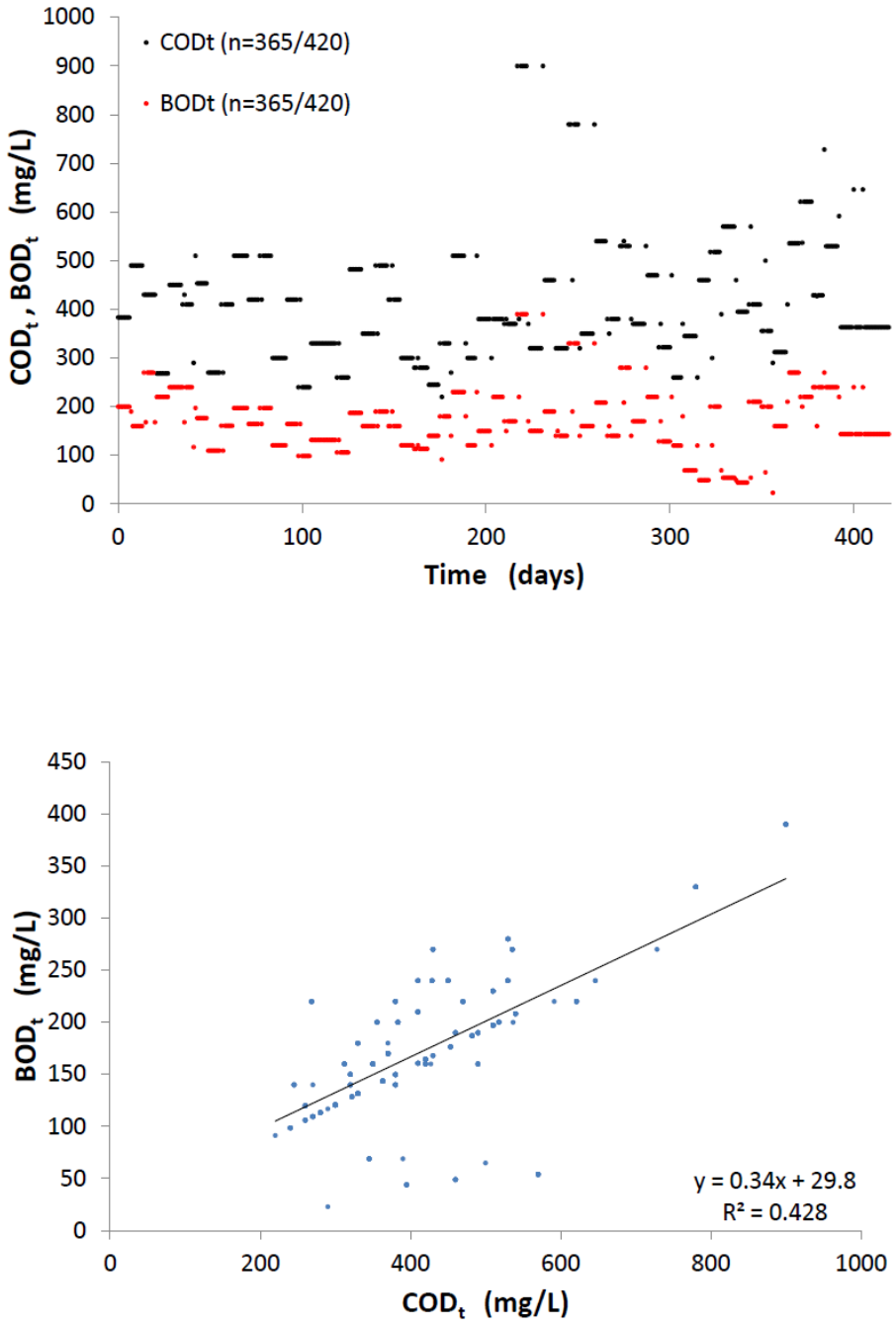


Figure 6.12: Complete (420 days) data set of BOD_t and COD_t values, including measured data, data obtained from linear regression and averages calculated weekly from the measured data.

Soluble organic matter

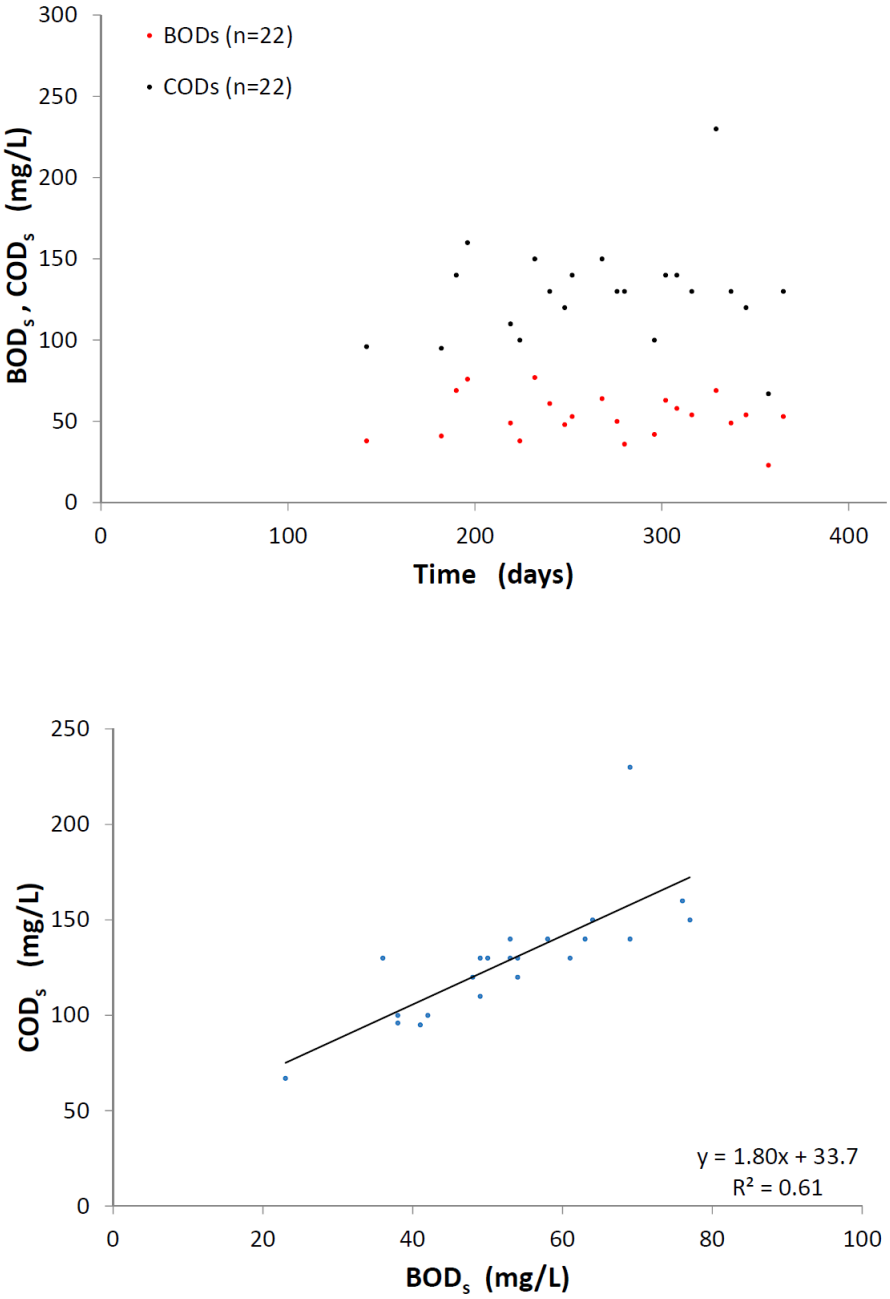


Figure 6.13: Initial available data set of soluble BOD and COD; time plot (top) and scatter plot (with linear regression).

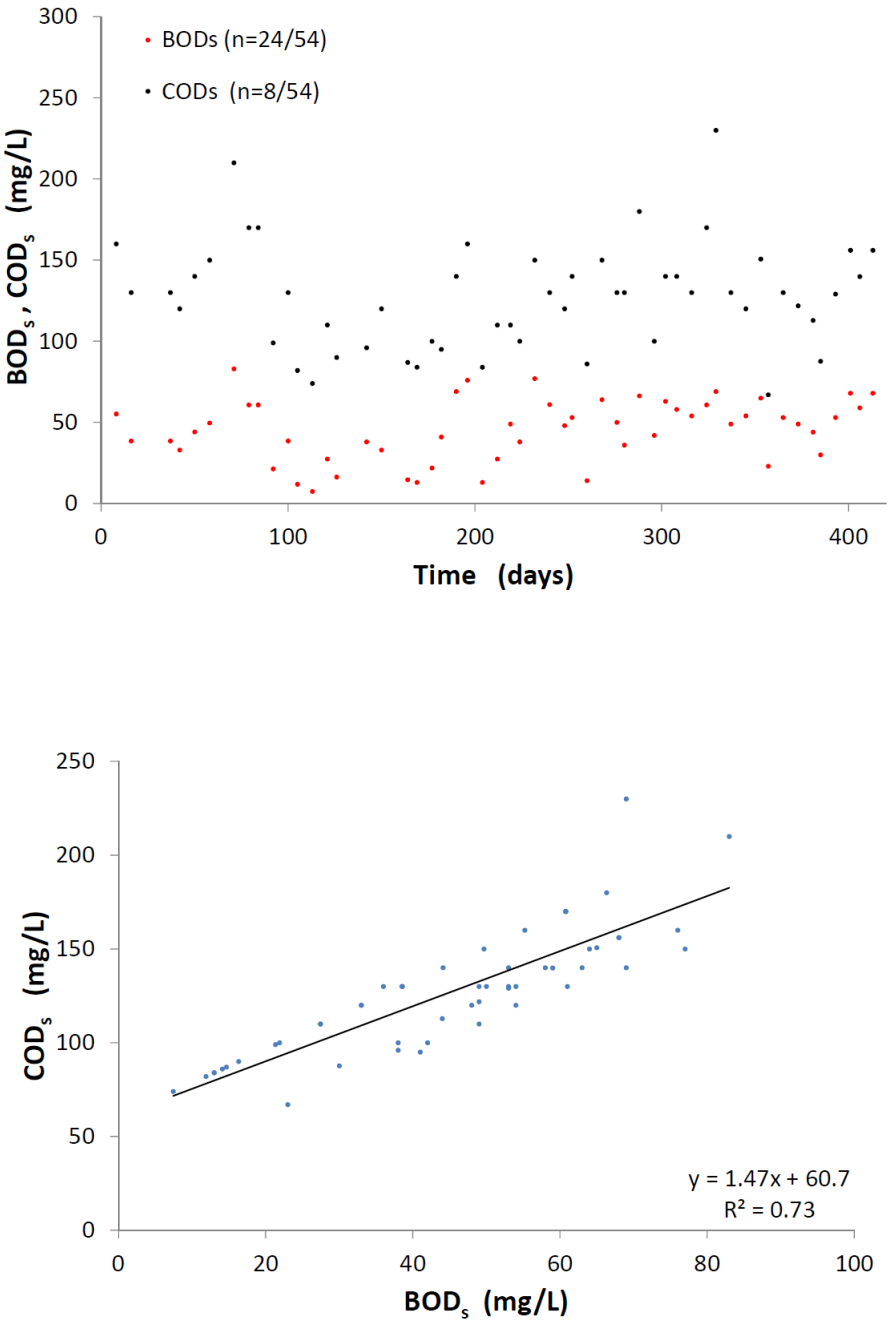


Figure 6.14: Time series (top) and scatter plot (bottom) with the best fit line including the BOD_s and COD_s measured and calculated (using linear regression) values.

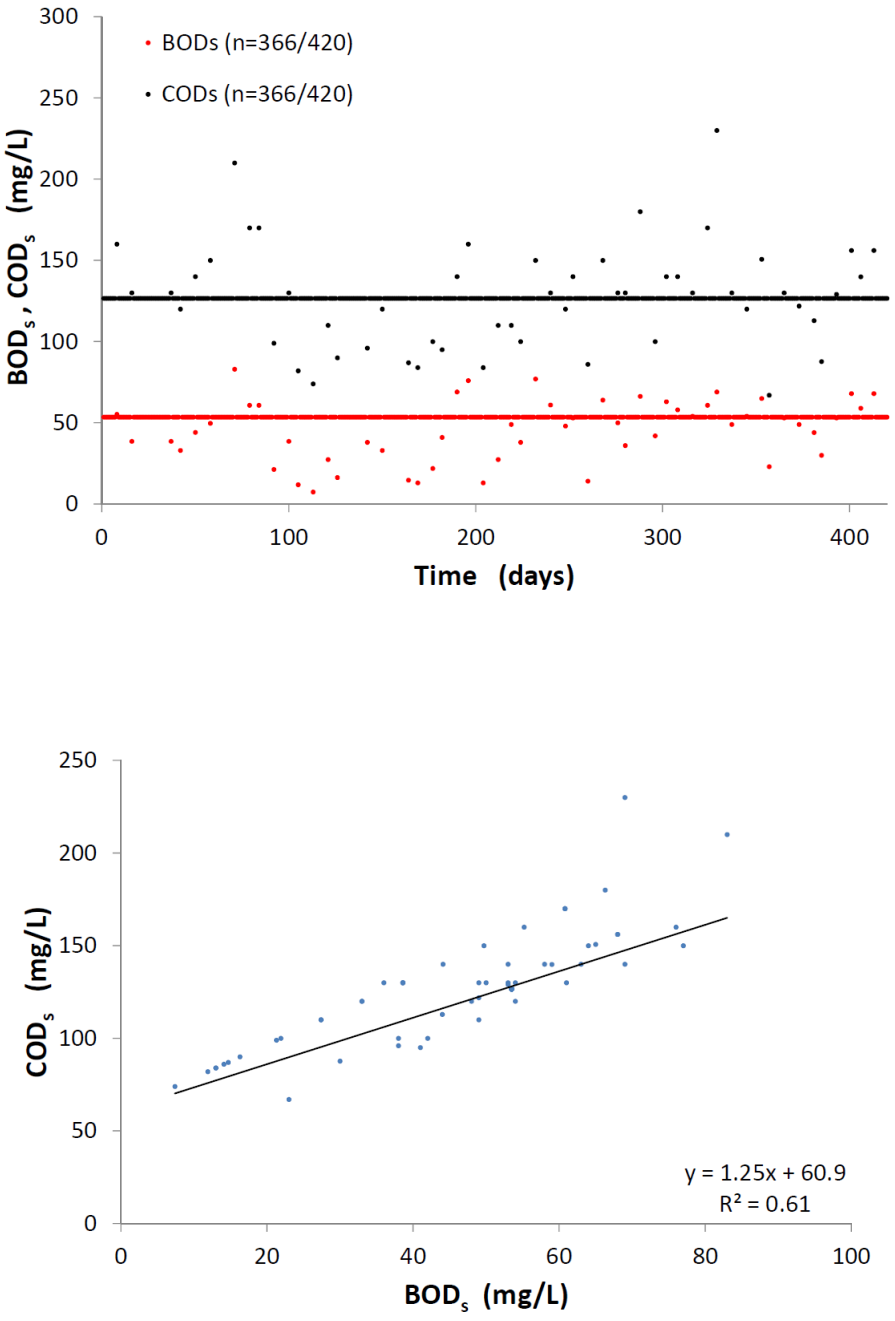


Figure 6.15: Complete (420 days) data set of BOD_s and COD_s values, including measured data, data obtained from linear regression and averages calculated from the complete series of the measured data.

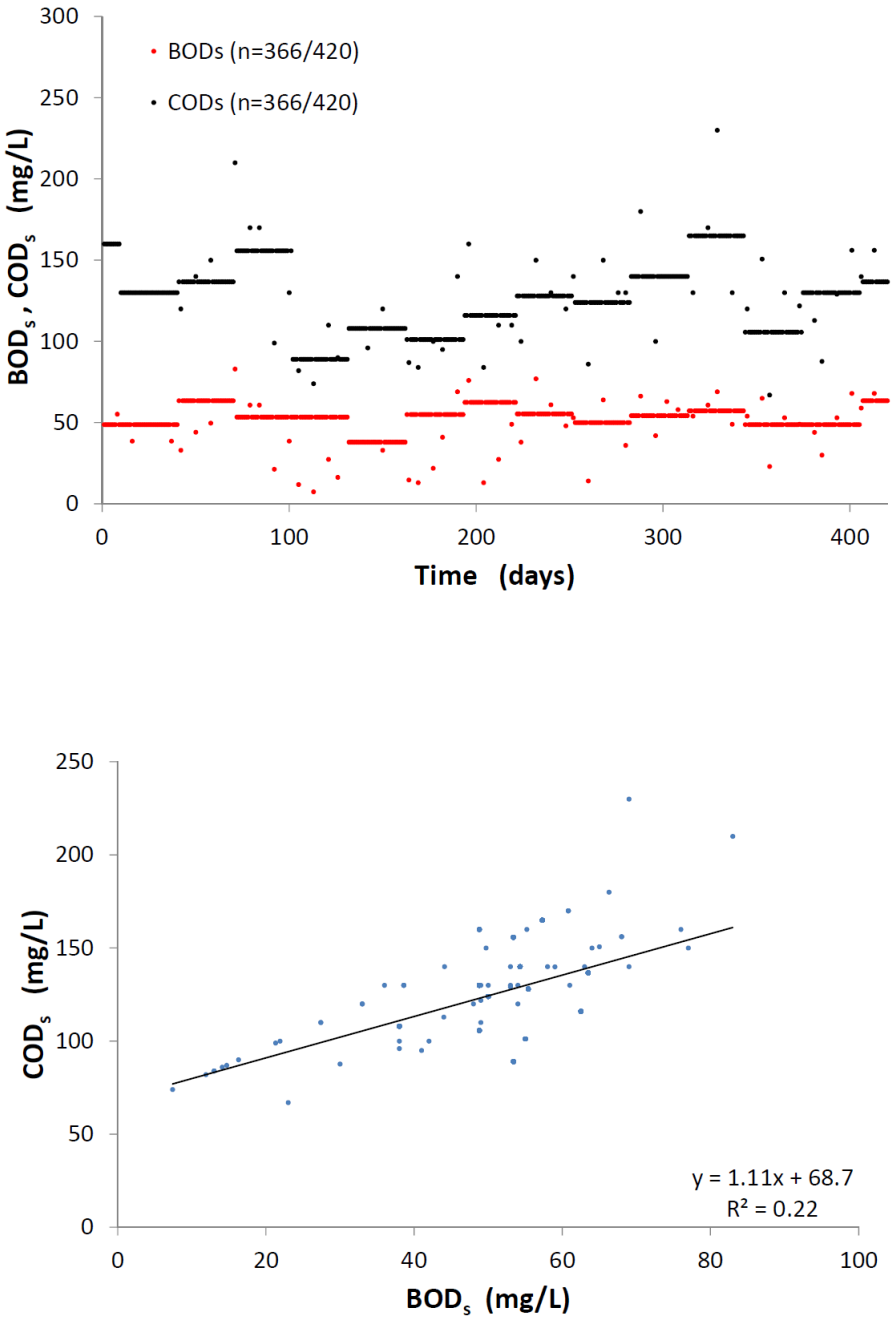


Figure 6.16: Complete (420 days) data set of BOD_s and COD_s values, including measured data, data obtained from linear regression and averages calculated monthly from the measured data.

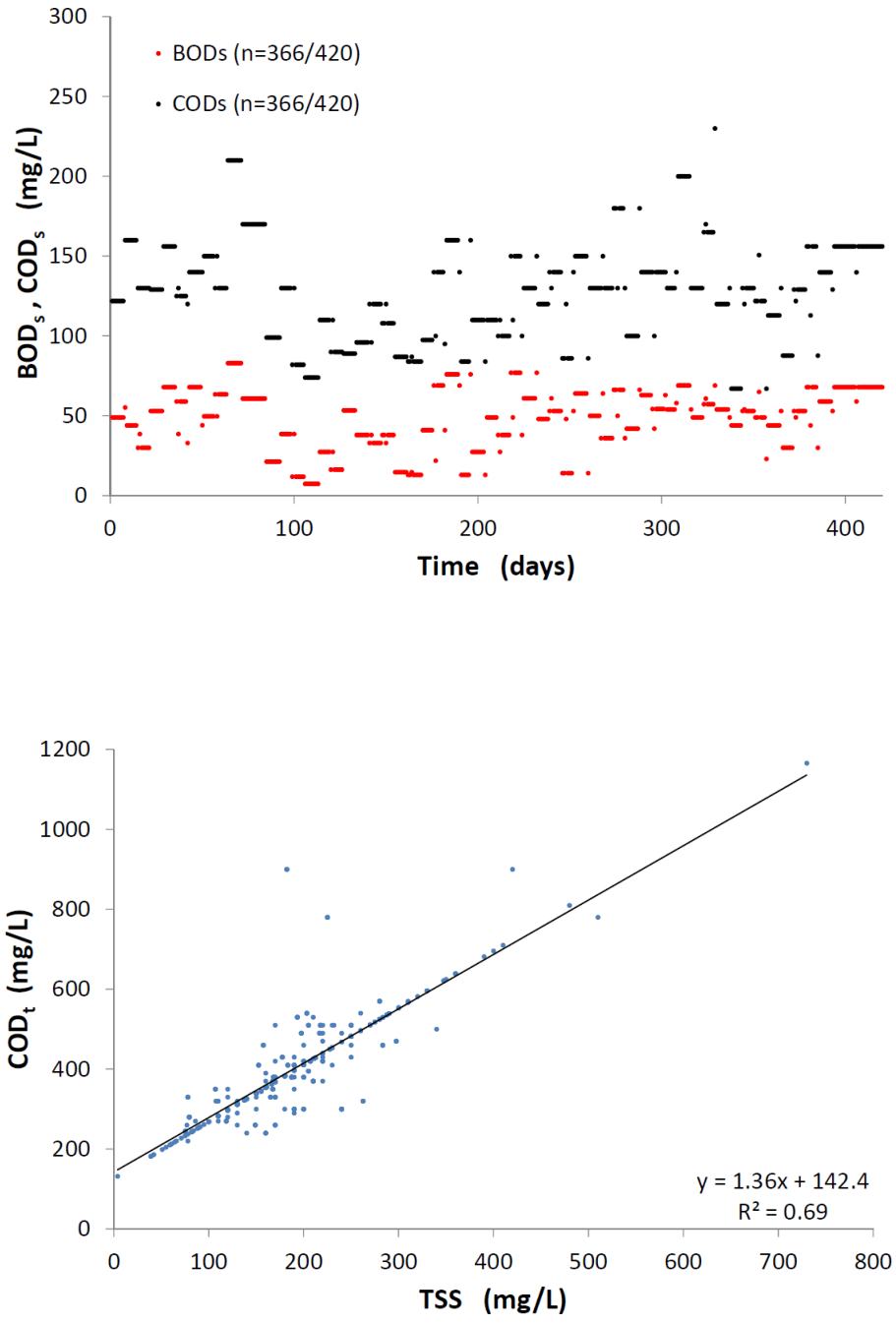


Figure 6.17: Complete (420 days) data set of BOD_s and COD_s values, including measured data, data obtained from linear regression and averages calculated weekly from the measured data.

Reference scenario results

Biological treatment line B2

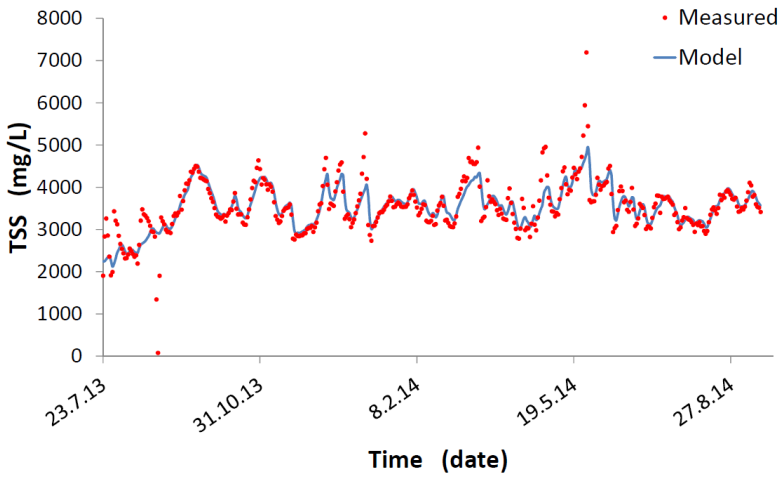


Figure 6.18: Comparison between model output (blue line) and measurements (dots) of TSS from line B2.

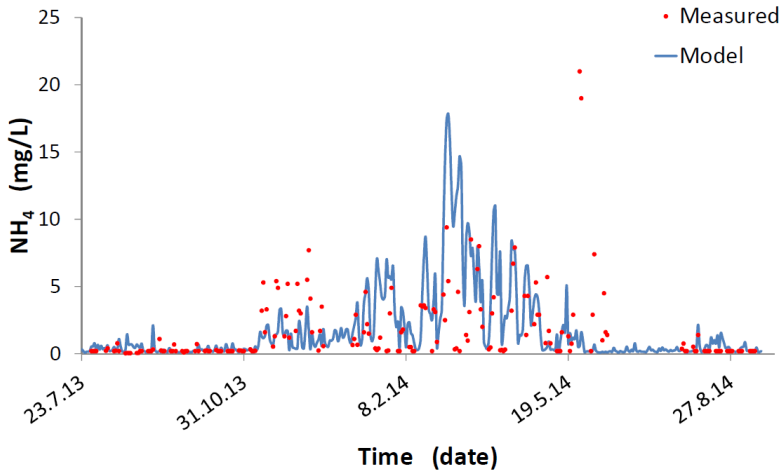


Figure 6.19: Comparison between model output (blue line) and measurements (dots) of NH_4-N from line B2.

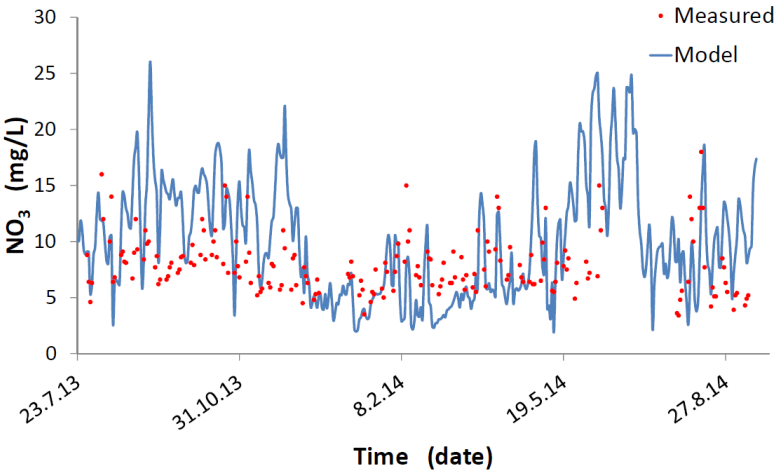


Figure 6.20: Comparison between model output (blue line) and measurements (dots) of NO_3-N from line B2.

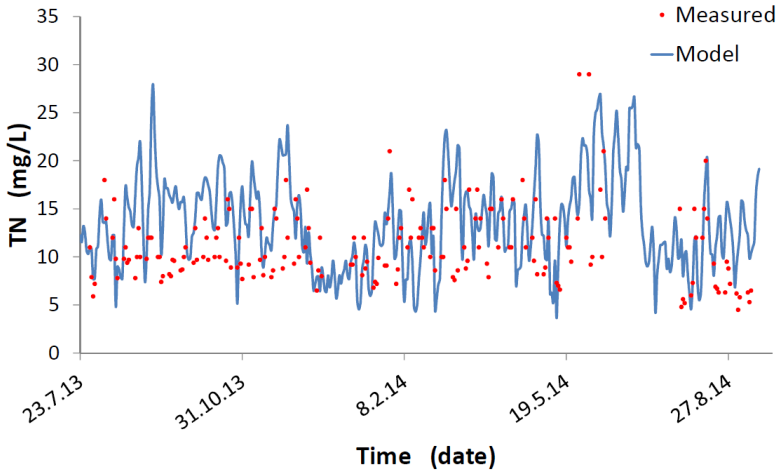


Figure 6.21: Comparison between model output (blue line) and measurements (dots) of TN from line B2.

Biological treatment lines B3 and B4

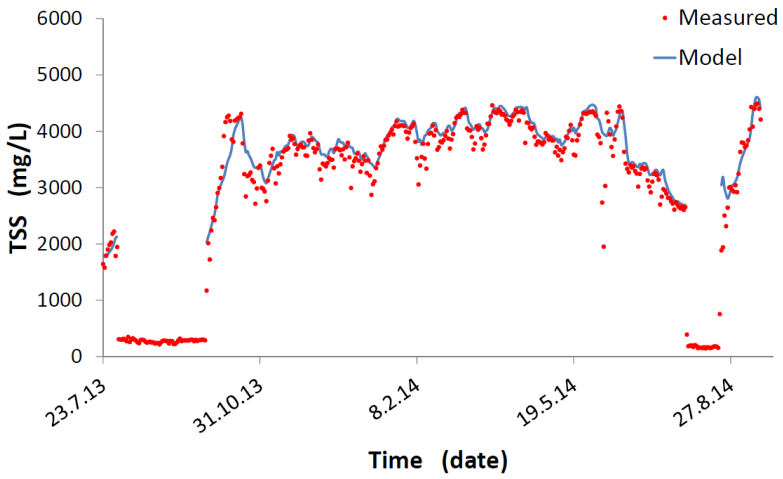


Figure 6.22: Comparison between model output (blue line) and measurements (dots) of TSS from line B3.

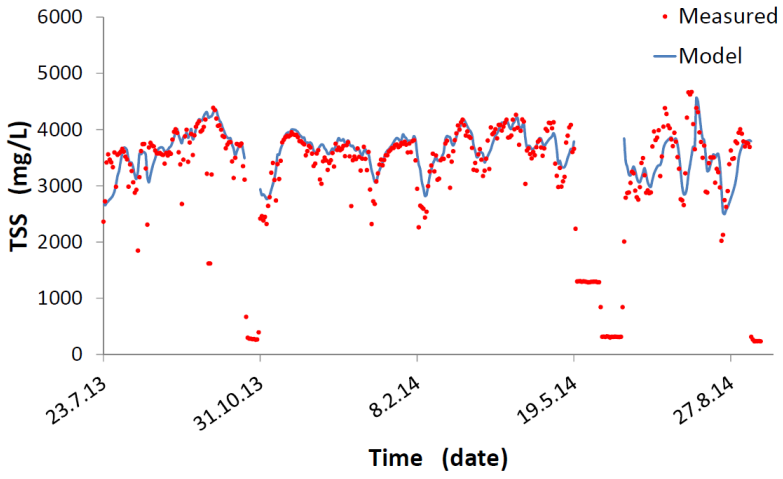


Figure 6.23: Comparison between model output (blue line) and measurements (dots) of TSS from line B4.

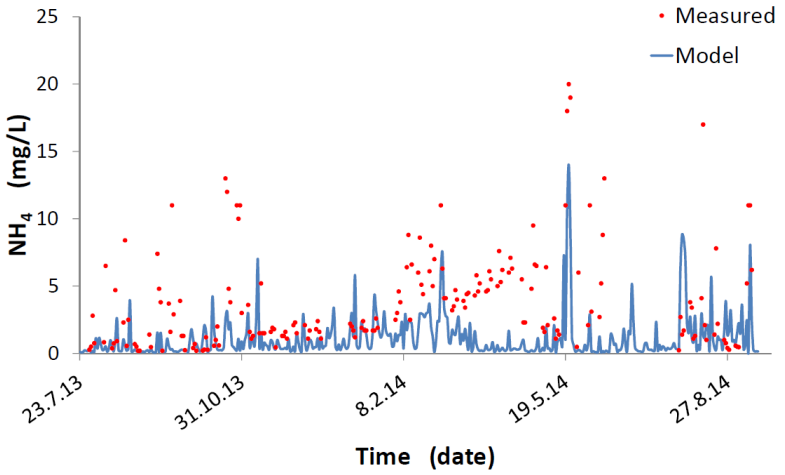


Figure 6.24: Comparison between model output (blue line) and measurements (dots) of NH_4-N from lines B3 and B4 combined.

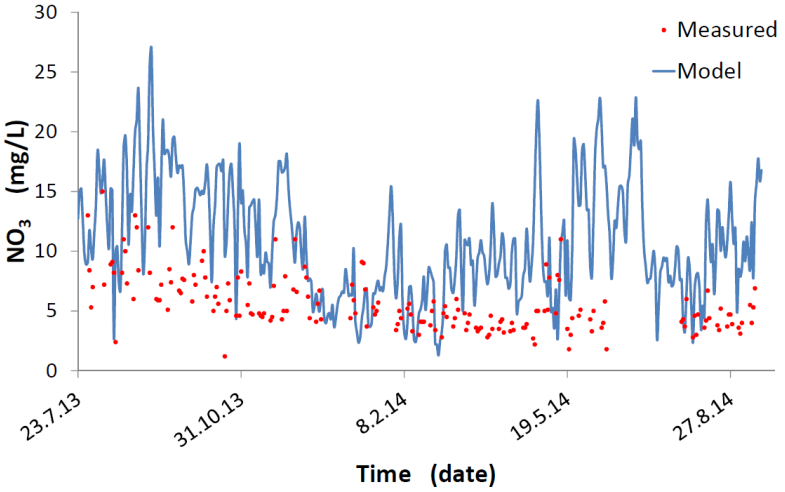


Figure 6.25: Comparison between model output (blue line) and measurements (dots) of NO_3-N from lines B3 and B4 combined.

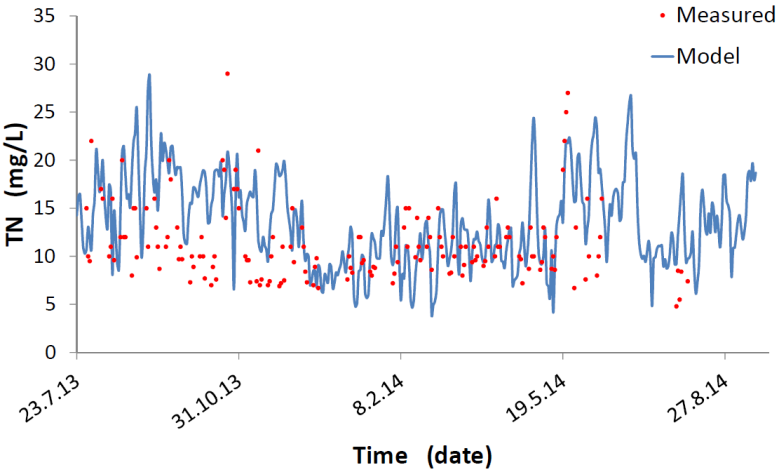


Figure 6.26: Comparison between model output (blue line) and measurements (dots) of TN from lines B3 and B4 combined.

Results of calibration

Table 6.2: Default values, calibrated values and literature ranges of different model parameters for ASM NO.1. Parameters changed are highlighted.

Symbol	Description	Default value [I]	Calib.	Lit. [II]	Unit
Stoichiometric parameters					
Y_h	Heterotrophic yeld	0.67	0.67	0.38-0.75	g cell COD formed/gCOD oxidized
Y_a	Autotrophic yeld	0.24	0.24	0.07-0.28	g cell COD formed/gN oxidized
f_p	Fraction of biomass converted to particulate prod.	0.08	0.08	-	-
i_{xb}	Mass N/mass COD in biomass	0.086	0.086	-	-
i_{xp}	Mass N/mass COD in endogenous mass	0.06	0.06	-	-
Kinetic parameters					
$\hat{\mu}_h$	Heterotrophic max. specific growth rate	6	6.6	0.6-13.2	d^{-1}
K_S	S_s half-saturation coeff. (hsc) for het.	20	20	5-225	g COD/ m^3
K_{oh}	Oxygen hsc for heterotrophs (het.)	0.2	0.2	0.01-0.2	g O_2/m^3
K_{no}	Nitrate hsc for denitrifying het.	0.5	0.4	0.1-0.5[II]	g NO_3-N/m^3
b_h	Heteroptrophic decay rate	0.62	0.62	0.05-1.6	d^{-1}
η_g	Correction factor for anoxic growth of het.	0.8	0.8	0.6-1.0	-
η_h	Correction factor for anoxic hydrolysis	0.4	0.4	-	-
k_h	Max. specific hydrolysis rate	3	3	-	g slowly biodeg. COD/(g cell COD d)
K_X	Hsc for hydrolysis of X_s	0.03	0.03	-	g slowly biodeg. COD/g cell COD
$\hat{\mu}_a$	Autotrophic max. specific growth rate	0.8	0.72	0.2-1.0	d^{-1}
K_{nh}	Ammonia hsc for autotrophs	1	1	-	g NH_4-N/m^3
b_a	Autotrophic decay rate	0.15	0.15	0.05-0.2	d^{-1}
K_{oa}	Oxygen hsc for autotrophs	0.4	0.4	0.4-2.0	g O_2/m^3
k_a	Ammonification rate	0.08	0.08	-	m^3/(g COD d)

[I] according to Henze *et al.* (2000a) and [II] according to Jeppsson (1996)