NTNU – Trondheim
Norwegian University of
Science and Technology

Modeling Biological Nutrient Removal in a Greywater Treatment System

Ivar Soares Urdalen

Civil and Environmental Engineering
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Supervisor: Stein Wold Østerhus, IVM
Co-supervisor: Viggo Bjerkelund, IVM

Norwegian University of Science and Technology
Department of Hydraulic and Environmental Engineering

Sammendrag

Mange bymiljø opplever vannmangel pga. befolkningsvekst og tørkeperioder. I den siste tiden har det vært en økt interesse for å utvikle alternative vannkilder som et supplement til den eksisterende vannforsyningen og for å redusere vannforbruket i byer. En mulighet for å redusere vannbruket i by områder er å kildeseparere husholdnings avløpsvann i gråvann og svartvann. Gråvanns fraksjonen har vist seg å kunne representere opp til 70% av volumet fra husholdningsavløpsvannet. Derfor representerer gråvannsrensing et stort potensiale for å redusere vannforbruket hvis det kan bli gjenbrukt til dovann, hagevanning/irrigasjon eller for rekreasjons formål.

Gråvanns kvalitet har vist seg å ha stor variasjon fra ulike lokaliteter. Enkelte lokaliteter har gråvann med relativ høy total fosfor (Tot-P) konsentrasjon (e.g 7.5 mg P/L). Ofte har total nitrogen (Tot-N) vist seg å være ganske lav for gråvann. Hvis gråvann skal bli gjenbrukt for formål som krever lav Tot-P og Tot-N konsentrasjoner, så er det helt avgjørende å utvikle et bærekraftig gråvannsrenseanlegg som er i stand til å oppnå dette.

Tot-P og Tot-N kan fjernes biologisk og biologisk næringsstoff rensing (BNR) er en vel etablert teknologi som er utbredt for kommunale avløpsrenseanlegg, men den har til gode å bli implementert for gråvanns rensing.

For urban områder med høy tetthet så er det behov for rense system med et lavt fotavtrykk og høy kapasitet. Membran Bioreaktor (MBR) systemer har i det siste blitt en populær teknologi for gråvanns rensing, siden det er et robust system med et lavt fotavtrykk som produserer avløpsvann med en høy kvalitet som kan bli gjenbrukt.

Derfor er et innovativt gråvannsrensesystem, som er basert på Integrert Fast film Aktiv slam (IFAS), BNR og MBR, undersøkt med aktivslam modellen ASM2d. Modellen ble implementert i WEST (et simuleringsprogram for avløpsrensing). Rensesystemet var en pilot som var satt opp ved Norges teknisk-naturvitenskaplige universitet (NTNU), og brukte en modifisert UCT-MBR konfigurasjon for BNR.

Et litteratur studie for gråvannsrensing, BNR, IFAS, MBR, ASM modeller og hvordan gjennomføre en modelleringsstudie er presentert. Modellen er utviklet basert på operasjonelle målinger fra piloten, og er videre kalibrert ved å justere innløps karakteriseringen og de kinetiske parameterne. Modellen ble brukt til sensitivitets analyse av de operasjonelle parameterne og til å foreslå en optimalisert konfigurasjon av lufte innstillinger, interne returstrømmer, volumer og «wastage rates». Den ikke-kalibrerte modellen var i stand til å simulere vannkvalitetsparameterne COD, Tot-P og Tot-N i utløpet. Men det anoksiske P opptaket og den løste COD konsentrasjonen i den anaerobe tanken ble ikke simulert med tilfredsstillende nøyaktighet.

Abstract

Many urban centers suffer water scarcity due to increased population growth and dry periods. There has been an increased interest in developing alternative water sources for supplementing the existing urban water supply and for reducing urban water demand. One possibility for reducing urban water demand is by source separation of domestic wastewater into greywater and blackwater. The greywater fraction has been found to be responsible for up to 70% of the domestic wastewater volume. Therefore, greywater treatment represent a big potential of reducing the urban water demand if it can be reused for toilet flushing, garden/agricultural irrigation or for recreational use.

Greywater characteristics have been found to vary a great deal from different locations. Certain locations contain greywater with relatively high total phosphorus (Tot-P) concentration (e.g 7.5 mg P/L). Often total nitrogen (Tot-N) have been found to be quite low in greywater. If the greywater is to be reused for purposes that require low Tot-P and low Tot-N concentrations, it is essential to develop a sustainable greywater treatment system that is able to achieve this.

Tot-P and Tot-N can be removed biologically and biological nutrient removal (BNR) is an well-established technology that been widely applied for municipal wastewater treatment, but has yet to be implemented in full-scale for greywater treatment.

For high density urban areas there is a need for treatment systems with a low footprint and high capacity. Membrane Bioreactor (MBR) systems have lately emerged as a popular technology for greywater treatment, as it is a robust system with a low footprint that produces a high quality effluent that can be reused.

Therefore, a novel greywater treatment system based on Integrated Fixed-Film Activated Sludge (IFAS), BNR and MBR, is investigated with the activated sludge model ASM2d. The model was implemented in WEST (a wastewater treatment simulator software). The system was a pilot operated at the Norwegian University of Science and Technology (NTNU), and employed a modified UCT-MBR configuration for BNR.

A literature review of greywater treatment, BNR, IFAS, MBR, ASM models and how to conduct a modelling study is presented. The model is developed based on operational measurements of the pilot plant, and further calibrated by adjusting the influent characterization and the kinetic parameters. The model was used for sensitivity analysis of the operational parameters, and for proposing an optimized configuration of aeration settings, internal recycle streams, volumes and wastage rates. The uncalibrated model was able to successfully predict the effluent quality variables COD, Tot-P and Tot-N. However, the anoxic P uptake and soluble COD concentration in the anaerobic tank were not predicted successfully.

Preface

This master thesis has been completed at the Department of Hydraulic and Environmental Engineering at Norwegian University of Science and Technology (NTNU), spring 2015. The topic was selected in collaboration with Professor Stein W. Østerhus, and out of my interest of utilizing mathematical models to investigate complex systems and biological wastewater treatment.

Greywater treatment and decentralized reuse schemes has received increased interest in many urban environments due to highly concentrated population leading to water scarcity. It has been shown that it can be a promising intervention to augment already stressed water supplies. Greywater containing high concentrations of nutrients is susceptible to biological treatment, however the system needs to be designed properly to function well.

Mathematical models can help explore different operational setups and help better understand the flexibility and stability of the process. Modelling biological systems such as a wastewater treatment plant is a very intellectual challenge due to a high number of processes and interrelation between the effluent quality and the parameters of the system. The modeling of a greywater treatment pilot with the configuration in this study has to my knowledge never been done before, and it has been very interesting to be at the frontier of biological greywater treatment.

I would like to thank Professor Stein W. Østerhus and PhD student Viggo Bjørklund at NTNU for providing guidance for this master thesis. I am grateful for the opportunity to investigate the pilot plant set up by Viggo and for the flexibility to combine the work in this thesis with my job as a consulting engineer.

I would like to thank DHI for providing a student license for the modelling software WEST for the duration of the thesis. Without this software it would have been very difficult to do the necessary analysis.

My thanks also goes to Asplan Viak and my colleagues there for the flexibility to combine work with this thesis work.

Finally, I would like to thank my wonderful wife, Luana, for always being supportive and providing motivation during this thesis.

16.06.2015 Sandvika, Norway

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List of Terms and Abbreviations

ADM1	Anaerobic Digestion Model 1
ASM	Activated Sludge Model
BNR	Biological Nutrient Removal
BOD	Biochemical Oxygen Demand
CAS	Conventional activated sludge
COD	Chemical Oxygen Demand
CSTR	Completely Stirred Tank Reactors
DO	Dissolved Oxygen
EBPR	Enhanced Biological Phosphorus Removal
GMP	Good Modelling Practice
HRT	Hydraulic Retention Time
IFAS	Integrated Fixed-Film Activated Sludge
IWA	International Water Association
LHS	Latin Hybercube Sampling
MBBR	Moving Bed Bioreactor
MBR	Membrane Bioreactor
MC	Monte Carlo
MLSS	Mixed Liquor Suspended Solids
PAO	Phosphorus Accumulating Organisms
PHA	Polyhydroxyalkanoate
PP	Poly phosphate (internal storage product)
SBR	Sequencing batch reactor
SMP	Soluble Microbial Products
SRT	Sludge Retention Time
TKN	Total Kjeldahl Nitrogen
TSS	Total Suspended Solids
UCT	University of Cape Town
WWTP	Wastewater Treatment Plant

List of ASM2d Symbols and Parameters

This thesis contains many parameters and symbols that are used in the wastewater treatment models. This thesis uses the ASM2d model, thus the relevant state variables are listed here. The kinetic and stoichiometric parameters are presented in Appendix B.

Notation

As models can be very complex with many parameters and state variables there is need to have a consistent notation scheme. The principle for the first capital letter is the following:

- S = soluble (generally < 0.45 μm)
- X = particulate (generally > 0.45 μm)

This thesis does not utilize a separate variable for the colloidal fraction, therefore the colloidal fraction is considered included in the variables named X.

State variables for the ASM2d model

Symbol	Description	Unit
S_A	Fermentation products, considered to be acetate.	mg COD/L
S_{ALK}	Alkalinity of the wastewater	mol HCO_3^-/L
S_F	Fermentable, readily biodegradable organic substrates.	mg COD/L
S_I	Inert soluble organic material	mg COD/L
S_{N2}	Dinitrogen, N_2	mg N_2-N/L
S_{NH}	Ammonium plus ammonia nitrogen	mg NH_4-N/L
S_{NO}	Nitrate plus nitrite nitrogen	mg NO_3-N/L
S_O	Dissolved oxygen	mg O_2/L
S_{PO}	Inorganic soluble phosphorus, primarily ortho-phosphates.	mg P/L
S_S	Readily biodegradable substrate	mg COD/L
X_{AUT}	Nitrifying organisms	mg COD/L
X_H	Heterotrophic organisms	mg COD/L
X_I	Inert particulate organic material	mg COD/L
X_{PAO}	Phosphate-accumulating organisms: PAO	mg COD/L
X_{PHA}	A cell internal storage product of PAO. Poly-hydroxyalkanoates (PHA)	mg COD/L
X_{PP}	Poly-phosphate stored in PAO	mg P/L
X_S	Slowly biodegradable substrates	mg COD/L
X_{TSS}	Total suspended solids, TSS	mg TSS/L

1. Introduction

1.1 The Big Picture

Many urban centers are facing increased water stress due to population growth, urbanization and increased water demand per capita. In 2014, 54% of the world's population live in urban areas, while it is projected that the number will increase to 66% in 2050, with a global population of 9 billion (UN, 2014). This will lead to an increased pressure on the water supplies for the urban centers, especially in arid or semi-arid areas. Many cities will need to develop new water sources such as surface water, groundwater or seawater desalination. These expansions of the water supply are often capital-intensive solutions, thus there has been an increased interest in developing alternative water sources or implement measures to decrease the urban water demand.

Household greywater treatment and reuse is one possible conservation technique that is able to decrease the urban water demand. In this thesis, greywater is defined as all non-toilet household wastewater (Figure 1.1). Various authors does not consider the kitchen sink to be included in the greywater definition due to high concentration of organic matter.

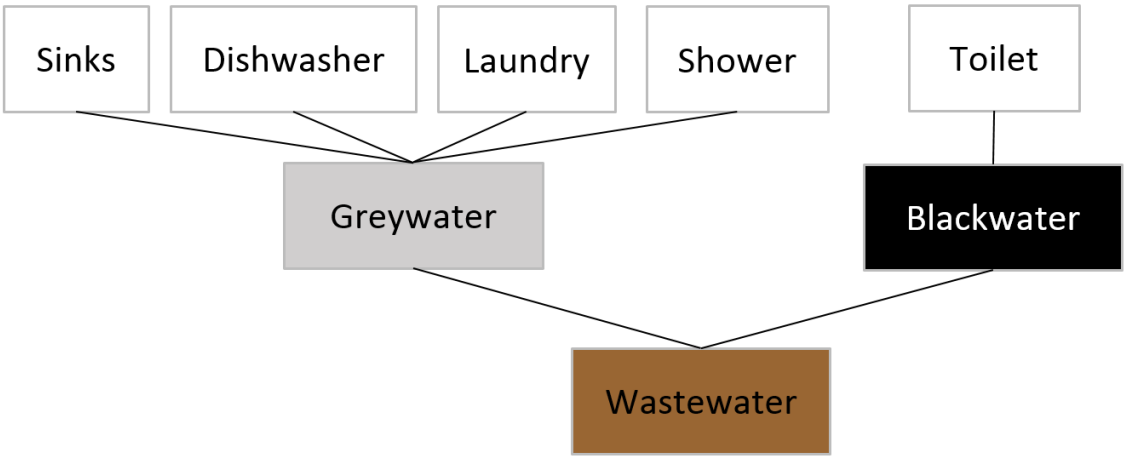

Figure 1.1 - Definition of Greywater

The greywater might be responsible for 50-70% of the total wastewater volume from a household (Revitt et al., 2011). Thus, greywater reuse has big potential to reduce the urban water demand.

The greywater water quality characteristics vary from different locations and depends on what fractions of the household wastewater is separated. But, often greywater is polluted with 500-650 mg COD/L, 330 mg BOD_5/L turbidity up to 70-100

NTU, total phosphorus up to 10 mg/L, total nitrogen up to 20 mg/L, personal care products and detergents (Meinzinger and Oldenburg, 2009).

Thus if greywater reuse is to be applied, the relevant pollutants needs to be removed as these can cause environmental, health and aesthetic problems. Many different technologies have been tested for greywater reuse, and most technologies combine biological and physiochemical treatment stages (Ghunmi et al., 2011). Recently, MBR systems have been applied for on-site greywater treatment, as it provide a system with small footprint and an effluent with high quality.

1.2 Why model biological greywater treatment systems?

Pilot studies of biological treatment system are often time consuming and expensive to set up, especially if various configurations and operational strategies are to be evaluated.

An alternative and a complement to pilot studies is to establish a mathematical model of the system. A mathematical model can also be used to help design a pilot plant. There are various objectives to modelling (Henze et al., 2008):

- Investigate the plant performance
- Evaluate possible configurations for upgrading or new design
- Evaluate and predict the impact of different input scenarios to the plant
- Develop and evaluate process control scheme
- Provide operator training
- Support management decisions (“what-if” scenarios can be examined further)
- Investigate novel process configurations

Models can be used for quick testing of various configurations at a fraction of the time and cost compared to laboratory and pilot tests. With a model of a treatment system, it is also possible make quantitative performance comparisons among different configurations (such as 5% lower sludge production, 10% need for more oxygen). Quantitative information can be much more valuable and objective than qualitative statements such as “better”, “lower” or “increased”.

For design of new municipal wastewater treatment plants (WWTP) to include biological nutrient removal (BNR), it has now been become common practice in the USA to use simulators and models to evaluate process design. This is due to the complex nature of BNR (several recycle flows, aeration settings, distribution of biomass in the reactors, etc.) and the wide range of configurations available (U.S. EPA, 2010). If models can lead to a more optimal design of greywater system, these systems may increase their usage in the urban water cycle. This thesis will investigate a pilot plant

running a BNR configuration and explore the benefits and limitations of modelling BNR in a greywater treatment system.

1.3 Project description

The aim of this master thesis is to establish an activated sludge model for a pilot biological greywater treatment system, without recycling. The treatment system includes biological nutrient removal and a membrane bioreactor. The thesis includes the following tasks:

1. *Evaluate different models (ASM2d, ASM3) and modeling programs that are applicable for modeling biological greywater treatment systems, and choose an appropriate model and software for this thesis.*

2. *Calibrate an activated sludge model for the greywater treatment pilot without recycling, and perform a sensitivity analysis to identify the most sensitive parameters (both kinetic/stoichiometric parameters and operational parameters).*

3. *Compare the results of the simulation model and the experimental data, and evaluate the predictability of the model.*

4. *Perform a sensitivity analysis of the operational parameters and suggest an optimized setup of operational parameters (internal recycle flows, aeration, volumes and SRT).*

1.4 Outline of the thesis

The experimental pilot system that is investigated in this thesis is a novel biological treatment system that is based on UCT-MBR configuration with an IFAS reactor configuration in the anoxic and aerobic reactor. This is a complex biological system and application of a mathematical model to such a system is quite a challenge.

Therefore, an extensive literature is presented in Chapter 2 to highlight the properties of the system, the procedure to apply an mathematical model and to provide a survey of the recent knowledge relevant to this system.

Chapter 3 describes the methodology applied for the model development, calibration, influent characterization, sensitivity analysis and investigation of the operational parameters. Chapter 4 presents the results and discusses the results from

the model of the greywater treatment system and Chapter 5 provides the conclusion. For describing the ASM2d model and other modelling results, several Excel spreadsheet are provided as part of the thesis.

2 Literature Review

This thesis is investigating many different aspects of wastewater treatment, such as MBR, BNR, IFAS, greywater and mathematical of biological wastewater treatment systems. Therefore, a literature review was conducted to explore the theory of these technologies and find an appropriate model and software to apply to the greywater pilot that is the focus of this thesis.

2.1 Greywater Treatment

This section provides a short overview over the greywater quality, an example of greywater reuse standard, treatment methods and challenges for biological nutrient removal.

2.1.1 Water quality

Greywater characteristics are often highly variable, because it is generated from different sources and depends on the products used in a household. Thus, there is a wide range of values reported in the literature.

Table 2.1 presents typical greywater characteristics based on a literature review of more than 130 references. These values are for mixed greywater from various sources (laundry, dishwasher, kitchen sink, shower, etc.).

Table 2.1 - Greywater Quality based on data from the literature

Parameter	**Median**[a]	**Range (min-max)**[a]	**Range (min-max)**[b]
pH	-	-	6.3 - 8.1
Turbidity (NTU)	-	-	29 - 375
TSS (mg/l)	228	-	25 - 183
BOD5 (mg/l)	329	205 - 449	47 - 466
COD (mg/l)	535	350 - 783	100 - 700
Total Nitrogen (mg/l)	13.0	6.7 - 22	1.7 – 34.3
Total Phosphorus (mg/l)	4.6	0.4 – 8.2	0.11 – 22.8
Potassium (mg/l)	8.8	-	-
Sulphur (mg/l)	72	-	-
COD:N:P	100:2.4:0.9		

a: Meinzinger and Oldenburg (2009)

b: Li et al. (2009)

As can been seen from Table 2.1, greywater quality has great variation and can include high concentrations of organic pollutants and nutrients (nitrogen and phosphorus). It is important to identify the greywater quality and treatment requirements as it is essential for deciding on treatment method.

An example from Germany of a typical distribution of nitrogen, phosphorus, potassium and COD from greywater, urine and faeces is shown in Table 2.2. As can be seen from the distribution of pollutants most of the nitrogen in household wastewater is concentrated in the urine. Most of the phosphorus originates from the urine and feces, while a major part of COD originates from greywater.

Table 2.2 - Distribution of pollutants in greywater, urine and faeces (Otterpohl, 2002)

Component	**Specific load** kg/(P*year)	**Greywater**	**Urine**	**Faeces**
Nitrogen	~ 4-5	~ 3%	~ 87%	~ 10%
Phosphorus	~ 0.75	~ 10%	~ 50%	~ 40%
Potassium	~ 1.8	~ 34%	~ 54%	~ 12%
COD	~ 30	~ 41%	~ 12%	~ 47%

2.1.2 Treatment requirements

If greywater is to be reused, it should fulfill at least four criteria (Nolde, 2000):

- Hygienic safety
- Aesthetics
- Environmental tolerance
- Economical feasibility

The degree of treatment and quality of the effluent depends on the application of the reclaimed greywater. There are few national or international established guidelines quality requirements for greywater reuse. Based on a review of various national and international water reuse standards, a grey water reuse standard for non-potable uses has been proposed (Li et al., 2009).

Table 2.3 – Proposed standard for non-potable grey water reuse (Li et al., 2009)

	Recreational, lakes	**Urban reuse and agricultural irrigation**		
	Unrestricted	**Restricted**	**Unrestricted**	**Restricted**
BOD_5 (mg/l)	< 10	< 30	< 10	< 30
TN (mg/l)	< 1	< 1	-	-
TP (mg/l)	< 0.05	< 0.05	-	-
TSS (mg/l)	-	< 30	-	< 30
Turbidity (NTU)	< 2	-	< 2	-
pH (-)	6 – 9	6 – 9	6 – 9	6 - 9
Faecal coliform (1/ml)	< 10	< 10	< 10	< 10
Total coliform (1/ml)	< 100	< 100	< 100	< 100
Residual chlorine (mg/l)	-	-	< 1	< 1

Table 2.3 shows that very low phosphorus and nitrogen concentrations is necessary if the greywater is to be reused for recreational purposes or discharged to a small lake.

Medium/high strength greywater have high nitrogen and phosphorus concentrations, and therefore it is necessary to utilize a phosphorus removal technology if the greywater is discharged in a water body to prevent eutrophication. EU Directive 91/271/EEC gives phosphorus and nitrogen requirements for urban WWTPs that discharge for sensitive water bodies. Even though these requirements are for large WWTP (> 10 000 p.e.), these requirements for nutrient reduction give an indication of the necessary treatment level of a greywater treatment system.

Table 2.4 - Requirements for discharges from urban WWTP to sensitive areas, which are subject to eutrophication. EU Directive 91/271/EEC

Parameter	**Concentration**	**Min. percentage of reduction**
Total Phosphorus (mg/l)	2 mg/l P (10 000 – 100 000 p.e.) 1 mg/l P (more than 100 000 p.e.)	70 – 80 %
Total Nitrogen (mg/l)	15 mg/l N (10 000 – 100 000 p.e.) 10 mg/l N (more than 100 000 p.e.)	80 %

2.1.3 Treatment methods

Various physical, chemical, and biological treatment methods has been investigated for greywater treatment and reuse. Normally, pre-treatment units such as screens, septic tanks, and filters are used to prevent clogging of the main treatment methods. If necessary, a disinfection step is also included. See Ghunmi et al. (2011) for an extensive review over different greywater treatment technologies, greywater characteristics and water quality standards in relation to greywater reuse.
Figure 2.1 presents a selection scheme based on the strength of the greywater and the usage of the treated greywater. A treatment system based on aerobic biological process and physical filtration has often been regarded as the most economical and feasible solution for a medium/high strength greywater. For lower strength greywater physical/chemical treatment solutions have proven more viable (Ghunmi et al., 2011; Li et al., 2009).

A COD:N:P ratio of 100:20:1 has often been reported as a requirement for aerobic treatment (Metcalf & Eddy et al., 2013). The literature values of greywater characteristics in Table 2.1 might suggest that aerobic treatment of greywater might suffer nitrogen deficiency (COD:N:P = 100:2.4:0.9). The kitchen sink may be included in the treatment of greywater, and a possible nitrogen deficiency for aerobic treatment suggests that the kitchen sink should be included to provide macro and trace nutrients for aerobic biological treatment.

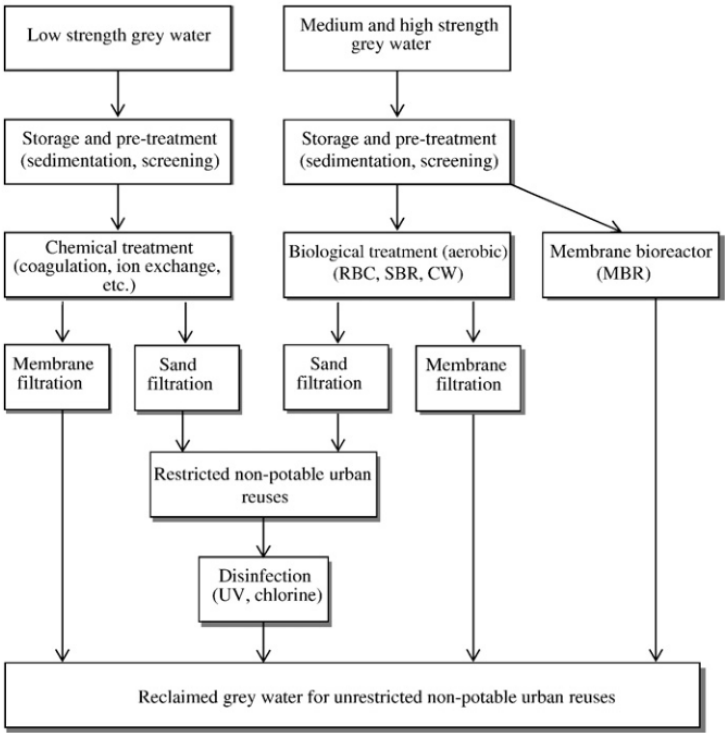

Figure 2.1 - Treatment selection scheme based on greywater quality (Li et al., 2009)

2.1.4 Biological nutrient removal

Biological nutrient removal and especially phosphorus removal is very dependent on the characteristics of the influent greywater, particularly VFAs and readily biodegradable COD (rbCOD). Various influent parameter ratios have been used to predict and assess the potential for biological phosphorus removal. Some of these are shown in Table 2.5. VFAs are consumed by PAOs in the anaerobic zone and therefore VFA:P is a good predictor for proliferation of PAOs and the efficiency of the phosphorus removal (Metcalf & Eddy et al., 2013). According the greywater quality presented in Table 2.1, biological phosphorus removal should be feasible with respect to BOD:P and COD:P ratios. Further investigations of VFAs and the rbCOD needs to be done to evaluate the feasibility of biological phosphorus removal of greywater.

Table 2.5 - Minimum influent ratios for achieving S_{PO4} < 0.5 mg/L in the effluent

Influent parameter ratio	Minimum value	Reference
VFA:P	8	Wentzel et al. (1989)
rbCOD:P	18	Barnard (2006)
BOD:P	15-20	Janssen et al. (2002)
COD:P	60	U.S. EPA (2010)

2.1.5 MBR for greywater

MBR has been especially popular for greywater treatment, due to various benefits such as:

- Process stability
- Removal pathogens because of micro/ultrafiltration
- High quality effluent
- Small footprint
- Low excess sludge production
- High organic loading rate
- Able to favor nitrifiers for nitrogen removal due to high sludge age

Typically MBR is used with a screen for pre-treatment (removal of coarse material), and a tank is used to maintain the biomass. The membrane is submerged in the tank, and can be put in either as a flat sheet membrane or a hollow fiber membrane.

MBR Case studies

Various studies have been conducted to investigate the feasibility of MBR as a greywater treatment technology. Atasoy et al. (2007) ran a 600 L MBR in Turkey with an HRT of 18 h for 50 days. The average removal efficiencies were found to be 95% for COD, 92% for T-N, and 99% TSS. Lesjean and Gnirss (2006) ran a 35 L MBR pilot in Berlin with real greywater for 8 months. It was operated at a low SRT of 4 d. An average removal efficiency for COD and TKN removal was found to be >85% and >80%, respectively.

2.2 University of Cape Town Process – Membrane Bioreactor (UCT-MBR)

The pilot plant that is the focus of this study utilize a biological nutrient removal (BNR) configuration known as University of Cape Town process. Traditionally, the configuration have been used with a sedimentation tank as a solid separation unit. The pilot in this study utilizes a submerged membrane in the aerobic reactor as the separation unit. This configuration is called UCT-MBR. See Figure 2.2 for a schematic of the system configuration.

The system can achieve a high effluent quality with > 90% COD, > 90% NH_4-N, > 90% P removal and achieve an P concentration of < 0.5 mg/l. The removal efficiency of P is very dependent on the influent characteristics (Metcalf & Eddy et al., 2013).

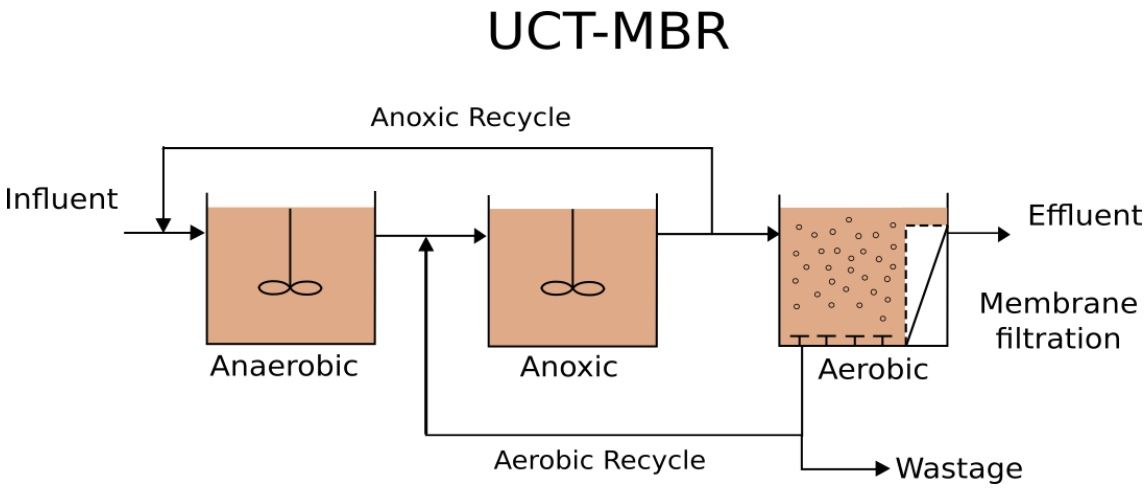

Figure 2.2 - Schematic for UCT-MBR system configuration

The fundamental principle of biological phosphorus removal is based on the cultivation of a group of organisms called phosphorus-accumulating organisms (PAOs), who are able to store more phosphate than they need for their cellular requirements. PAOs store the phosphorus as polyphosphate under aerobic/anoxic conditions, and use

stored PHA as an energy source to store polyphosphate. Under aerobic conditions, oxygen is used as an electron acceptor, while under anoxic conditions nitrate is used as an electron acceptor.

Under anaerobic conditions, PAOs use polyphosphate as an energy source to convert VFAs (acetate, etc.) to PHA. Either the VFAs are converted from fermentable COD or they are already present in the influent. See Figure 2.3 for a simplified biochemical model. Due to this kind of metabolism, PAOs are able to outcompete other organisms in alternating anaerobic and aerobic/anoxic conditions.
Therefore, it is expected to find a high phosphorus concentration in the anaerobic tank and a low phosphorus concentration in the aerobic tank in a WWTP running the UCT-MBR process. See Figure 2.4 for an illustration of phosphate, poly-P, PHA and glycogen in the different tanks. The PAOs can store more phosphorus than they release, and this results in a net P removal when the sludge is wasted. Care must be taken during the sludge treatment as the PAOs release the phosphorus under anaerobic treatment.

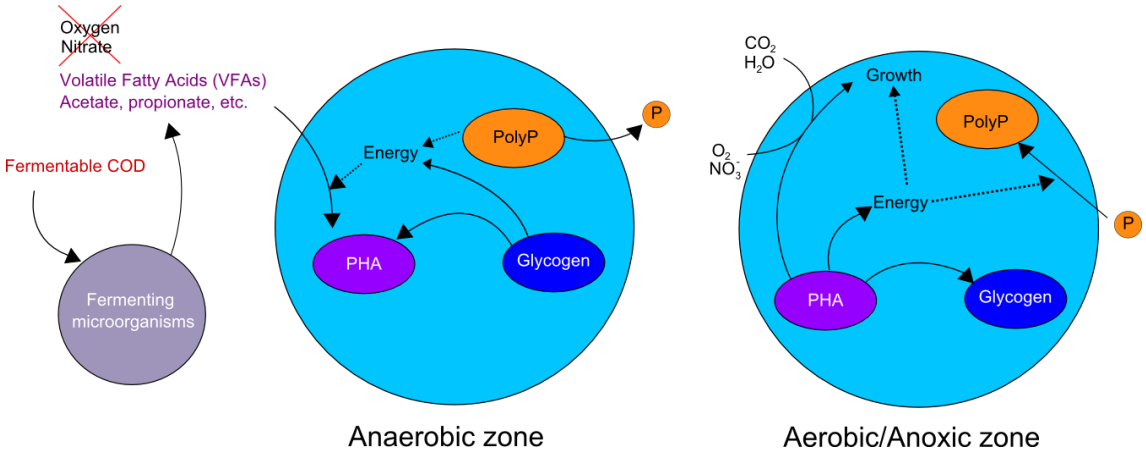

Figure 2.3 - Simplified biochemical model for PAOs in anaerobic and aerobic/anoxic environment (Henze et al., 2008)

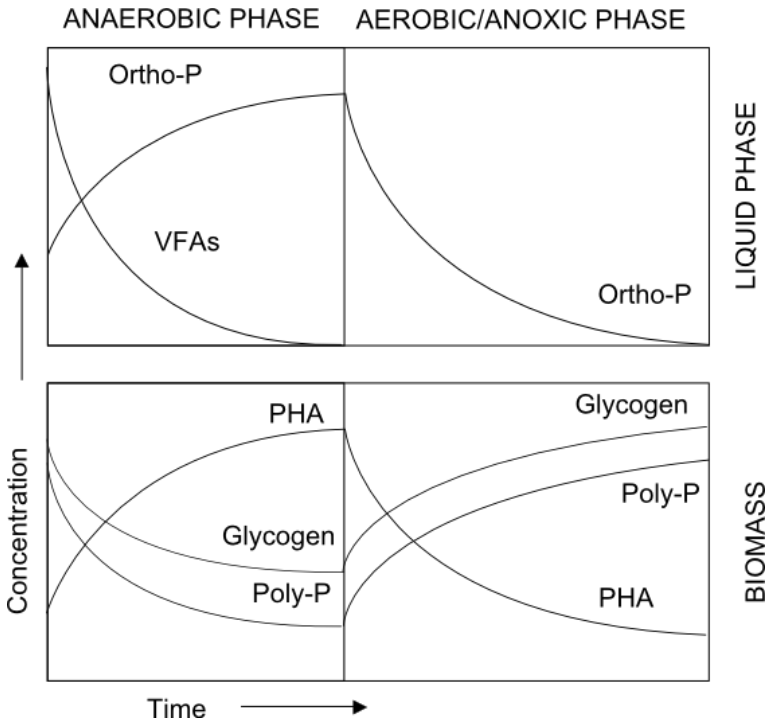

Figure 2.4 - Concentrations of phosphate, PHA, Poly-P and Glycogen in different tanks (Janssen et al., 2002).

The PAOs are able to store as much as 0.38 g P/g VSS (0.17 g P/g TSS), which is much higher compared to what can be typically stored in the sludge mass: 0.02 g P/g VSS (0.015 g P/g TSS). For BNR systems with good operation, the sludge can reach as high as 18% g P/g TSS. Typical phosphorus concentration in the sludge is 5% g P/g TSS (Henze et al., 2008).

In the UCT configuration, the sludge is recycled from the aerobic tank to the anoxic tank, and further recycled to the anaerobic tank. The nitrogen is converted to nitrate through nitrification in the aerobic tank and subsequently denitrification converts the nitrate to nitrogen gas in the anoxic tank. If there is low denitrification in the anoxic tank, nitrate can be recycled to the anaerobic tank and that can be detrimental to the process. If nitrate is present in the anaerobic tank, the heterotrophic organisms utilize the fermentable COD for growth and the nitrate as an electron acceptor. Thus, the fermentable COD is not converted to VFAs, which is essential for the PAOs for storage of PHAs. Thus, nitrate in the anaerobic tank will hinder the proliferation of PAOs and needs to be prevented.

The anoxic P uptake in BNR systems have been widely studied, and there are variable results in the literature. Some exhibited close to zero anoxic P uptake (Clayton et al., 1991), while other have found that anoxic P uptake was dominant over aerobic P uptake (Hu et al., 2001; Patel et al., 2005; Šorm et al., 1996). If the anoxic P uptake can

be increased, that would lead to less sludge production and less aeration costs compared to BNR systems with dominant aerobic P uptake (Henze et al., 2008).

Sludge retention time

There is a conflict between the factors that control nitrifying bacteria and PAOs. Nitrifiers have a slow growth rate and therefore need a long SRT to proliferate, while the PAOs favor a short SRT (3-5 days) (Onnis-Hayden et al., 2011). MBR systems are typically run with a long SRT (> 20 days) and systems with a long SRT typically have a low net biomass growth, and thus PAOs have limited storage of phosphorus in new cell material and the system therefore have low phosphorus removal.

Thus, there is a need to find a balance to achieve good N and P removal, and decrease the SRT in UCT-MBR systems compared to the typical MBR system. Many systems have operated well with a SRT of 10 days, and up to 20 days (Patel et al., 2005).

Membrane as the solid separation unit

Ramphao et al. (2005) investigated the impact of membrane as the solid separation unit in a UCT configuration for BNR and highlighted several advantages:

1. The solid separation is not dependent on the sludge settability and sludge bulking. Poor settling sludge occurs often in BNR systems, when aerobic mass fraction is low (< 60%)
2. Footprint reduction, due to lower reactor volumes (possibility to maintain higher MLSS concentrations) and membranes have lower footprint than sedimentation tanks
3. It is possible to adapt the mass fractions in the different reactors to variable influent wastewater characteristics, by varying the recycle ratios.
4. High quality effluent is produced, reducing the requirement for tertiary treatment.

Monti et al. (2006) did a comparative study on conventional UCT pilot and a UCT-MBR pilot operated at University of British Columbia, Canada. The pilots were fed with primary effluent from municipal wastewater. Both pilots maintained satisfactorily P removal when favorable COD:P ratio was maintained in the influent. The UCT-MBR pilot exhibited lower sludge yield and it was possible to run the UCT-MBR with a low HRT (7 h). The conventional UCT pilot demonstrated better denitrification capability and better P removal when VFAs in the influent was limiting. This was likely due to low nitrate concentration, so that the PAOs were able to efficiently use the VFAs in the anaerobic zone. These aspects are important for design of UCT-MBR systems.

2.3 Integrated Fixed Film Activated Sludge (IFAS) for nutrient removal

An IFAS system is a combination of activated sludge and attached growth system, and is a popular modification/upgrade of conventional activated sludge systems instead of building new aeration/settling tanks. A carrier media (suspended plastic wheel/sponge or fixed media) is added to the aeration tank, where the biofilm can attach and grow. Figure 2.5 shows an example of plastic media with biofilm.

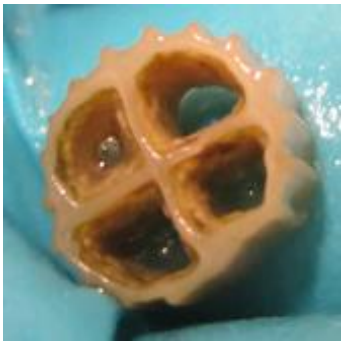

Figure 2.5 - Plastic media with biofilm

This process demonstrates various benefits compared to conventional activated sludge systems (Metcalf & Eddy et al., 2013):

- Increase the effective MLSS concentration (by 1.5 – 2.0 times)
- Higher effective SRT (favorable for nitrifiers)
- Decouples the growth rate of nitrifying populations and the suspended mixed liquor phase SRT (MLSRT)
- Higher treatment capacity for the same volume
- Robust operation and resistance to load variations
- Lower sludge production

IFAS systems normally require a DO concentration of 4 to 6 mg/L, for the oxygen to diffuse fully into the biofilm.

It is possible to achieve biological phosphorus removal with similar configurations that are used for conventional activated sludge systems, where the carrier media is placed in the anoxic and/or aerobic tank (Majed et al., 2008).
Few studies have investigated biological phosphorus removal with IFAS system, however Christensson and Welander (2004) achieved a phosphorus removal of 95% (reduction from 6.5 mg/l to 0.3 mg/l, with a UCT configuration with carrier media in the aerobic tank.

Onnis-Hayden et al. (2011) investigated one of the few full scale IFAS-EPBR operating in the world. It is located at Broomfield, Colorado, USA. This study showed

that the phosphorus removal and PAOs were mainly associated with the mixed liquor and the nitrifiers and nitrification were associated with the biofilm at the carriers. This enables a separate control of SRT for fast growing PAOs and slow growing nitrifiers to achieve simultaneous nitrogen and phosphorus removal. PAOs need to be exposed to alternating anaerobic and aerobic conditions and thus are favored through the recycle streams, while the nitrifiers are maintained in the aerobic tank due to the carrier media.

2.4 Mathematical models for Biological Wastewater Treatment

This section discusses the different mathematical models relevant to this thesis, such as ASP, MBR, MBBR/IFAS, and BNR models.

2.4.1 Model applications

This section will elaborate on the specific applications of mathematical models for biological wastewater treatment systems.

A family of models have been published for activated sludge systems, where the most popular is still the first model, ASM1. One of the main motivations for the development of the ASM models were practical use by engineers and consultants in design and optimization studies. Especially for complex WWTPs that utilize biological nutrient removal, and where the recycle side streams from the sludge treatment needs to be considered, modelling has been shown to be a very useful tool.
For a certain system configuration, various aspects can be investigated by a model, such as:

- Effluent quality
- Aeration requirements
- Sludge production
- Concentration of MLSS in the bioreactor
- Optimal internal recycle streams and recycling of activated sludge

With dynamic simulators, it is also possible to investigate situations for taking a tank out of service and storm events.

Mathematical models have also been used for industrial wastewater treatment. The direct application of ASM type models for industrial wastewater should be done with great care. The ASM models where developed with regard to municipal wastewater treatment and industrial wastewater may contain compounds that will affect the treatment process in a way that is not considered in the model. There is a greater need to characterize the influent to the plant and do experimental investigations to estimate important kinetic parameters for the model (Rieger et al., 2012).

However, various authors have used models successfully with few modifications to ASM models for evaluating industrial WWTP. Moussa et al. (2004) used a modified ASM1 to evaluate possible extensions to a tannery. Bentancur et al. (2015) used the BioWin ASDM model to investigate pulp mill WWTP extension, and Pardo et al. (2007) used the ASM3 model to describe and evaluate extensions to a WWTP treating oil refinery effluent. These studies have shown that the ASM models

are robust and are able to successfully simulate wastewater treatment with quite different influent characteristics.

2.4.2 Modelling Framework

A wastewater treatment system is a complex system involving physical, chemical and biological processes, where there are numerous internal interactions between compounds and the biomass.
Figure 2.6 shows a schematic representation of the different submodels involved in a complete WWTP model.

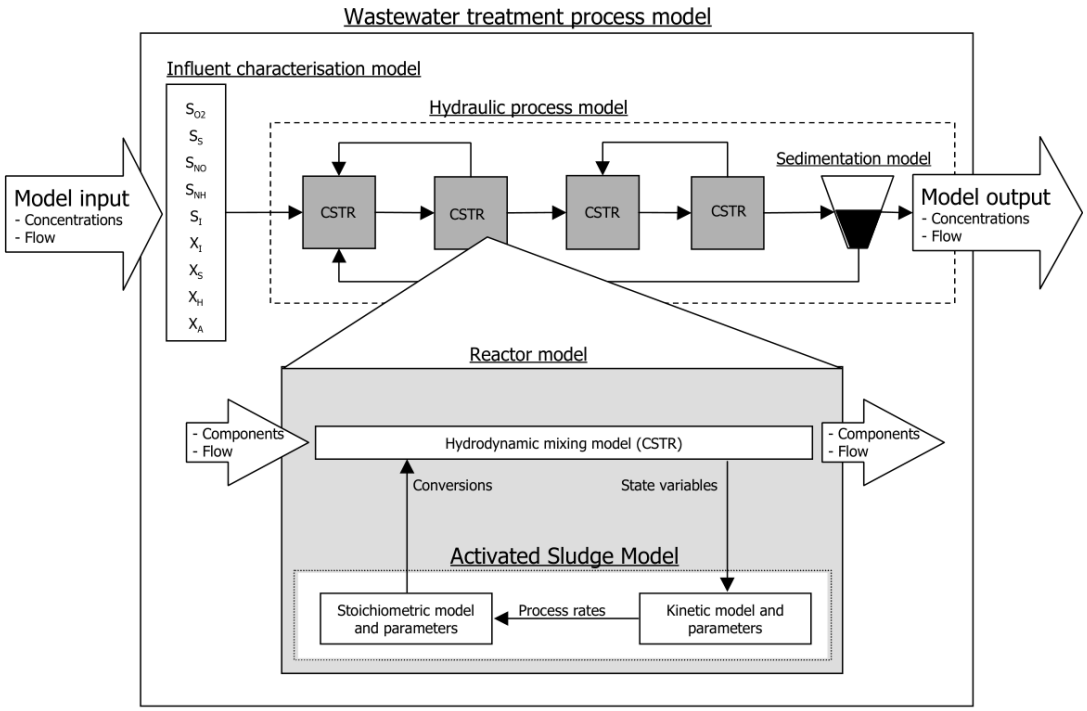

Figure 2.6 - Schematic representation of a WWTP model (Meijer, 2004).

2.4.2.1 Influent wastewater characterization model

The parameters that is typically measured at a WWTP does not immediately convert to components or state variables that are used in activated sludge models. Therefore, it is necessary to define a conversion or fractionation from the measured parameters to the components that are used in the model. There are several models that have been proposed for this conversion and this is discussed more in Chapter 2.5.2.

2.4.2.2 Hydraulic/Transport model

The hydraulic model represents the flow through the plant, and includes the connections and recycle streams between the reactors in the WWTP model. Normally, the pipes are not modelled with volume or friction losses. Mass moves with a defined time step between the compartments. A full scale WWTP can have different hydraulic regimes, such as several CSTR physically separated by compartments or long tanks without walls with aerated and unaerated zones (oxidation ditch, etc.). Most modelling studies and simulators have used CSTR tanks-in-series for modelling the hydraulic regime. With this approach, it is possible to utilize a biokinetic model such as ASM to model a wide range of hydraulic regimes and maintain a simple model. If not, the ASM equations and model had to be adopted to a dispersed or plug flow regime resulting in complex partial differential equations (Chambers and Jones, 1988).

It can be difficult to decide on the number of CSTR tanks that represents the real WWTP, and various approaches have been used in the literature, such as empirical equations, tracer experiments, CFD studies or expert assessment (Petersen et al., 2002). If there exists concentration gradients within a tank, the tank should be modelled by a tank-in-series model. Measuring the concentration for compounds such as nitrate, ammonia, oxygen or phosphate throughout the tank can help determine how the tank should be divided into several compartments in the model (Henze et al., 2008).

Figure 2.7 shows some examples of conversion from real flow scheme to a modelled flow scheme.

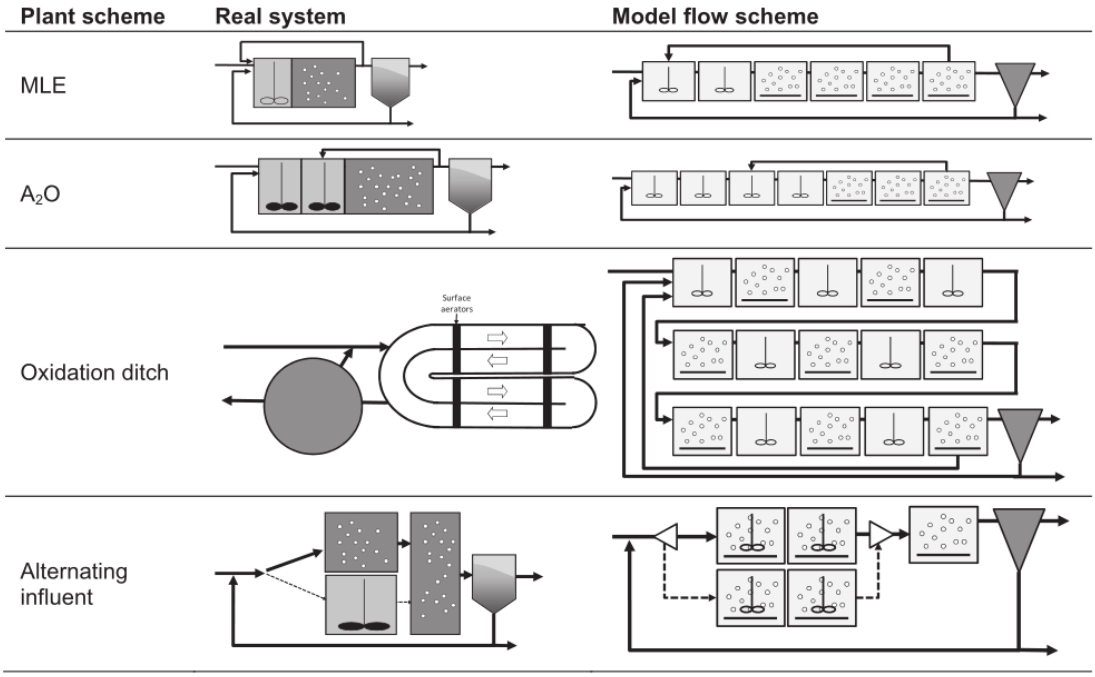

Figure 2.7 - Differences between full scale WWTP and the model implemented (Rieger et al., 2012)

Chambers and Jones (1988) presented an empirical equation (2.1) for estimating the number of tanks-in-series for representing dispersed flow systems:

$$N = \frac{7.4 \cdot L \cdot q_s(1+r)}{W \cdot H} \qquad 2.1$$

Where N = Number of tanks-in series

W = Width of tank (m)

H = Depth of tank (m)

L = Length of tank (m)

r = Recycle ratio (-)

q_s = Average flowrate (m^3/s)

2.4.2.3 Reactor model

The reactor model is the compartment and is typically modelled as a CSTR. This means that the concentrations of the components are equally distributed throughout the tank. This model can include an aeration model and gas transfer equations to represent the gas exchange with the atmosphere. For advanced modelling studies, the temperature variations can also be included in this submodel (Makinia, 2010).

2.4.2.4 Biokinetic / Activated Sludge model

This submodel is considered the workhorse of a biological wastewater treatment model. All the biological processes and conversions are considered here. It consists of equations for process rates for the different biokinetic conversions. The activated

sludge model (ASM) is elaborated in Chapter 2.4.3. The biokinetic model can also contain a biofilm model or a combination of biofilm and activated sludge model. These types of models are discussed in more detail in Chapter 2.4.5.

2.4.2.5 Separation model

For a typical activated sludge system, the separation model consists of a sedimentation model. One of the most popular sedimentation models is a simple dynamic 1-D model, often referred to as the Takács model (Takács et al., 1991). The sedimentation model can also be combined with an ASM model if biological reactions in the sedimentation tank has a significant effect on the performance of the WWTP. As the experimental system that is the subject of this thesis does not utilize a sedimentation tank, sedimentation models will not be elaborated further.

For MBR systems, the membrane filter is used as the separation unit. If the fouling process or cake formation is of no interest, the filter is often modelled as an ideal separation point or point settler (Naessens et al., 2012). The ideal separation model separates the incoming flow into two streams, and the user specifies the solids capture efficiency. For ultrafiltration or microfiltration, membranes that means 99-100% solids capture rate. The soluble components are divided proportionally to the outgoing flows.

2.4.3 Activated sludge models

Biokinetic models considers time-dependent (kinetic) transformations of compounds by organisms in the wastewater. The ASM models are a group of biokinetic models that considers separate groups of organisms (heterotrophic, autotrophic, phosphorus accumulating organisms (PAOs), and nitrifiers), substrates (readily biodegradable substrate, slowly biodegradable substrate), and other relevant components.

Short history of ASM1/2/2d/3

The first ASM model was published in 1987, and it represented an important breakthrough for wastewater treatment models. It was developed in an IWA Task Group formed in 1983. Previously, there existed various modeling frameworks and there was no common platform for WWTP modeling. The ASM1 represented a consensus model that was established based on work from different research groups (USA, Denmark, South Africa, Japan and Switzerland). The goal was to find the simplest model that could provide realistic predictions and thus would be widely applicable for engineering practice. The ASM1 includes 8 processes and 13 components for

describing activated sludge system for organic matter and nitrogen removal (nitrification/denitrification) (Henze et al., 1987).

For the next published ASM model (ASM2) phosphorus removal mechanisms was included. The ASM2 model includes both chemical and phosphorus removal processes. The model was expanded to include 19 processes and 19 components, due to the inclusion of PAO organisms and cell internal storage products such as poly phosphate and PHA. Total suspended solids (TSS) was also introduced as a component for describing phosphate precipitates and mineral particulate solids (Gujer et al., 1995). Later, ASM2 was expanded with 2 processes to include denitrification by the PAO organisms (anoxic P removal). This model was published as ASM2d (Henze et al., 1999).

The latest "official" ASM model is the ASM3 model. The ASM3 model was developed to describe organic matter and nitrogen removal, as was the case for ASM1. The ASM3 model contains 12 processes and 13 components. The main difference between ASM1 and ASM3 is that heterotrophic organisms grow on storage polymers (such as glycogen) instead of directly on substrate as was the case with ASM1. In ASM3 the readily biodegradable substrates (S_s) are stored as storage polymers before the are consumed by the heterotrophic organisms (Gujer et al., 1999). Later, ASM3 was expanded to include biological phosphorus removal mechanisms similar to ASM2d (Rieger et al., 2001). This expansion is often referred to as ASM3-bioP.

Fundamentals

This section describes the fundamentals for the ASM models. For the specific models the reader is encouraged to read the individual model reference papers.
The ASM models are considered mechanistic models since they are based on physical-chemical-biological fundamental mechanisms. The ASM model are built on a framework that consists of a 6 essential parts. See Table 2.6 for the essential parts of an activated sludge model with a short description and an example.

In other contexts, parameters and variables are often used interchangeably, but in the context of ASM models, parameters refer to kinetic and stoichiometric coefficients that are defined at the start of the simulation and remains constant for the simulation period. State variables refer to the different components (e.g. COD, N, and P components) in the model and changes throughout the simulation period.

Table 2.6 - Essential parts of activated sludge model

Part	Description	Example	Example of Units
State variables / Components	Represents concentrations of defined components	Soluble oxygen (S_{O2}), Readily biodegradable substrate (X_S), Ammonia (S_{NH})	mg O_2/l, mg COD/l, mg N/l, mg P/l, Mole
Kinetic parameters	Conversion rate for process that acts on the state variables	Autotrophic growth $\hat{\mu}_A$	1/d, mg O_2/l, g P/l
Stoichiometric parameters	Describe the conversion of state variables to others	Heterotrophic yield Y_H	g COD/g COD, g P/g COD
State variable composition	N, P, COD content, or charge is defined in the composition matrix to allow mass balance continuity.	Fraction of nitrogen in X_S (i_{NXS}), Fraction of phosphorus in X_H (i_{PBM})	g N/g COD, g P/g COD
Mass balance/continuity equations	The models include mass balance equations for essential elements.	COD balance N and P balance Ionic charge balance	
Processes	A distinct event acting on one or more components such as S_O, X_S.	Aerobic growth of heterotrophs, 'Decay' of autotrophs, 'Decay' of heterotrophs	

The basis for the ASM models is a mass balance, where a single bioreactor is the system boundary. A mass balance is setup for each component (oxygen, ammonia, slowly biodegradable substrate, etc) according to the basic equation 2.2.

$$Input - Output + \boldsymbol{Reaction} = Accumulation \qquad 2.2$$

The core of the ASM models is the definition of the reaction term of the mass balance. Since the introduction of the ASM1 model, the reaction terms have been presented in a Gujer matrix format.

Due to the high complexity of biokinetic models, a Gujer matrix notation has become standard way for publishing and communicating the processes, state variables and parameters involved in the model. Before ASM1 was published, it was increasingly difficult to follow the thought process of the authors of different models. ASM1 helped define a basis and a unified notation that modern wastewater treatment models are based upon. See Appendix A – Matrix for ASM2d for a description of the Gujer matrix format and the ASM2d model used in this thesis. The matrix can also be viewed in the attached Excel sheet.

The matrix format enables the description of the reactions term in a compact format instead of a long list of reactions terms. It would be redundant and extremely tedious to write out the different reactions term, but the reaction term for heterotrophic organisms (X_H) from ASM2d is included here as an example (Equation 2.3). This expression includes the processes for aerobic/anoxic growth and hydrolysis of heterotrophic organisms. As can be observed these expression can be quite complex and thus there is a need for a compact presentation framework.

$$
\begin{aligned}
r = {} & \mu_H \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_F}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H \\
& + \mu_H \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_A}{K_A + S_A} \cdot \frac{S_A}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H \\
& + \mu_H \cdot \eta_{NO_3} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_F}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \\
& \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H \\
& + \mu_H \cdot \eta_{NO_3} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{S_A}{K_A + S_A} \cdot \frac{S_A}{S_F + S_A} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{PO_4}}{K_P + S_{PO_4}} \\
& \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H \\
& + q_{fe} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \cdot \frac{S_F}{K_F + S_F} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot X_H \\
& - b_H \cdot X_H
\end{aligned}
\qquad 2.3
$$

Equation 2.3 also shows that ASM relies heavily Monod kinetics and switching functions. Switching functions are used to turn processes on/off based on the environmental conditions. For example, Equation 2.4 shows a switching function, which is turned on in aerobic conditions (S_O is positive). When K_O is small compared to S_O, this expression is close to 1 and will not influence the full process term a lot under

aerobic conditions. When S_O is small, the term will go towards zero and the process will be "turned off".

$$\frac{S_O}{K_O + S_O} \quad 2.4$$

Assumptions

The various ASM models are based on individual assumptions, and it would be too extensive to elaborate on all of them here; nevertheless, there are some common assumptions:

The pH is an important variable for biological activity and species distribution for ammonia, phosphate, acetate, and various other compounds. Therefore, it would be beneficial if the pH could be accurately modelled. However, pH modelling is difficult due to numerous reactions that are fast and complex. The approach to date in activated sludge models has been to track alkalinity changes instead, and the pH is assumed to be constant and is not inhibiting the biological processes. The alkalinity is used as an indicator for potential pH instability problems.

The nature of the influent does not change. As previously noted, the influent is fractionated into different ASM components (X_S, X_I, S_I, etc), and this relation to the influent data is assumed to be maintained for the simulation period. For municipal wastewater, this might not be entirely accurate throughout the year as the seasons and temperature might affect the degradation of the organic matter in the sewer network before it arrives at the WWTP.

Temperature is usually assumed to be in the range of 10 – 25 ^oC.

For further review of activated sludge modelling, Hauduc et al. (2013) should be consulted.

2.4.4 Biological Phosphorus removal

This section reviews the most popular models that are used for biological phosphorus removal. Table 2.7 shows an overview over four popular models in terms of the number of processes, state variables, kinetic parameters, stoichiometric parameters and composition factors. These properties are important to get a quick overview over the complexity of the models.

In terms of number of elements considered in Table 2.7, the ASM2d model is the least complex model. The TUDP model (Meijer, 2004) is a combination of metabolic model and the ASM2d model. A main difference from the ASM2d model is the addition of cell internal glycogen (X_{GLY}) as a component. Under anaerobic conditions X_{GLY} and X_{PP} is consumed, as X_{PHA} is stored. Subsequently, under aerobic conditions, X_{GLY} and X_{PP} is taken up as X_{PHA} is oxidized for energy.

The ASM3 model does not include a fermentation step, and does not model volatile fatty acids (S_A) as a separate state variable. Hydrolysis is considered as the rate-limiting step, so that fermentation does not need to be represented explicitly. However, this can be a model limitation where hydrolysis no longer is the rate-limiting step (for application where the influent is already contains a high amount of hydrolyzed compounds).

Table 2.7 – Published models that include biological phosphorus removal (Makinia, 2010)

	Model			
Elements of model	**ASM2d**	**ASM3+bioP**	**TUDP**	**UCTPHO+**
Processes	21	23	22	35
State variables	19	17	17	16
Kinetic parameters	45	43	50	28
Stoichiometric parameters	9	12	18	14
Composition factors	13	15	18	12
Reference	(Henze et al., 1999)	(Rieger et al., 2001)	(Meijer, 2004)	(Hu et al., 2007)

Two highly complex models that includes BNR have been implemented in commercial simulators, and the number of processes and state variables in these models are shown in Table 2.8. These models are used for plant wide modelling that includes sludge treatment/anaerobic digestion and therefore result in a high number of processes and state variables. See Chapter 2.5.4 for a short discussion of these models.

Table 2.8 - Models that are implemented in commercial simulators

	Model	
Simulator	**GPS-X**	**BioWin**
Elements of model	**Mantis2**	**ASDM**
Processes	56	> 70
State variables	48	> 50
Reference	(Hydromantis, 2014)	(EnviroSim, 2014)

Zuthi et al. (2013) reviewed different models for biological nutrient removal in MBR systems, and reader is encouraged to consult this reference for more in-depth discussion on the differences between the different models.

2.4.5 Biofilm/MBBR/IFAS models

During the last 20 years, there have been published various biofilm models. An extensive review on different types of modes has been made by an IWA Task group and published in a report (Wanner et al., 2006). That report describes five different biofilm model classes:

- Pseudo analytical
- Analytical
- 1 dimensional numerical (1-D)
- 2 dimensional numerical (2-D)
- 3 dimensional numerical (3-D)

Pseudo analytical and analytical models are only feasible for simple problems and 2-D/3-D models have been limited to advanced research questions. It has been found that 1-D numerical models with heterogeneous biomass distribution are sufficient for usage in engineering design and modelling of full-scale systems (Henze et al., 2008). Different variation of 1-D numerical models have been implemented in the commercial WWTP simulators for biofilm reactor simulation and this review will focus on this class of biofilm models.

For design and simulation of biofilm reactors there are several aspects that can be elaborated by a biofilm model, beyond the aspects that are of typically of interest (effluent quality, aeration requirements, sludge production) (Takács et al., 2007):

- Distribution of particulate and soluble components in the biofilm
- Biofilm thickness
- Active biomass contained in the biofilm
- Required surface area to achieve the treatment objective
- Aerobic, anoxic and anaerobic sections of the biofilm

There is no consensus model that can be applied for biofilm reactors as is available for activated sludge systems, and biofilm modelling is more complex than activated sludge reactors due to various factors (Boltz et al., 2010):

- Biofilm diffusional resistance
- Impact of bulk-liquid hydrodynamics
- More complex fate of particulate and soluble components
- Biofilm reactor configuration

There have been several different modeling approaches applied in biofilm modeling, resulting in various models with different model structures (e.g.

heterogeneous vs. homogeneous biomass distribution). This differ from the ASM models where the same modeling structure is similar, but the processes included in the model differs in the different models (Morgenroth et al., 2000). Different modelling approaches also complicates the decision to chose an appropriate model for a given application.

However, even though there are some differences, there are also some essential features that are common for the 1D biofilm models (Wanner et al., 2006):

- Compartments that represents the biofilm, the bulk and the mass-transfer boundary layer.
- Components that represent the substrate, biomass and other constitutents similar to the ASM models.
- Processes that represent transformation of the different components.
- A mass balance equation is utilized to calculate the change in concentrations of the components, where processes and a reaction term is included.

The mass transfer boundary layer compartment is used to represent the strong concentration gradients that have often been observed between the biofilm surface and the bulk liquid. It includes the resistance of mass transport for soluble components outside of the biofilm. In cases where there is a high flow velocity in the bulk liquid, the mass transport boundary layer have been found to be insignificant (Wanner et al., 2006).

The components are similar to the ASM models and is divided in particulate and dissolved. Similar transformation processes that are used in ASM model are also used in biofilm models.

Essential processes that are typically defined for a biofilm model are:

- Attachment and detachment of particulate components in the biofilm and at the surface
- Diffusion processes for attached particulate components in the biofilm
- Diffusion of dissolved components from the liquid phase to the biofilm and/or through the mass-transfer boundary layer.

Parameters that need to be set up or calibrated for application of biofilm model are the following:

- Kinetic and stoichiometric parameters for transformation processes (similar to ASM models)
- Diffusion coefficients
- Coefficients for attachment and detachment rate functions
- Thickness of mass-transfer boundary layer

- Geometric and hydraulic data (Biofilm surface area, Bulk liquid volume, inflow rate, etc.)

Figure 2.8 illustrates the different parts of a biofilm model as discussed above, and indicates that the uncertainty in the modelling results is more likely to originate from the mass-transfer boundary layer or the interaction between the bulk-liquid and the biofilm (Boltz et al., 2010).

L_L = Mass-transfer boundary layer thickness, L_F = Biofilm thickness, S = Substrate.

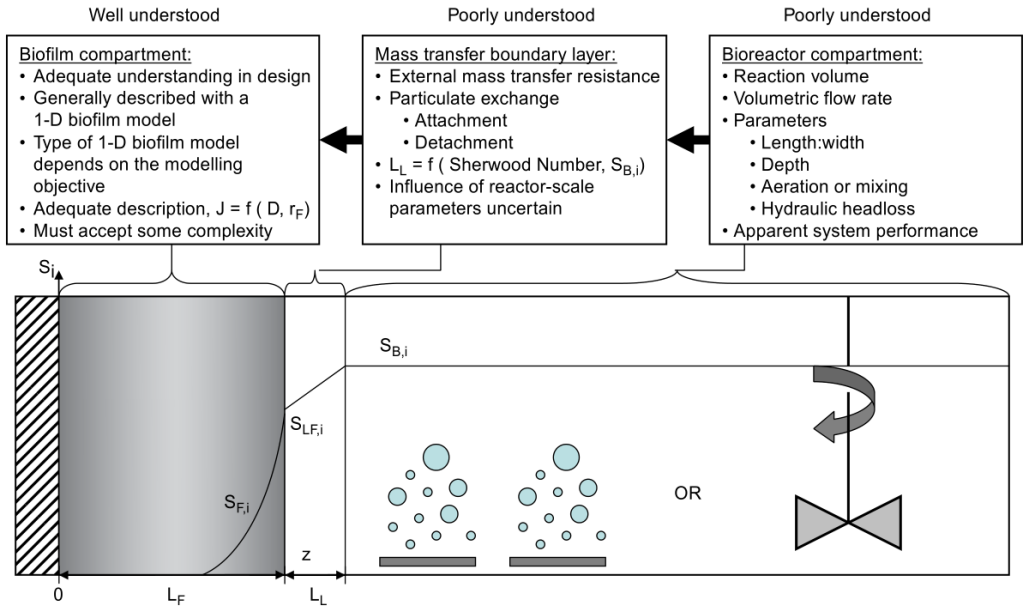

Figure 2.8 - Biofilm model with compartment for biofilm, mass-transfer boundary layer and bulk-liquid (Boltz et al., 2010)

IFAS systems are a combination of activated sludge models and attached growth systems as discussed in Chapter 2.3. To be able to successfully model IFAS systems there is a need to combine biofilm and ASM models. During the last decade two such 1D biofilm and ASM hybrid models have been published and applied for engineering purposes (Boltz et al., 2009a, 2009b; Sen and Randall, 2008a, 2008b). One of them will be discussed here.

Boltz et al. (2009a) presents a steady-state model that uses an extended ASM2d model for the biokinetic transformation processes in the suspended biomass and the biofilm. The same kinetic and stoichiometric parameters are used for both the biofilm and the suspended biomass. The biofilm thickness and biofilm concentration is assumed to be constant throughout the simulation period and needs to be specified by the model user. The mass-transfer boundary layer is also included and the thickness needs to be specified. A special feature of the model is the inclusion of two populations of methanol-degrading heterotrophs (methylotrophs). Boltz et al. (2009b)

evaluated the model on four different MBBR and IFAS applications with COD removal and nitrification, and the predictions fitted reasonably well with the experimental results. However, due to lack of measurements on the biofilm thickness and biofilm concentration it was difficult to validate this aspect of the model.
Different Models for hybrid systems has also been implemented in each of the popular commercial simulator such as GPS-X, BioWin and WEST. See the description for the individual simulators in Chapter 2.5.4 for a more detailed discussion of the biofilm models.

Even though various biofilm models have been developed during the last decade, no consensus model have emerged and therefore the decision for which model to use is difficult. An increase in case studies of biofilm model applications might help increase the understanding of the application of these types of models.

2.4.6 Membrane bioreactors (MBR)

When only the separation of solids is of interest in the MBR configuration, the filtration model is heavily simplified to an ideal separation point, which have complete retention of solids. Soluble compounds are divided proportionally between the outflow streams of the reactor.

Compared to conventional activated sludge systems, MBR systems often employ a high MLSS concentration (7 - 13.5 g SS/L) and a high SRT (15 – 40). MBR also tend to apply high aeration rates for scouring and accumulate soluble microbial products (SMP) due to the membrane filtration step. These aspects make it questionable whether the ASM models can be directly applied to MBR configurations as these might cause a different microbial composition with different kinetic parameters to develop (Fenu et al., 2010; Hai et al., 2013). The kinetics for nitrification might change due to high SRT as this will most likely cause a high retention of nitrifiers. Many authors have utilized modified ASM models that include SMP for modelling of MBR systems. Fenu et al. (2010) concluded that the inclusion of SMP in the ASM models where justified if the following objectives where part of the modelling study:

1. Prediction of membrane fouling
2. Soluble COD predictions in the tanks
3. Modelling of MBR systems employing a high SRT (> 40 days)

When the objective is optimization of the operational settings (e.g. aeration, sludge wastage, recycle flows), it is important to include the cake layer formation, backwash and fouling into the filtration model. The filtration model is typically a mechanistic model based on Darcy's law and a resistance-in-series concept. The Darcy law helps

relating the flux to the TMP, and helps calculate the resistance. The resistance is typically modelled as a combination of clean membrane resistance, irreversible resistance, and a reversible resistance. The reversible resistance is increases during the filtration period and is reset after backwash (Naessens et al., 2012).

Parco et al. (2007) found that the kinetic parameters for phosphorus removal in a MBR system were comparable to that in conventional systems. Further, they concluded that high MLSS concentration had little to no effect on the denitrification and phosphorus removal kinetics, and thus parameters used for ASM models could be applied to MBR systems.

For further reading, an extensive review over the state-of-the-art modeling of MBR can be found in Hai et al. (2013).

2.4.7 Magnesium and Potassium

None of the standard ASM models nor biofilm models consider micronutrients as separate state variables and track their changes in the treatment system. Typically, magnesium (Mg) and potassium (K) are assumed to be in concentrations that are not limiting for the organisms. The lack of Mg and K might inhibit the polyphosphate storage of PAO organisms and thus the PAOs are not able to proliferate and the P removal capacity of the treatment systems deteriorates.
Barat et al. (2005) extended the ASM2d to include, and added switching functions to the PAO processes for storage of polyphosphate under aerobic and anoxic conditions.

1. Two new components, inorganic soluble Mg and K.
2. Additional switching functions for Mg and K.
3. Additional stoichiometric parameters for Mg and K for storage and lysis of polyphosphates.

This extension demonstrated successfully the deterioration of the PAO biomass and P removal capacity, when there was a lack of Mg and K.

2.5 Usage of Activated Sludge Models

2.5.1 Protocols

Due to a high number of modelling studies since the publication of the first ASM model there is a need for protocols that help provide a format for structuring the modelling study. A modelling survey found that most model users are self-thought and have not participated in an organized model training (Hauduc et al., 2009). Therefore, it is not surprising to find a variety of modeling approaches in the literature. This makes it difficult to compare and evaluate the modelling study, and there is a need for a standardized protocol. Different research group and organizations have developed their own protocol for conducting wastewater treatment modelling studies, and only recently have a unified protocol been established. The names, countries and references are summarized in Table 2.9. The protocols have been essential for increasing the usage of wastewater treatment models for consulting engineers (Rieger et al., 2012).

Table 2.9 - Standardized protocols for wastewater treatment modelling

Name	Country	Reference
STOWA	Netherlands	Hulsbeek et al. (2002)
BIOMATH	Belgium	Vanrolleghem et al. (2003)
WERF	USA	Melcer et al. (2003)
HSG	Germany	Langergraber et al. (2004)
GMP Unified Protocol	-	Rieger et al. (2012)

The protocols include information about data collection, influent characterization, model-setup and calibration procedures. Some of the protocols are more focused on practioners (STOWA, WERF) while others have been developed with a focus on application for research purposes (BIOMATH). The Good Modelling Practice (GMP) Unified Protocol combined the experiences with the different protocols, and can be called a consensus protocol. The five overall steps in the protocol are (Figure 2.9):

1. Project definition
2. Data collection and reconciliation
3. Model set-up
4. Calibration and validation
5. Simulation and result interpretation

Even though the steps are listed in a sequential manner, the steps are interrelated and might be revisited after a subsequent step has been performed. For example a

preliminary model can be setup to identify which data that are necessary for collection, or closer investigation of the model-setup might be necessary after a failed calibration and validation. A detailed discussion and comparison of the different protocols can be found in Makinia (2010) or Sin et al. (2005).

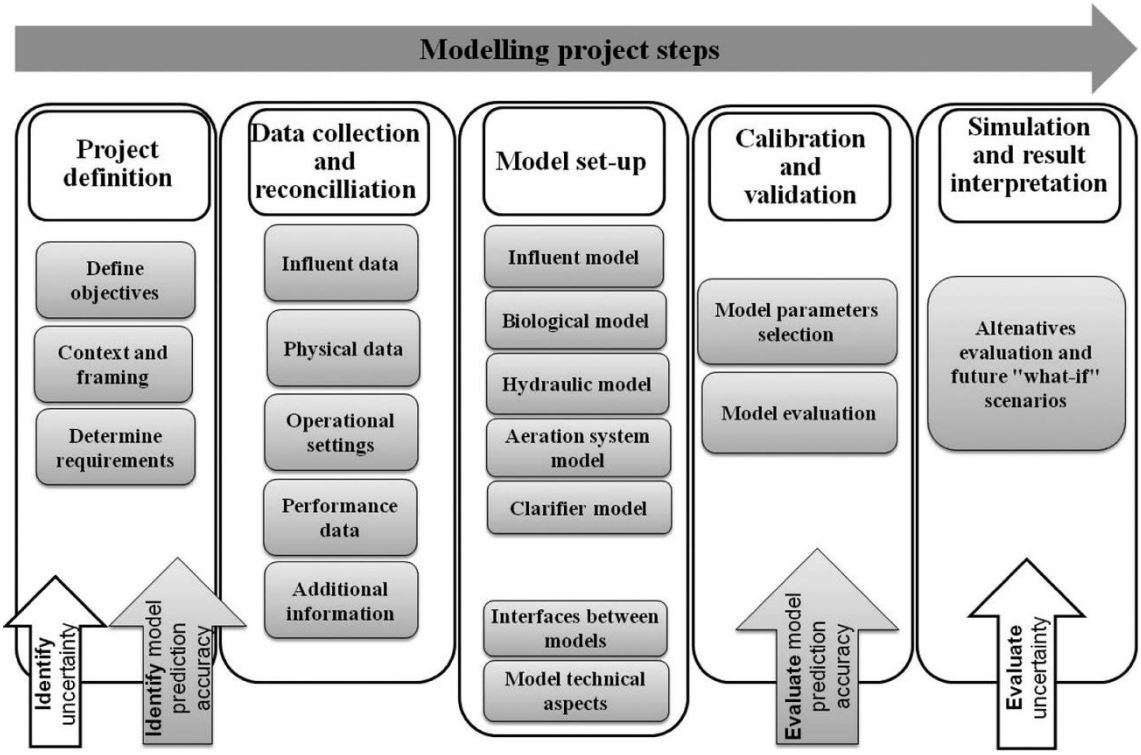

Figure 2.9 - The overall GMP Unified Protocol steps

2.5.2 Influent Characterization

Influent characterization is one of the most important modelling steps, and is a dominant factor for the quality of the predictions made by the model (Rieger et al., 2012). Modern approaches for measuring the characteristics of wastewater for modelling is mainly focused on COD, as BOD cannot be used for mass balancing because it is not conserved. BOD is typically defined as the oxygen demand for biological degradation after 5 days. Normally, the degradation processes are only partially completed in 5 days, and therefore the BOD value does not represent the complete oxygen need of the biomass and organic material. If only BOD values are available, they need to be converted to COD values to be used for mass balancing the model.

For every time the model is to be applied, it is necessary to define a COD fractionation scheme (How is the total COD divided into different fractions?).
For the ASM2d model, the total COD includes the following components:

$$C_{\mathrm{TCOD}} = S_{\mathrm{A}} + S_{\mathrm{F}} + S_{\mathrm{I}} + X_{\mathrm{I}} + X_{\mathrm{S}} + X_{\mathrm{H}} + X_{\mathrm{PAO}} + X_{\mathrm{PHA}} + X_{\mathrm{AUT}}$$

Often X_{H}, X_{PAO}, X_{PHA}, and X_{AUT} can be considered to be close to zero, and therefore are not considered in the influent (Henze et al., 2000). Thus, the total COD can be simplified to:

$$C_{\mathrm{TCOD}} = S_{\mathrm{A}} + S_{\mathrm{F}} + S_{\mathrm{I}} + X_{\mathrm{I}} + X_{\mathrm{S}}$$

A schematic representation of the COD fractionation in the ASM2d model is shown in Figure 2.10.

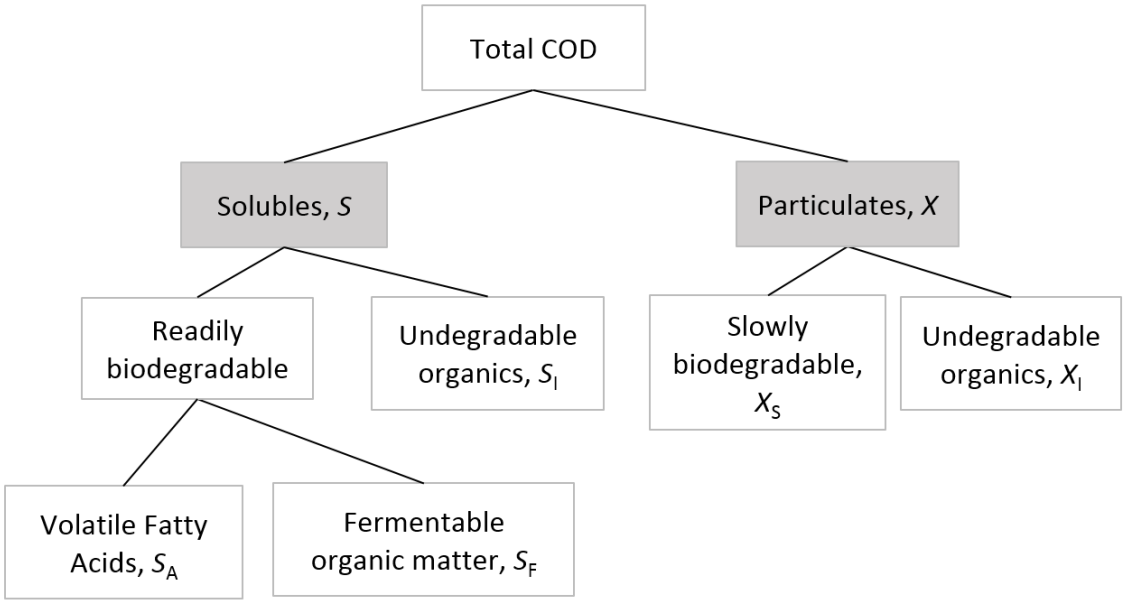

Figure 2.10 – COD fractionation scheme for ASM2d model.

Currently, there doesn't exists a standardized COD fractionation method. In general, two approaches have typically been used for COD fractionation: respirometric methods or physiochemical methods.

Respirometric methods involves setting up a batch or flow-through aerobic experiment and measuring the oxygen utilization rate (OUR) (Ekama et al., 1986). A flow-through aerobic test typically involves setting up a pilot reactor and letting it stabilize for 3 SRT. For aerobic batch test, the procedure can be done in 4-5 hours, depending on the amount of readily biodegradable COD. The total undegradable COD fraction, the total biodegradable COD fraction, heterotrophic biomass, and readily biodegradable COD can be identified by respirometric methods.

Physical-chemical methods involves filtration with 1.2, 0.45 or 0.1 μm filters, and sometimes flocculation with iron ($FeCl_3$) or zinc (Zn). These methods assume that the size of organic matter and their biodegradability is directly linked. These methods are used to identify the readily biodegradable COD or undegradable organics.

The S_A fraction (VFAs) are typically measured directly using gas chromatography.

For practical applications, the long term BOD test have also been applied for determining the total biodegradable COD fraction. The STOWA protocol utilizes the BOD test, COD test of filtrated influent wastewater with 0.45 μm filter or 0.1 μm filter with flocculation and COD test of filtrated effluent wastewater to determine the different COD fractions (Roeleveld and van Loosdrecht, 2002).

Various comparative evaluations have concluded that the different characterization methods lead to different results, and therefore it is difficult to choose which method to utilize (Fall et al., 2011; Gillot and Choubert, 2010; Ruiz et al., 2014). Physical-chemical methods are most often used because of the ease of laboratory work, and then the resulting COD fractions are used as an initial value for further calibration against the measured data.

Phosphorus

The phosphorus in the wastewater influent is typically classified into orthophosphate, and organic phosphate (e.g. sugar phosphate, phospholipids and nucleotides). Total phosphorus and orthophosphate can be measured, while the organic phosphate can be estimated based on the difference between the orthophosphate and total phosphorus.

The ASM2d model is a fraction-based model, where several composition factors are used that models the organic phosphorus fractions as a fixed ratio of the COD state variables.

Table 2.10 shows the values of the composition factors used in ASM2d, and Equation 2.5 can be used to estimate either the orthophosphate or total phosphorus concentration based on the typical values of composition factors. Figure 2.11 illustrates the different phosphorus fractions in the influent. In this figure, the phosphorus fractions based on soluble inert (S_I) and volatile fatty acids (S_A) are left out, as they often are considered negligible in the influent.

Table 2.10 – Composition factors for phosphorus used in ASM2d

Fixed ratio of COD variable	Symbol	Typical value[a]	Range[b]
S_I	$i_{P,SF}$	0.00	0.002-0.008
S_A	$i_{P,SA}$	0.00	0.00
S_F	$i_{P,SF}$	0.01	0.010-0.015
X_I	$i_{P,XI}$	0.01	0.005-0.010
X_S	$i_{P,XS}$	0.01	0.010-0.015
Biomass (X_H, X_{PAO}, X_{AUT})	$i_{P,BM}$	0.02	

a (Henze et al., 1999)

b (Roeleveld and van Loosdrecht, 2002)

$$TotP = S_{PO_4} + S_F \cdot i_{PSF} + S_I \cdot i_{PSI} + X_S \cdot i_{PXS} + X_I \cdot i_{PXI} + (X_H + X_{AUT} + X_{PAO}) \cdot i_{PBM} + X_{PP} \quad 2.5$$

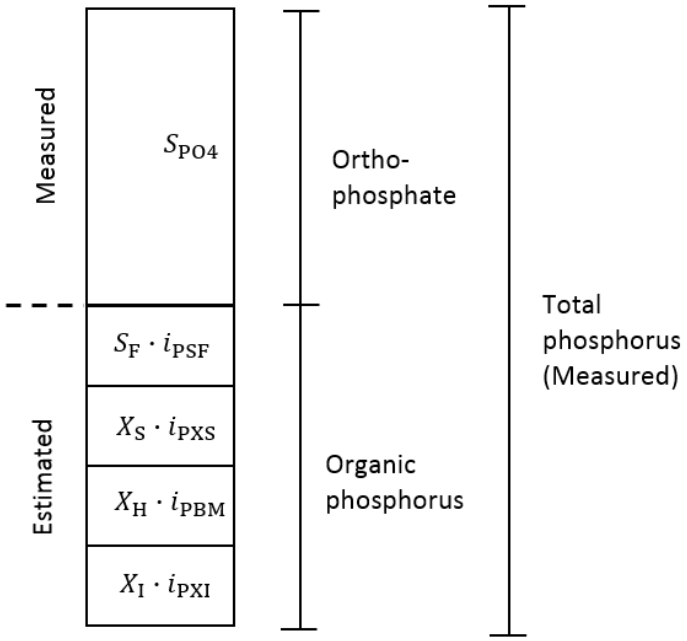

Figure 2.11 – Phosphorus fractionation of influent wastewater in the ASM2 model (Henze et al., 1995).

Nitrogen

For the fraction-based models such as the ASM2d model, the nitrogen is fractionated in a similar way as phosphorus. ASM2d contains state variables for nitrate (S_{NO3}) and ammonium (S_{NH4}) and these can be directly measured and used as influent values. The organic nitrogen is modelled as fractions of the COD state variables. The total nitrogen or total Kjeldahl Nitrogen (TKN) can be used to adjust the composition factors if necessary. However, this should be done with care as these factors also control the

organic nitrogen fractions in the reactors and should be controlled against the nitrogen content in the sludge. The composition factors for nitrogen in ASM2d are shown in Table 2.11 and Figure 2.12 illustrates the different nitrogen fractions. Equation 2.6 shows the calculation of total nitrogen

Table 2.11 – Composition factors used for nitrogen in ASM2d

Fixed ratio of COD variable	Symbol	Typical value[a]	Range[b]
S_I	$i_{N,SI}$	0.01	0.01-0.02
S_F	$i_{N,SF}$	0.02	0.02-0.04
X_I	$i_{N,XI}$	0.03	0.01-0.06
X_S	$i_{N,XS}$	0.04	0.02-0.06
Biomass (X_H, X_{PAO}, X_{AUT})	$i_{N,BM}$	0.07	

a (Henze et al., 1999)

b (Roeleveld and van Loosdrecht, 2002)

$$Tot\ N = S_{NO_3} + S_{NH_4} + S_F \cdot i_{NSF} + S_I \cdot i_{NSI} + X_S \cdot i_{NXS} + X_I \cdot i_{NXI} + (X_H + X_{AUT} + X_{PAO}) \cdot i_{NBM} \quad 2.6$$

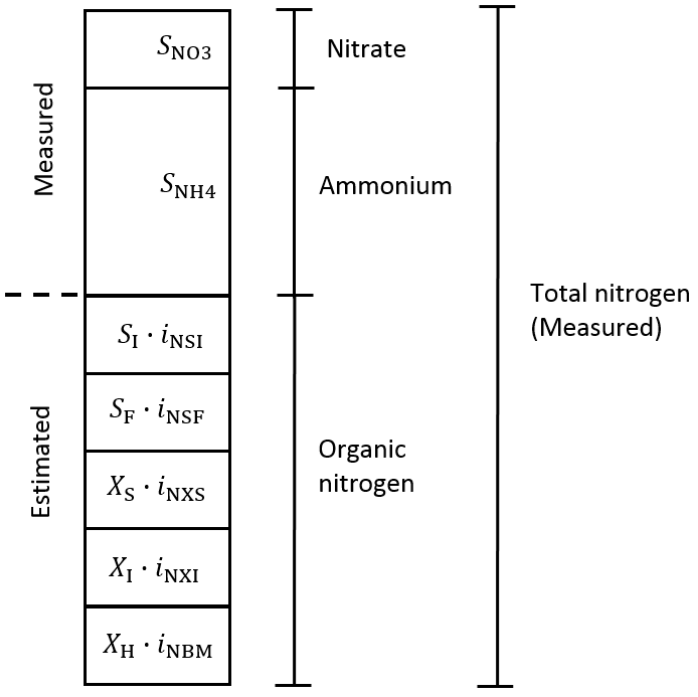

Figure 2.12 – Nitrogen fractionation for influent wastewater in ASM2 model (Henze et al., 1995).

2.5.3 Calibration

Calibration of activated sludge models is a very complex process due to many interrelating factors in the models such as influent characterization, kinetic/stochiometric parameters and operational parameters (pump flows, aeration settings, wastage rates). The ASM models contain many more parameters than can be uniquely identified by typical measurements in a WWTP (overparameterized). Thus, there exists many combinations of parameters that are able to produce the same results. This has resulted in many studies looking at the identifiability of the parameters in the ASM models, and used sensitivity analysis to identify the most important parameters for different aspects of the model (Brun et al., 2002; Cosenza et al., 2013; Ruano et al., 2007). Sensitivity analysis aims to quantify how the model output changes due to parameter variation.

Calibration can be done in a manual step wise, ad-hoc manner that relies on expert engineering knowledge of the system. This involves visual comparison of simulation and measured results, and adjusting assumed relevant parameters until a satisfying result is obtained. This is often done in practice and depending on the objective, can be an efficient calibration method. However, if one tries to calibrate the model against a complex simulation objective (e.g. N/P distribution in the activated sludge tanks), the process typically involve too many parameters and ends up being a very time consuming process. This method requires in-depth knowledge of how the model is setup and the consequence of changing a parameter in the model.

Preferably, the parameter that needs to be calibrated should be measured directly or indirectly to justify the change in value. Various experiments have been proposed for measuring the yield coefficients and growth rate of the different organisms.

Instead of using a manual calibration, an automatic calibration procedure can be followed. Different automatic calibration procedures have been proposed. Brun et al. (2002) suggests using sensitivity analysis for identification of the most important parameters, and subsequently utilize a parameter estimation algorithm for model parameter adjustment. Sin et al. (2008) and Mannina et al. (2011) both proposed a calibration procedure based on sensitivity analysis and Monte Carlo simulations and choosing the model parameters from the best simulation among a large number of simulations (> 10,000).

2.5.4 Commerical simulator software

In order to make the model accessible to a wide range of users, such as professors, engineers, students, operators and managers, several companies and research groups began developing software programs in the 1990s. These programs are called simulators and have several powerful features that allows the modeler to perform various tasks, such as:

- Plant-wide modelling (includes sludge treatment)
- Investigate various variables in the different unit processes with graphs and statistics
- Scenario analysis
- Influent generation
- Influent fractionation
- Data Handling
- Report generation
- Develop and optimize control strategies (aeration, recycle streams, etc).
- Steady state simulation
- Dynamic simulation

All the commercial simulators provide tools for
The review of the simulators focuses the relevant capabilities for biological nutrient removal, IFAS/MBBR models and membrane separation. The commercial simulators contain many of the similar features, such as:

- Sensitivity analysis
- Parameter estimation for calibration and optimization purposes
- Standard activated sludge models (ASM1, ASM2d, ASM3)

Therefore, this review will focus more on the differences and special features of the individual simulators.

Several of the simulators include anaerobic digestion and sludge treatment (dewatering, aerobic digestion) models, and thus makes it possible to model the whole WWTP with nutrient rich recycling streams. This is especially important when modelling BNR plants. The simulators also contains models for pre-treatment (screening), sedimentation and disinfection. However, this review will not go into depth on this part.

2.5.4.1 GPS-X (Hydromantis, Canada)

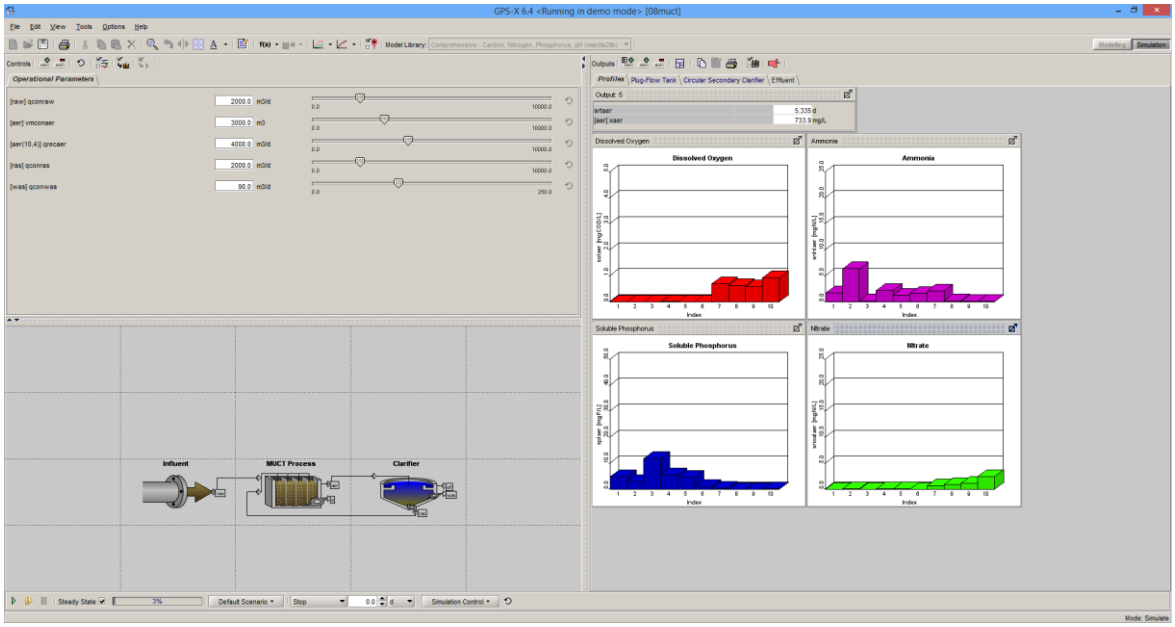

Figure 2.13 - UCT configuration in GPS-X

GPS-X is a powerful simulator developed by Hydromantis, Canada. It was first developed in 1992, and is one of the most popular simulators in North America. This review is based on the 6.4 version (2014). It comes with a large number of sample layouts for different purposes (nitrogen removal, phosphorus removal, only carbon removal, process configuration comparisons between IFAS, AS and MBR).
It is able to use the standard biokinetic models ASM1, ASM2d and ASM3 for modelling activated sludge reactors. However, GPS-X has also a couple of other models that has only been implemented in this software.

Mantis2 is the most comprehensive model in GPS-X and is developed by Hydromantis. It is based on the ASM2d, ADM1 and numerous extensions from the literature, and it is intended to be used for plant wide modelling with anaerobic digestion and nutrient rich recycle streams. It contains 48 state variables and 56 processes, which is considerably more complex than ASM2d (19 state variables and 21 processes). Some of the unique processes that are considered in the model are pH, precipitation of struvite and other compounds and anammox process among others. For more information about Mantis2 the reader is encouraged to see GPS-X Technical Reference (Hydromantis, 2014).

NewGeneral model is based on (Barker and Dold, 1997) with some adjustments. This model includes biological phosphorus removal, fermentation and nitrate as a nitrogen source for cell synthesis. In various full-scale BNR plants, there has been found an imbalance in the COD mass balance (more COD enter that plant than

leaves). This effect has been incorporated in this model as a “COD loss” in hydrolysis and fermentation.
For a quick overview of the processes considered in the different models in GPS-X, see Table 2.12.

Table 2.12 - Processes in models implemented in GPS-X (Hydromantis, 2014)

Process	ASM1	ASM3	Mantis	ASM2d	New General	Mantis2
Fermentation step				**X**	**X**	**X**
Nitrification/Denitrification	**X**	**X**	**X**	**X**	**X**	**X**
Aerobic Denitrification			**X**			
Aerobic Substrate Storage		**X**				
COD “Loss” (less COD leave the model than enters)					**X**	
2-Step Nitrification/Denitrification						**X**
NO_3^- as a N source for cell synthesis			**X**		**X**	
Alkalinity consumption/generation	**X**	**X**	**X**	**X**		**X**
Alkalinity (as a limiting factor for growth processes)						
Biological phosphorus Removal				**X**	**X**	**X**
Precipitation of P with metal hydroxides				**X**		**X**
Temperature dependency	**X**	**X**	**X**	**X**		**X**
pH						**X**
Struvite, other Calcium and Magnesium ppt.						**X**
Anammox						**X**
Methylotroph						**X**

GPS-X has also the ability to model MBR reactors. The MBR reactor is modelled with a submerged separation filter, and is combined with a suspended growth activated sludge model such as one of the ASM models or Mantis2/NewGeneral. The reactor can be modelled as CSTR or plug flow, as shown in Figure 2.14.
There are 3 different MBR model modes: simple, intermediate and advanced. Simple ignores the filter operation and the separation is only defined by a solids capture efficiency. Intermediate includes filter operation such trans-membrane pressure (TMP), cake formation, fouling, backwashing and membrane resistance. Advanced mode is similar to the intermediate, but includes the possibility for variation in volume based on the permeate flux.

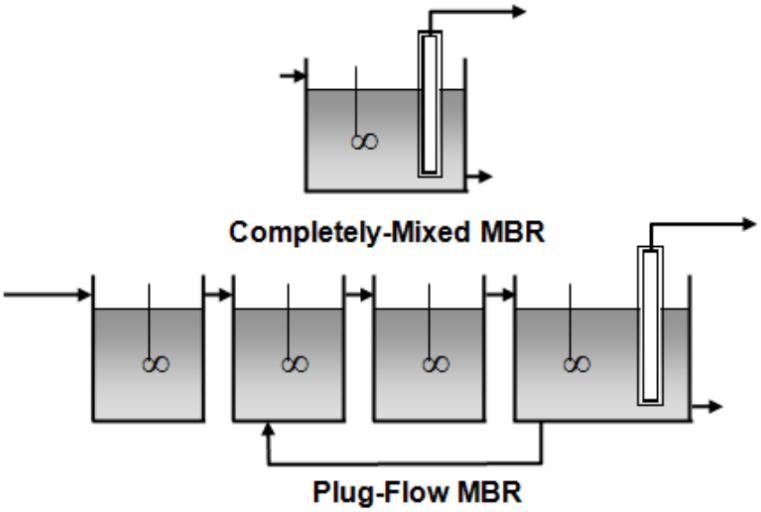

Figure 2.14 - MBR model structures in GPS-X

An IFAS model has been implemented, which combines an activated sludge model with an attached growth model. The attached growth model is a biofilm model that was developed for modelling RBC reactors, and is adapted to IFAS systems. The biofilm model handles soluble material diffusion, biofilm growth, and particulate attachment and detachment (Spengel and Dzombak, 1992). The biofilm is based on 6 layers (1 liquid layer), and each layer is modelled as an small CSTR with biological reactions similar to the ASM models. The user specifies the maximum biofilm thickness.

The user is also able to edit and develop his own model through a Model Developer. The Model Developer uses the same matrix notation that is typical for the standard biokinetic models.

More information about the different models in GPS-X can be found in the Technical Reference for GPS-X (Hydromantis, 2014).

2.5.4.2 *BioWin (EnviroSim, Canada)*

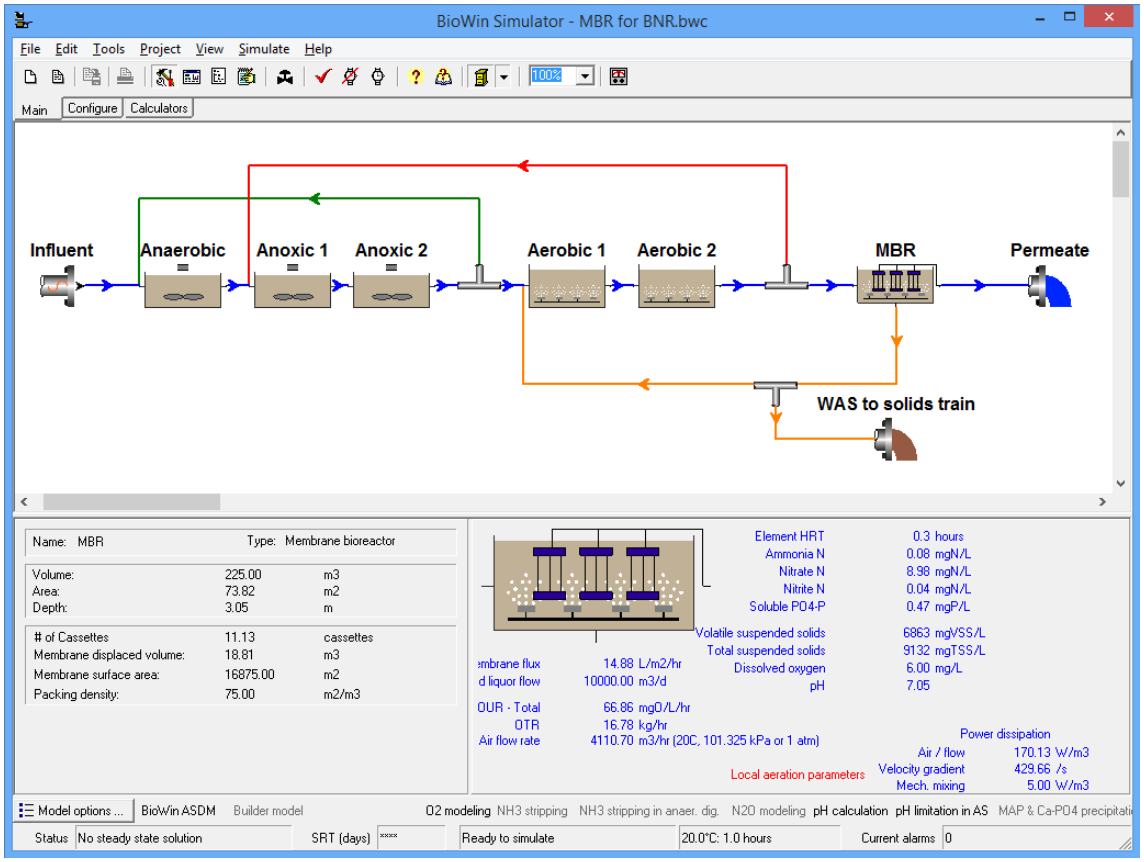

Figure 2.15 – UCT configuration with MBR in BioWin

BioWin is another popular simulator in North America, and contains many of the same features as GPS-X. This review is based on the 4.1 version.

One of the unique features of this simulator is the Activated Sludge/Anaerobic Digestion Model (ASDM). It is a highly complex model for plant wide modelling, and is the default model for BioWin. The ASDM model contains over 50 state variables and over 70 processes. This model contains all the components and processes relevant to model anaerobic digestion and activated sludge in the same model, without the need to convert between ASM components to ADM components. It is beyond the scope of this thesis to discuss this model in detail, but some of the unique features of this model are:

- Growth and Decay of Methylotrophs
- Growth and Decay of Anaerobic Ammonia Oxidizers (AAO)
- Ammonification
- pH modelling
- Struvite and calcium phosphate precipitation
- Two step nitrification/denitrification
- Anammox

It is also possible to replace this model with the standard activated sludge models if the user wishes to do so.

MBR

BioWin models the MBR reactor with a combination of activated sludge and submerged separation unit. The model is a simple point separator, where it is possible to define the solids capture efficiency. It does not model TMP, fouling, cake formation, nor backwashing routine.

Biofilm/IFAS model

The biofilm model in BioWin is included in the general ASDM model, and can be used to model MBBR/IFAS systems. The biofilm model is a 1D dynamic numerical model. The fundamental equations are based on (Wanner and Reichert, 1996) and (Reichert and Wanner, 1997), but the ASDM biofilm model is improved with other processes to be able to simulate a variety of configuration with little modification. The model includes calculation of turbulence, diffusion of soluble and particulate components, particulate attachment/detachment, biofilm density and porosity.
More information can be found in the BioWin 4.1 Model Reference (EnviroSim, 2014).

2.5.4.3 WEST (DHI, Denmark)

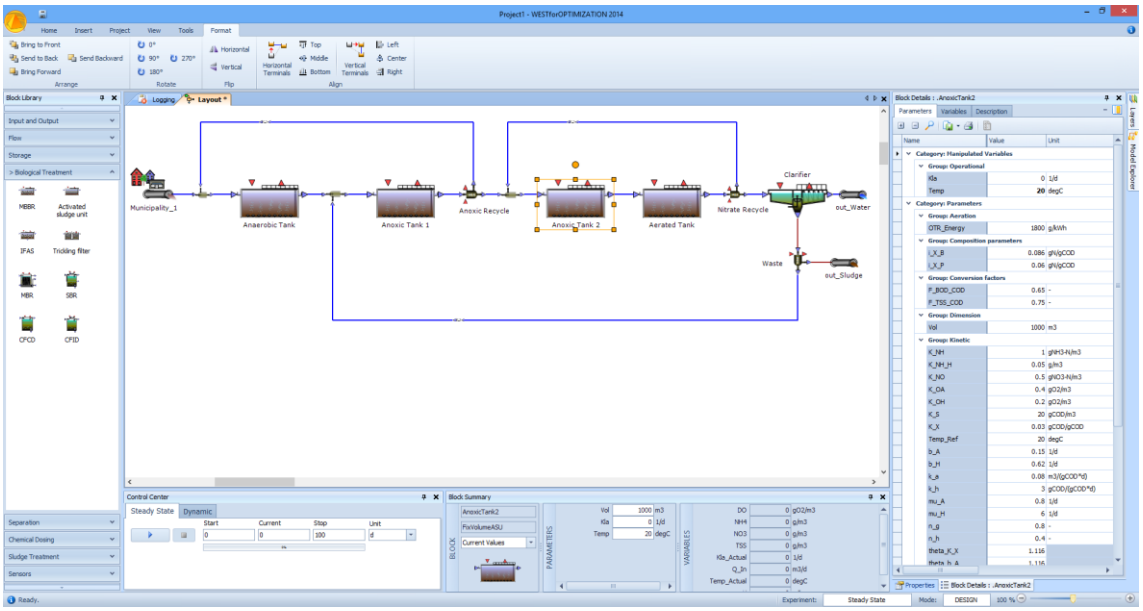

Figure 2.16 - Modified UCT configuration in WEST

WEST is a simulator that is developed by DHI, and is a popular simulator among researchers because of its flexibility to include user defined models and the simulator is transparent in terms of showing the code for the different unit processes. This review is based on the WEST 2014 version.

The simulator special features are a special modelling language called MSL that makes it possible for users to develop their own models. It is also possible to use WEST for integrated urban wastewater systems, where sewers and the river catchment is also taken into account in the model.
It includes the standard ASM models (ASM1/2d/3), and anaerobic digestion (ADM1).

MBR

MBR reactors can be modelled as a submerged membrane bioreactor or with a side stream setup. The operation of the membrane can be modelled with backwash and relaxation periods. The membrane is modelled as an ideal separation unit, where the solids capture efficiency is defined, and the soluble components are divided proportionally between the concentrate and the permeate.
The MBR model can also include the process of fouling and calculates the resulting TMP. For simulating the fouling process, the user is required to provide the concentration of SMP and membrane characteristics (resistance, critical flux, etc.). The models uses an empirical relationship to calculate build-up of cake resistance in the membrane.

IFAS

The IFAS model in WEST is a combination of ASM model and 1D dynamic numerical biofilm model. The biofilm model consists of 10 layers that are completely mixed and the biological processes in each layer is modelled according to the ASM model used. The interaction between the bulk phase (suspended growth model) and the biofilm is modelled through attachment/detachment for particulate components and diffusion processes for soluble components. The detachment is occurs in each layer when it reaches the maximum biofilm thickness (0.05 mm) set in the model.
More information can be found in the WEST 2014 Models Guide (DHI, 2014).

2.5.4.4 Simba# (ifak, Germany)

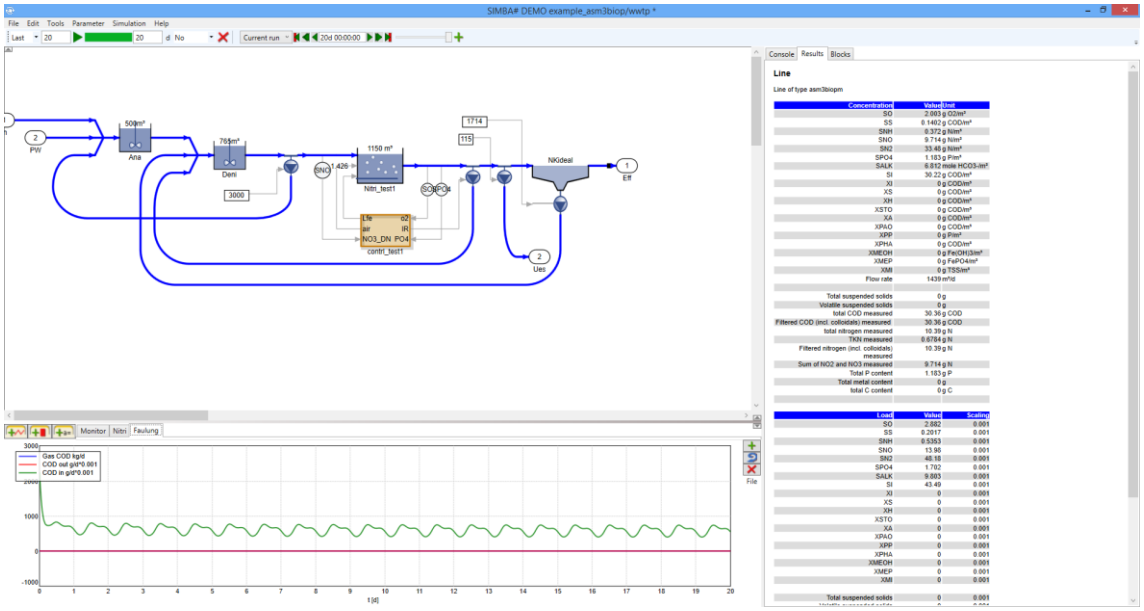

Figure 2.17 - UCT configuration in Simba#

Simba# simulator is developed by ifak system, Germany. It was previously based on Matlab/Simulink, but it is now a stand-alone program based on C#. It does not provide as many modelling unit blocks as the competitors. The unique feature about Simba is an integrated simulation with sewer, wastewater treatment, sludge treatment and river quality.

|It comes with ASM1 and ASM3/bioP included and anaerobic digestion modelling. It does not have any modelling units for IFAS or MBR processes. It does include an biofilm model, but it is developed for fixed bed biofilm processes. More information can be found in the Simba# Manual (ifak, 2015).

2.5.5 Free simulator software

Various simulators have been released as free software during the last years, due to different reasons. One of the main reasons are that they are currently not being actively updated.

2.5.5.1 *STOAT (WRc, England)*

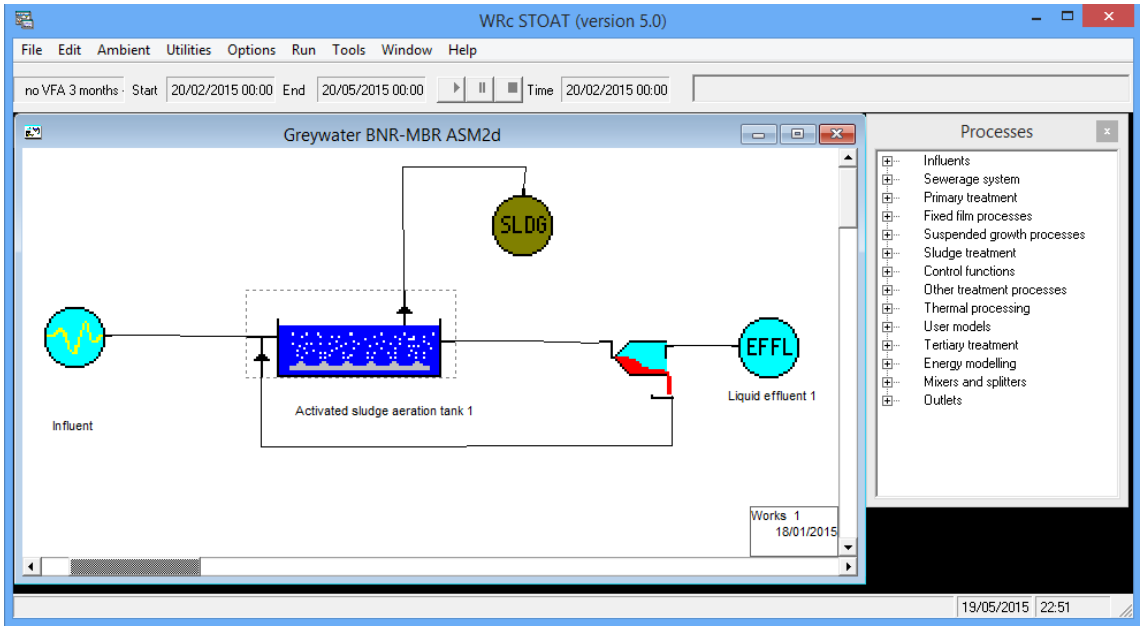

Figure 2.18 - UCT configuration with MBR in STOAT

STOAT has been developed by WRc in England since 1994. This review is based on STOAT 5 (2013). The STOAT simulator has recently been released as free software and thus have experienced increased usage.

A unique feature is that it contains a group of models similar to the ASM family, which is called ASAL. This group of model can be based on BOD, instead of COD. However, the ASAL models have not been tested as extensively as the ASM models and should therefore be used with more caution. It does not include a model editor, such as the other simulators.

It contains a variety of unit processes, such as biofilm processes (trickling filter, biological aerated filter), sludge treatment (anaerobic digestion, dewatering), chemical phosphorus removal

It provides capabilities for sensitivity analysis, calibration and optimization. However, the tools are implemented with less flexibility in terms of which parameters can be calibrated, compared to the commercial simulators.

IFAS or MBR unit processes are not included as models in the STOAT software. However, membrane separation can be modelled as an ideal separation model, similar to the other simulator.

2.5.5.2 ASIM (Eawag, Switzerland)

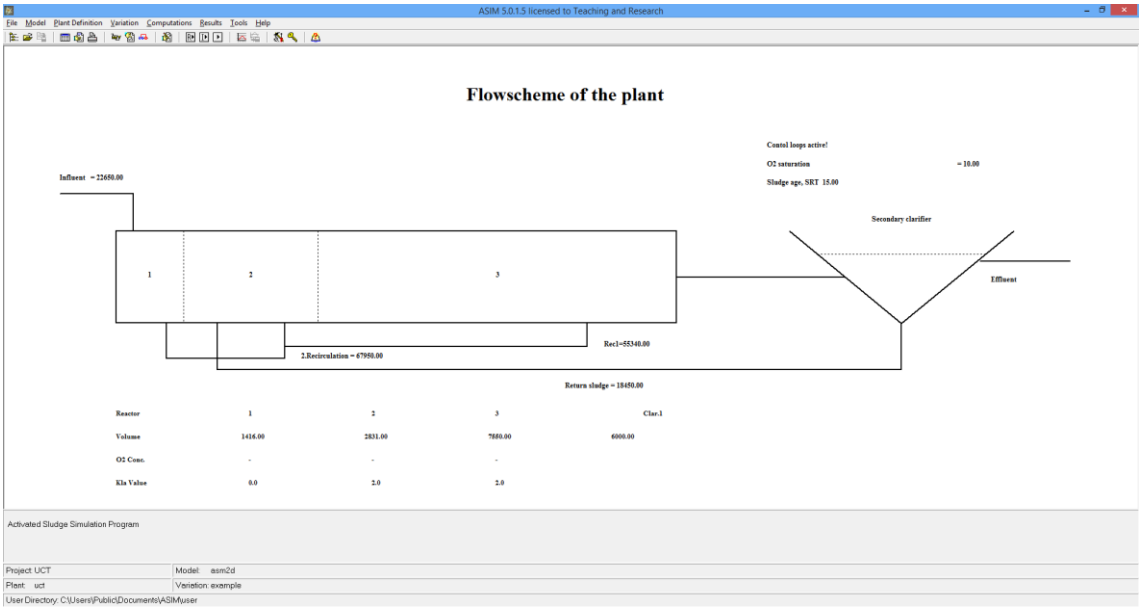

Figure 2.19 - UCT configuration in ASIM

The ASIM (**A**ctivated Sludge **SIM**ulation program) was developed at the Swiss Federal Institute of Aquatic Science and Technology (Eawag) in Switzerland. This review is based on the ASIM 5 version. It was one of the first simulators to implement the ASM1 model.

It is not as flexible as the commercial simulators. It is able to simulate up til 10 anaerobic/anoxic/aerobic reactors in sequence with a sedimentation tank for separation step. It can include internal recycle streams and return sludge.

ASIM comes with a model editor where the user are able to define the biological processes, kinetic/stoichiometric parameters and state variables considered in the model. It includes the standard ASM models 1/2/2d/3/3+bioP.
Simple control loops with proportional and on/off type controllers can be implemented.

ASIM does not come with a biofilm model or a membrane bioreactor model. It does not include any tools for automatic calibration, sensitivity analysis or scenario analysis.

2.5.5.3 *Aquasim (Eawag, Switzerland)*

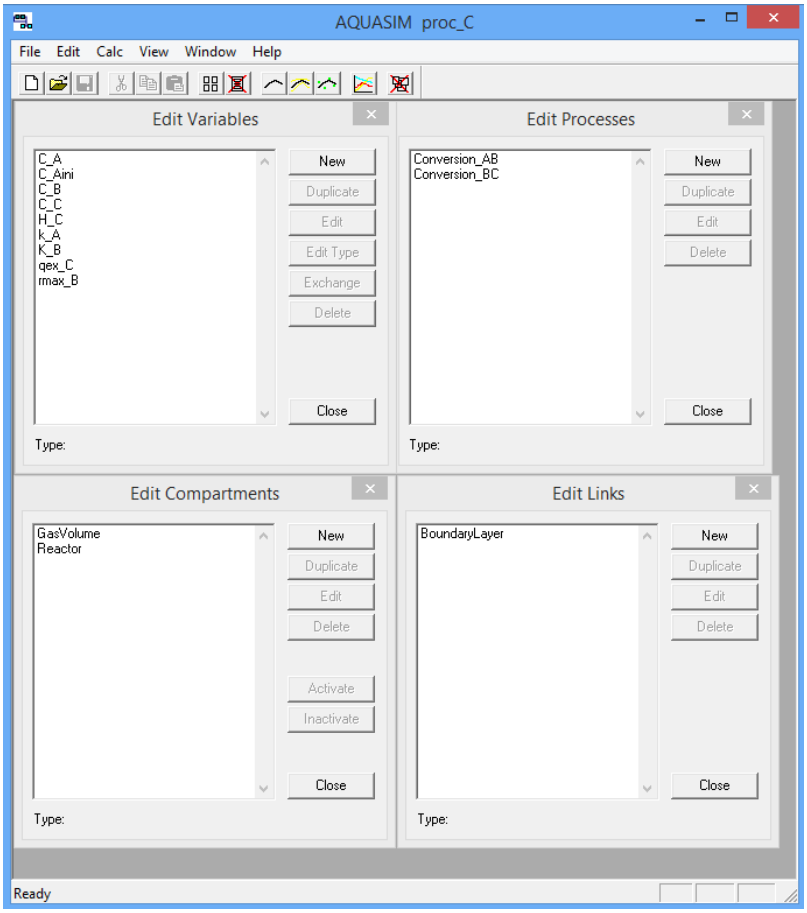

Figure 2.20 - Aquasim User Interface

Aquasim is also a simulator developed at Eawag in Switzerland. It is a flexible simulator that does not come with any ASM models pre-defined. The simulator consists of compartments (e.g. reactors, biofilm, river section), processes, variables and links. The program can be utilized for any kind of biokinetic model and have been used to activated sludge modelling, biofilm and river water quality modelling (Reichert, 1994).

It does not include a user-friendly interface with dragging connections between the different tanks, as is the case with the commercial simulators, and thus has a higher learning curve. The connections needs to be defined in a list where start and end is defined.

It includes powerful tools to perform sensitivity analysis, parameter estimation and uncertainty estimations.

2.6 Further reading

For further information about mathematical modeling of wastewater treatment plants, the reader are encouraged to look up these resources:

Biological Wastewater Treatment: Principles, Modelling and Design – (Henze et al., 2008) This textbook give an short introduction the ASM model framework (notation, simulators, model setup and history).

Guidelines for Activated Sludge Models - (Rieger et al., 2012)
This is an IWA Scientific Technical Report published by the "Good Modelling Practice (GMP) Task Group". This report hopes to establish a Unified Protocol for modelling studies, and provide a list of steps necessary for carrying out a cost effective modelling study of high quality that is well documented and comparable to other modelling studies. It also provides suggestion to sources of measurement errors and uncertainty.

Activated Sludge Models: ASM1, ASM2, ASM2d and ASM3 - (Henze et al., 2000)
This is an IWA Scientific Technical Report published by the "Mathematical modelling for Design and Operation of Biological Wastewater Treatment Task Group". It contains the reports for the original models of ASM family models and contains essential information about the details and development of the models. The default values of kinetic and stoichiometric parameters for several of the ASM models are published here.

Mathematical Modelling and Computer Simulation of Activated Sludge Systems - (Makinia, 2010)
This book gives a broad overview to the usage of models to WWTP, and gives practical details for unit process models, calibration, different simulators, experimental analysis and a review of the protocols for conducting a modelling study.

2.7 Limitations

Until now, a lot of advantages and possibilities for wastewater treatment modeling have been highlighted and discussed. However, even though the field of mathematical modeling of wastewater treatment processes has come a long way in the last 30 years, there are certainly some fundamental limitations to the use of models (Makinia, 2010):

- Wastewater flow rate and composition is constantly varying and is of a complex nature. To find a correct influent characterization for the model is a challenging task, and typically, the model assumes that the fractionation of COD, P and N species in the beginning of the simulation is maintained throughout the analysis period. If the simulation period is long and there is a varying

contribution of industrial wastewater and stormwater, the real fractionation might change during the simulation.

- It is not possible to measure directly or exactly many of the state variables such as phosphate accumulating organisms (X_{PAO}), autotrophic organisms (X_{AUT}), and stored poly phosphate for PAO (X_{PHA}). Therefore, it is difficult or sometimes impossible to validate the simulation results regarding some state variables.
- Even though modelling a WWTP can be done with less work than setting up a pilot plant, the modelling effort can be extensive due to data collection, model development, analysis and calibration.
- A biological WWTP is a highly complex system that is difficult to measure accurately. Therefore, simulations based on incomplete and erroneous data might easily be misleading and inaccurate.
- Approximations are made during the model development and set-up, therefore the simulations results should be used as approximate results and not interpreted as exact results.
- The kinetic/stoichiometric parameters can be adjusted to unreasonable values to fit observed data, however then the model most likely will not be able to predict other situations.

2.8 Case studies of modelling greywater treatment

As previously emphasized, most modelling studies and application of ASM has been on municipal and industrial wastewater treatment. However, there are a few examples of modelling studies on greywater treatment systems.

Friedler et al. (2008) investigated a side-stream MBR onsite pilot that was treating greywater from a campus building in Israel. The model was based on ASM1 and predicted COD and N removal successfully. The model was implemented in Matlab and was utilized to investigate the reliability of the system with a stochastic failure framework (including pump, electronic, membrane and aeration failures). The influent characterization was based on literature values from (Dixon et al., 2000) and standard ASM1 model parameters were used.

Hocaoglu et al. (2013) utilized a simplified ASM1 model that only considered organic carbon utilization for modelling a submerged MBR operating in SBR mode. The greywater was provided from a campus building in Turkey. A detailed COD fractionation was employed with respirometric analysis for determining the biodegradable fractions. The model managed to simulate successfully the MLSS concentration, effluent COD and DO variation during operation of SBR mode. Nitrogen and phosphorus removal were not modelled.

Jabornig and Rauch (2015) investigated an MBBR-MBR reactor treating synthetic greywater. The model was based on Hocaoglu et al. (2013)/ASM1 and thus only considered COD removal. The model was implemented in a Excel spreadsheet. No model for biofilm flux kinetics was implemented due to the assumption that the biofilm was thin and full penetration could be assumed. A separate biomass component were included to represent the biofilm mass and was considered to have the same characteristics as the suspended heterotrophic biomass.

3 Materials and Methods

3.1 Experimental system description

An experimental pilot plant that was set up at the Department of Hydraulic and Environmental Engineering at NTNU. The system uses a biological nutrient removal configuration known as University of Cape Town (UCT) with IFAS configuration in the anoxic and aerobic tank. A membrane is used as the separation stage (Henze et al., 2008; WEF, 2010). The setup consists of an anaerobic tank, an anoxic tank and an aerobic tank in sequence. The membrane is submerged in the aerobic tank. There are two recycling streams, from the aerobic tank to the anoxic tank, and from anoxic tank to the anaerobic tank. The sludge is wasted from the aerobic tank. See Figure 3.1 for an illustration of the experimental set-up. The pilot was run in cycles of 2 days, where 200 L synthetic greywater was treatment during this period, and analyzes of the excess sludge and the effluent were done at the end of the period.

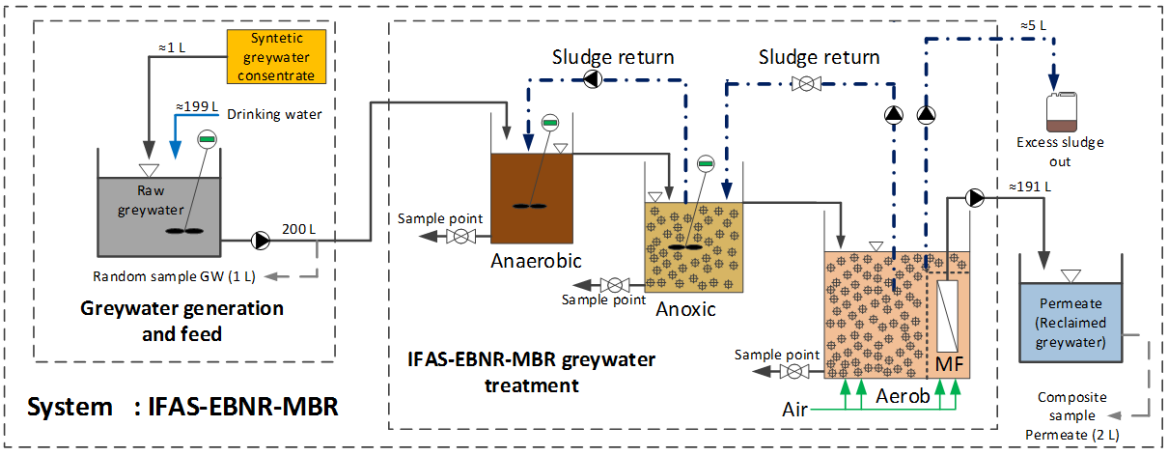

Figure 3.1 - Scheme of IFAS-EBNR-MBR setup (Bjerkelund and Østerhus, 2015)

The period for analysis was from 7/3/2014 - 7/4/2014. The system was inoculated with biomass from a BNR pilot running at Hamar, Norway. The pilot had run about 5 months before the analysis period. The SRT during the period was 14 days. Figure 3.2 shows the performance and MLSS concentrations of the pilot for 3 different operating periods. Period 3 is the subject of this thesis and the figure shows that a stable operation was obtained for that period.

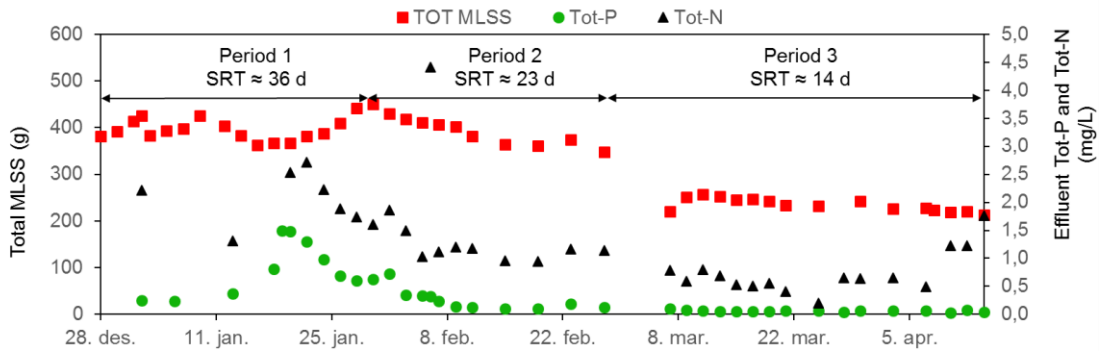

Figure 3.2 - MLSS concentrations and Tot-P/N effluent concentrations for different operation periods (Bjerkelund and Østerhus, 2015)

Table 3.1 shows the pilot plant operational characteristics during the period. The pumping for influent and recycle streams were done by peristaltic pumps (Masterflex Easy-Load II) and set at a constant rate. The inflow rate was set to 3.8 L/h (91.2 L/d). The excess sludge was wasted continuously at a rate of 0.105 L/h (2.52 L/d).

Table 3.1 - Pilot plant operational characteristics

	Anaerobic	**Anoxic**	**Aerobic**	**Total**
Volume [L]	12.74	10.35	20.78	43.87
Volume fraction	0.29	0.24	0.47	-
HRT [h]	3.2	2.6	5.25	11.1
Recycle into tank	1.2*Q_{in} from anoxic	5*Q_{in} from aerobic	-	-
MLSS [mg/L]	3680	5658	6456	-

The membrane was a flat sheet Kubota Type 203 micro-filtration (MF) with a nominal pore size of 0.4 µm. 3 plates were used with a total area of 0.33 m^2 (Figure 3.3). The membranes were operated with 9 minutes filtration time and 1 minute relaxation time. No backwash was implemented for the membranes. An average filtration flux of 0.2804 m^3/m^2*d is used and a vacuum is applied by means of a peristaltic pump (Masterflex Easy-Load II). The membrane plates were cleaned through soaking in solutions of sodium hypochlorite (0,25%) and citric acid (0,5%).

The aeration was provided by a coarse bubble system. 2 rotameters were used to control the air flow for the membrane plates (3 L/min), and 1 rotameter were used to control the air flow to the aerobic volume with media (ca. 10-12 L/min). The dissolved oxygen (DO) in the aerobic tank was maintained a level of 5 – 5.5 mg/L. The anaerobic and anoxic tank was mixed with mechanical mixers, while the aerobic tank was mixed by the aeration system.

The temperature in the system fluctuated between 16 and 19 ^{o}C, with an average temperature of 17 ^{o}C.

The anoxic and aerobic reactor was filled with K1 plastic media (Anox Kaldnes) with a specific surface area of 500 m^2/m^3, and the fill percentage was 50% in the anoxic and aerobic tank. Biofilm was established on the carriers in the anoxic tank, however low to none biofilm growth was observed in the MBR reactor (Figure 3.4).

More information about the experimental setup can be found in Bjerkelund and Østerhus (2015).

Figure 3.3 – Flat sheet membrane Kubota Type 203

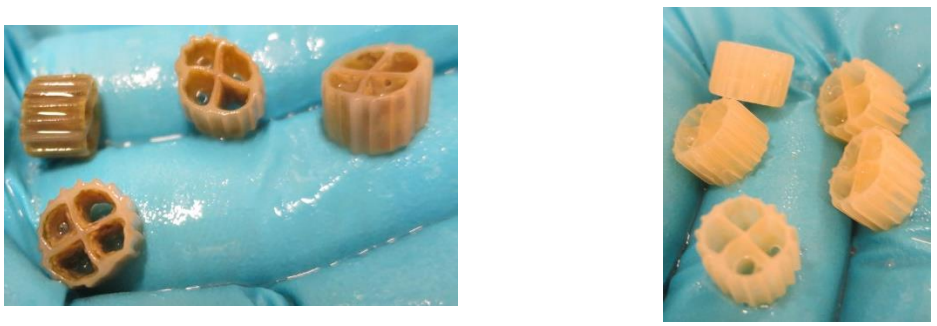

Figure 3.4 - Carrier with biofilm in anoxic tank (left) and carrier without biofilm in MBR tank (right)

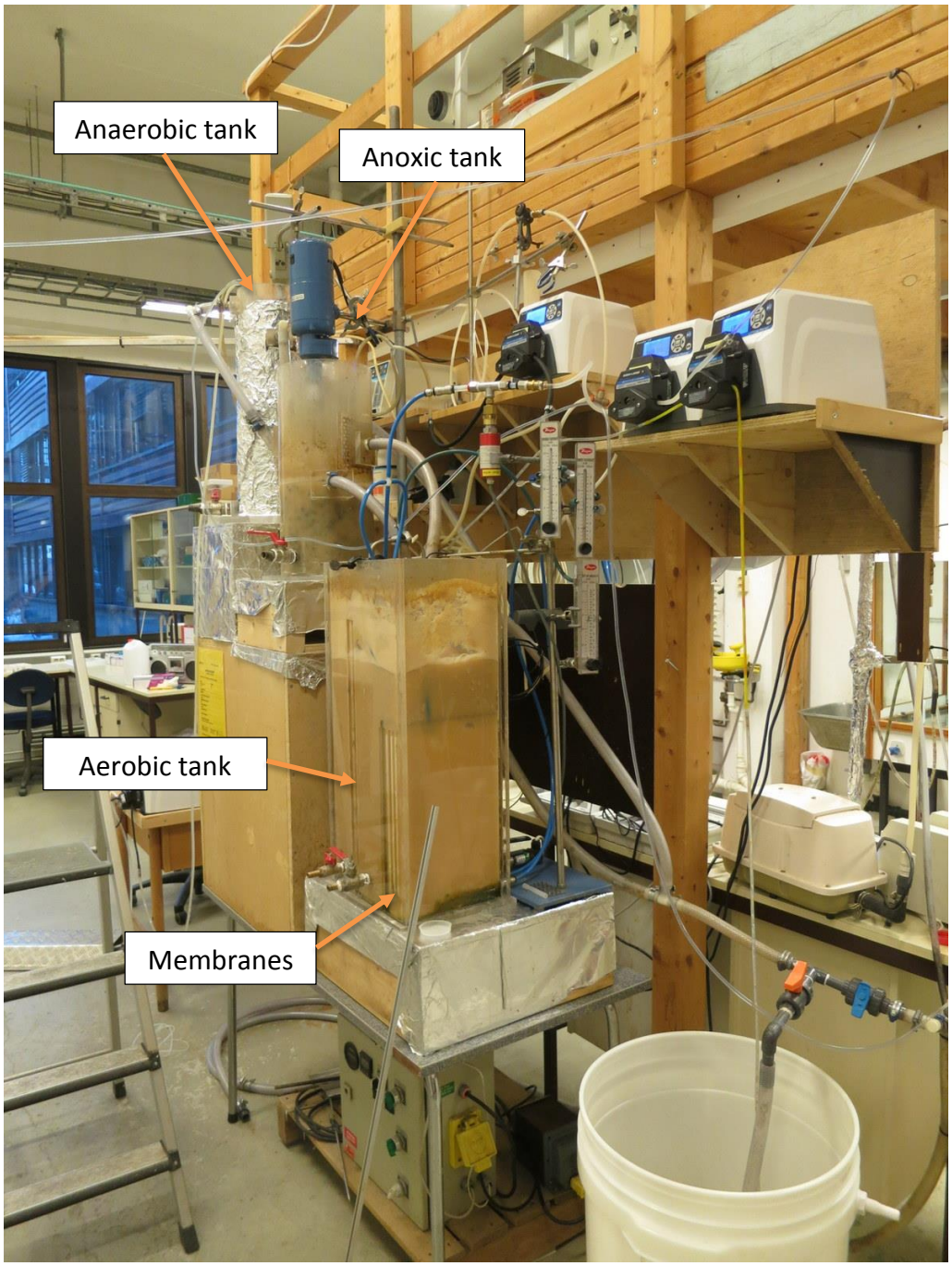

Figure 3.5 - IFAS-EBNR-MBR setup

3.2 Data Collection and Analytical methods

The analysis of the different parameters of the effluent, excess sludge and the reactors were conducted at the end of each cycle (2 days). The COD and concentration of nitrogen/phosphorus compounds were determined by Hach Lange cuvette tests, and measured with a DR 900 spectrophotometer. The BOD was measured continuously to establish a BOD curve. An overview of the relevant cuvette tests and standards are shown in Table 3.2.

Table 3.2 - Analytical procedures for greywater parameters

	Dr Lange LCK	Standard
BOD	-	NS-EN 1899-1
MLSS[a]	-	NS 4733
FCOD[b]	114, 414	ISO 6060
COD	114, 414	ISO 6060
NH_4-N	304	ISO 7150-1
NO_3-N	339	ISO 7890-3
Tot-N	138, 238	EN ISO 11905
Tot-P	348, 349	EN ISO 6878

a Filtered with Whatman GF/C 1.2 µm (55 mm) glass microfiber filter
b Filtered with Whatman GF/C 0.45 µm (55 mm) glass microfiber filter

Total biofilm solids on the biofilm carriers were measured by drying ten carriers at 105 °C for ≥ 2 h. The dried samples were weighed and the biofilm removed by placing the carriers in 37 % H_2O_2 in 10 min, before brushing them with a pipecleaner. The carriers were then rinsed with distilled water, dried for ≥ 2 h at 105 °C and then weighed. The difference in initial and final weight was used to calculate the biomass on the carriers (Bjerkelund and Østerhus, 2015).

3.3 Synthetic greywater

In this study, synthetic greywater was used. The mixture was prepared based on market reports providing overview over popular personal care and household products usage in Norway. It is a complex mix of 25 different products of shampoo, soap, toothpaste, detergents, bleach, body lotion, and general cleaning products. This concentrated mix of household products was then diluted with tap water. Potassium monohydrogen phosphate (K_2HPO_4), proteins, urea, whole milk, and hydrochloric acid (HCl) where added as a supplement to adjust the Tot-P, Tot-N, COD and pH to get a mixture similar to the greywater characteristics presented in the literature (Table 2.1). The raw greywater quality is presented in Table 3.3. The synthetic greywater mix was stored in a refrigerated room at a temperature of about 4 ^oC, and therefore it was assumed that no change in the greywater occurred during storage.

Table 3.3 - Influent water quality

Parameter	Raw greywater
pH	7.6
EC (µS/cm)	338
Alk (meq/L)	2.0
Turb. (NTU)	80
SS (mg/L)	62
VSS (mg/L)	31
COD (mg/L)	517
$COD_{0.45um}$ (mg/L)	325
BOD_5 (mg/L)	280
TOT-P (mg/L)	5.67
TOT-N (mg/L)	20
NH_4-N (mg/L)	1.38
NO_3-N (mg/L)	<0.23
COD:N:P	**100:3.5:1.1**

3.4 Model development

Based on the findings in the literature review, ASM2d and WEST by DHI were chosen as the model and simulator. The ASM2d model considers COD, nitrogen and phosphorus removal in activated sludge systems. It is the least complex model considering for BNR systems, which also considers the denitrifying PAO organisms. This is favorable due to the high amount of processes and parameters involved in ASM models. Hauduc et al. (2011) found it to be the most popular model for municipal WWTP employing a BNR configuration.

WEST

The WEST modelling software includes a user-friendly interface to construct the model and input the parameters. It also includes powerful analysis tools such as sensitivity analysis, parameter estimation and scenario analysis. The freeware simulator software were tested out for the model for this thesis, but due to lower usability and lack of a unit process model for submerged MBR, WEST was found a more favorable software for this study.

Modification of ASM2d in WEST

The ASM2d model that is implemented in WEST is extended to make the decay processes of the different organisms (heterotrophs, autotrophs, and PAOs) electron acceptor depending (oxygen or nitrate). With the default parameters that means that

the decay processes are slower under anoxic conditions than under aerobic conditions (Gernaey and Jørgensen, 2004).

Application of ASM2d to MBR system

The treatment system in this study does not utilize high MLSS concentration (> 10 g/L) and high SRT (> 40 days), which is typical for MBR systems. Therefore, it is possible an unmodified ASM2d model is able to successfully simulate the pilot plant, as discussed in Chapter 2.4.6. Various other studies have applied ASM2d successfully for evaluating nutrient removal in MBR configurations and thus it is possible to do comparative evaluations for municipal wastewater (Jiang et al., 2008; Nopens et al., 2007).

IFAS model

The experimental system utilizes an IFAS configuration. However, the field of biofilm models for IFAS systems is still a young field with no clear consensus model. In addition, there exists few case studies and guidelines for application of the published models.

The specific biofilm mass in the pilot for the analysis period was observed to be about 5.1 g/m^2 in the aerobic reactor and 11.5 g/m^2 in the anoxic reactor. Recently, Jabornig and Rauch (2015) applied a simplified ASM1 model to a MBBR-MBR configuration where no processes for biofilm flux kinetics were implemented based on the assumption that the biofilm was thin and full penetration of the substrate could be assumed. The specific biofilm mass was measured to be 9.3 g/m^2. The simplified ASM1 model did not include N or P removal. The model developed in this thesis also applies the same assumption, however because the biofilm is important for nitrifiers, a model with no biofilm flux kinetics might incorrectly model the nitrogen removal in an IFAS configuration.

Other studies have emphasized that the P removal is associated with the mixed liquor biomass in an IFAS configuration (Majed et al., 2008; Onnis-Hayden et al., 2011), and therefore it is likely that a ASM2d model with no biofilm flux kinetics is able to successfully model the P removal mechanisms in an IFAS configuration.

To facilitate the input and handling of values for membrane area, flows and volumes in WEST, all real values were multiplied by 1000, so that liters would be shown as cubic meter in the model.

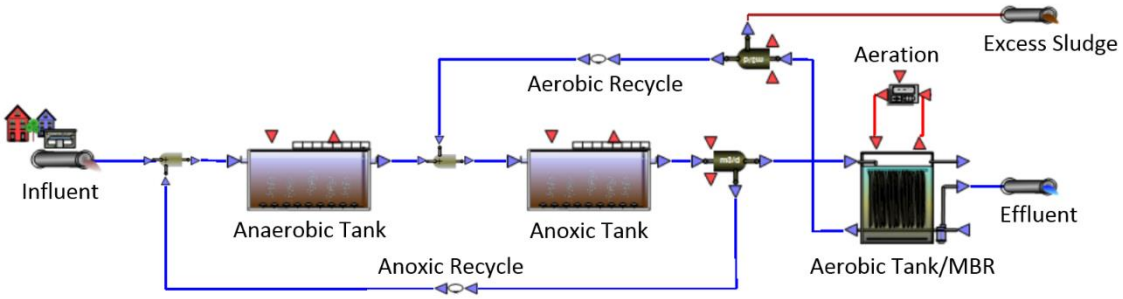

Figure 3.6 – Pilot plant layout in WEST

Hydraulic model

The experimental setup consists of small volumes compared to full-scale systems. No tracer tests were conducted to obtain better information about the mixing or flow regime in the pilot plant. The model was assembled by connecting 2 CSTR activated sludge tanks and an CSTR with an integrated ideal membrane separation model (MBR). The first tank represents the anaerobic tank; the second represents the anoxic tank and the third tank is the aerobic tank.

Separation model

The membrane separation is modelled as an ideal separation unit with complete retention of solids. It does not include modelling of fouling or removal of soluble compounds. The wastage flow is taken directly from the MBR tank. The flows, volumes and membrane area is set equal to the values described in Chapter 3.1.

The aeration in the MBR was modelled by a PI controller that maintained the oxygen concentration in the aerobic tank at 5.5 mg/l. The temperature was set to a constant value of 17 ^{o}C.

The TSS is calculated with the following expression that is defined in the ASM2d:

$$TSS = X_S \cdot i_{TSS,XS} + X_I \cdot i_{TSS,XI} + (X_H + X_{PAO} + X_{AUT}) \cdot i_{XSS,BM} + 3.23 \cdot X_{PP} + 0.6 \cdot X_{PHA}$$

3.5 Influent characterization

As mentioned in the literature review (Chapter 2.5.2), the influent characterization is the conversion of typically measured parameters such as COD, BOD, nitrogen and phosphorus into state variables that are used by the model. The influent characterization applied in this study was based on the STOWA protocol elaborated in

Roeleveld and van Loosdrecht (2002). It uses a combination of total COD test and BOD test to determine the biodegradable COD fraction. The effluent COD is used to determine the inert soluble fraction (S_I), and filtration is used to determine the soluble COD fraction. For the remaining fractions, mass balancing is used.

A preliminary simulation based on the default ASM2d parameters and the initial influent characterization were carried out to evaluate the predictability of the model. The influent characterization was then adjusted to fit the MLSS concentration according to the recommendations presented in Rieger et al. (2012). This adjustment included the calibration of the X_I fraction in the influent. This was based on comparison with other published greywater characteristics and trial-and-error.

3.6 Sensitivity analysis

For further calibration of the model, a sensitivity analysis was carried out to identify the most important kinetic and stoichiometric parameters for the anaerobic and anoxic bulk concentrations of phosphorus.

The sensitivity analysis utilized standardized regression coefficients (SRC), and was based on the procedure used by Sin et al (2011). First step was to define which variables that should be involved in the sensitivity analysis and their variation range. The distribution for each parameter was assumed uniform. A number of model outputs is used as a reference to measure the sensitivity of parameters with respect to these model outputs.

Then a set of 500 Monte Carlo (MC) steady state simulations with the Latin Hybercube Sampling (LHS) method was utilized. LHS is a type of stratified sampling, and provides the possibility to evenly explore the parameter space and thus run fewer simulations compared to random Monte Carlo sampling (McKay et al., 1979). The model was assumed to have reached steady state after 100 days, and the end values were used for analysis.

For each model output, a first order linear multivariate model was fitted according to the following equation:

$$y = a + \sum_i b_i \cdot \theta_i$$

Where y = Model output

a = Constant

b_i = Regression coefficient

θ_i = Model input/parameter

The regression coefficient is standardized by scaling with the standard deviations of model input and output of the Monte-Carlo simulations:

$$\beta_i = \frac{\sigma_{\theta_i}}{\sigma_y} \cdot b_i$$

Where β_i = Standardized Regression Coefficient (SRC)
b_i = Regression coefficient
σ_{θ_i} = Standard deviation of model input of the MC simulations
σ_y = Standard deviation of model output of the MC simulations

The SRC is used as the sensitivity measure and has the following interpretations:

1. A high absolute value indicates a large effect of the parameter on the model output
2. A negative sign indicates a negative effect and vice versa with positive sign
3. Coefficients close to zero indicates that the parameter have negligible effect on the model output.

The result of the sensitivity analysis was used to choose the most important parameters for calibration.

3.7 Calibration

The calibration of the kinetic and stoichiometric parameter were based on the most sensitive parameters found in the sensitivity analysis.
The calibration used the same variation range used in the sensitivity analysis, and employed a Simplex optimization algorithm with the same variation range (constraints) as the sensitivity analysis, where soluble COD effluent, anaerobic, anoxic and aerobic bulk phosphorus concentration were used as target variables.

3.8 Scenario analysis and optimization

The operational parameters (aeration, internal recycle flows, volumes and wastage) were investigated by scenario analysis. This means that a set of values is defined for each parameter and all combinations of these values are run. The simulations results were then investigated to find an optimal setup.

4 Modeling Results and Discussion

This section discusses the results from preliminary the influent characterization and steady state calibration of the model, and optimization by scenario analysis of the operational parameters.

4.1 Preliminary influent characterization

This section describes the conversion of COD, nitrogen and phosphorus compounds into ASM2d model state variables for usage in the model.

Organic fractions

The organic fractions X_S, X_I, S_A, S_F, S_I needs to be determined based on COD measurements. The following procedure that is used is based on the STOWA guideline (Roeleveld and van Loosdrecht, 2002):

1. Calculate soluble inert organic matter, S_I, based on effluent COD.

The effluent COD goes through membrane filtration of 0.4 μm and it is assumed that all readily biodegradable substrate is consumed in the treatment process. Thus, the effluent COD equals S_I.

$$S_{\mathrm{I}} = COD_{effluent} = 18.2\ mg/l$$

2. Calculate the readily biodegradable substrate, S_S (= S_F + S_A).

The ASM2d model includes volatile fatty acids (acetate) as a separate variable, S_A, and as a part of S_S. The S_A is considered negligible in the synthetic greywater mix. Thus, S_S = S_F.

$$S_{\mathrm{F}} = COD_{soluble} - S_{\mathrm{I}} = 325 - 18.2 = 307\ mg/l$$

3. Calculate the slowly biodegradable substrate, X_S, based on BOD measurement.

An estimation of X_S based on BOD analysis is a practical way to determine the biodegradable COD (bCOD). The BOD was measured over time until 7 days and a first order equation is fitted to the curve to determine the ultimate BOD (BOD_{tot}).

$$BOD(t) = BOD_{tot} \cdot (1 - \mathrm{e}^{-k_{BOD} \cdot t}) \qquad 4.1$$

k_{BOD} and BOD_{tot} is found by optimizing the equation by non-linear regression with the least squares method implemented in a spreadsheet. One of the BOD measurements with the fitting is shown in Figure 4.1.

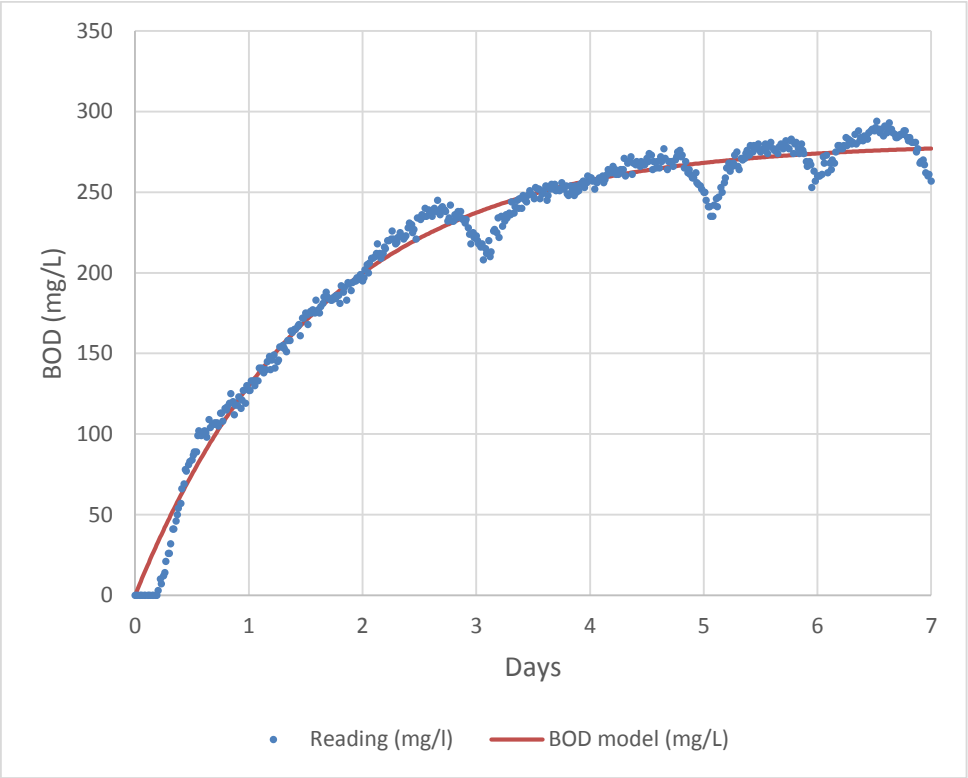

Figure 4.1 - BOD curve with BODtot equation

According to the STOWA guideline, the bCOD is determined by adjusting the BOD_{tot} with a correction factor, f_{BOD} according to Equation 4.2.

$$cBOD = \frac{1}{1 - f_{BOD}} \cdot BOD_{tot} \qquad 4.2$$

The summary of the calculation can be seen in Table 4.1.

Table 4.1 - bCOD calculation summary

Variable	Value	Units
BOD_5	280	mg/l
k_{BOD}	0.6	-
BOD_{tot}	295	mg/l
f_{BOD}	0.2	-
bCOD	368.3	mg/l

With bCOD determined, X_S can be calculated with the following equation:

$$X_S = bCOD - S_F = 368.3 - 307 = 61.5 \frac{mg}{l}$$

4. Calculate the inert particulate COD fraction, X_I.

The remaining fraction X_I is calculated from mass balance.

$$X_I = COD_{tot} - S_I - S_F - X_S = 517 - 18.2 - 307 - 61.5 = 130.5\ mg/l$$

Table 4.2 summarizes the different COD fractions and compares the relative fractions to other greywater characterizations. The COD fractions estimates compares well with the finding that greywater typically has a larger soluble fractions than municipal wastewater. With this preliminary influent characterization, the X_I fraction is calculated to 25% (compared to 9% and 1.5%) which is quite high for greywater. This might affect TSS concentrations in the simulation.

Table 4.2 - Summary and comparative evaluation of COD fractionation

COD fraction	This study	This study fractions[d]	Greywater[a]	Greywater[b]	Municipal wastewater[c]
$S_S = S_A + S_F$	307	59 %	45 %	29%	26 %
S_I	18.2	4 %	15 %	5 %	6 %
X_S	61.5	12 %	31 %	64 %	28 %
X_I	130.5	25 %	9 %	1.5 %	39 %

a (Dixon et al., 2000)

b (Hocaoglu et al., 2010)

c (Roeleveld and van Loosdrecht, 2002)

d The fractions are calculated as a percentage of the total COD in the influent

Nitrogen compounds

The standard composition factors for nitrogen for the ASM2d model is used, and the model ammonium influent is set to the measured ammonium value (S_{NH} = 1.4 mg/l)

Phosphorus compounds

The standard composition factors for phosphorus for ASM2d model is used for calculating the orthophosphate concentration in the influent (i_{PXS}, i_{PXI}, i_{PSF} = 0.01 g P/g COD).

$$S_{PO_4} = TotP - X_S \cdot i_{PXS} - X_I \cdot i_{PXI} - S_F \cdot i_{PSF}$$
$$= 5.67 - 61.5 \cdot 0.01 - 130.5 \cdot 0.01 - 307 \cdot 0.01$$
$$= 0.7\ mg\ P/l$$

The synthetic greywater mixture was diluted with tap water and therefore the oxygen concentration in the influent was set to 4 mg/L.

4.2 Preliminary Steady state simulation

After the initial influent characterization, the model was simulated with the default parameters presented with the original ASM2d model (Henze et al., 1999). These parameters are meant as a starting point, and a reliable model is not necessarily obtained.

Table 4.3 - Comparison between experimental results and preliminary steady state model simulation

		Anaerobic		**Anoxic**		**Aerobic**		**Effluent**	
Parameter	**Units**	**Exp**	**Sim**	**Exp**	**Sim**	**Exp**	**Sim**	**Exp**	**Sim**
COD_{tot}	mg/l	-	4990	-	8684	-	10325	*18.2*	18.2
$COD_{soluble}$	mg/l	*41.9*	126	*27.7*	24	*18.4*	19	*18.2*	18.2
MLSS	mg SS/l	*3680 ± 395*	3956	*5658 ± 311*	7167	*6456 ± 279*	8600	*0*	0
Tot-$P_{soluble}$	mg P/l	*22.9*	26.5	*1.9*	15.5	*0.246*	0.13	*0.07*	0.13
Tot-$N_{soluble}$	mg N/l	*4.79*	6.48	*1.8*	2.3	*2.07*	1.25	*<1*	1.25
NH_4-N	mg N/l	*2.92*	4.84	*0.88*	2.02	*0.07*	0.56	*0.04*	0.56
NO_3-N	mg N/l	*0.14*	0.0	*0.17*	0.02	*0.52*	0.49	*1.64*	0.49

The results from the preliminary steady state simulation is shown in Table 4.3. Several aspects can be highlighted from the preliminary state simulation:

1. The effluent quality parameters COD, Tot-P, Tot-N are predicted with a high degree of accuracy. This is remarkable considering the default ASM2d parameters that were applied is based on municipal wastewater and that the model does not include any biofilm flux kinetics.

2. The TSS concentration in the anoxic and aerobic tank is generally overestimated by 25-30%. This affects the sludge production to the same degree. Rieger et al. (2012) suggests that the influent particulate COD components (X_I and X_S) have the largest impact on the TSS concentrations and sludge production in the model. These values will be investigated further to calibrate the MLSS levels in the tanks.

3. The measured anoxic phosphorus uptake is much larger in the experimental system than simulated, leading to a higher simulated Tot-$P_{soluble}$ concentration

(1.9 vs. 15.5) in the anoxic tank. Denitrifying PAO or anoxic P uptake have been intensively studied in the past, however the current ASM models and other biokinetic models are unable to successfully simulate the anoxic P uptake when it becomes dominating over the aerobic P uptake (Henze et al., 2008).

4. The membrane model does not include separation of soluble compounds. From the measured values of the aerobic tank and effluent, it can be hypothesized that a biofilm on the membrane is able to reduce the Tot-$P_{soluble}$ in the effluent.

5. The system utilize an IFAS configuration in the anoxic and aerobic tank, therefore the nitrogen components might not be correctly simulated, due to the ability of nitrifiers to proliferate in a biofilm due to a slow growth rate. However, there is generally good agreement between the model and the experimental results for the nitrogen species in the different tanks and the effluent.

6. The simulated soluble COD concentration in the anaerobic tank is much higher that the measured in the experimental setup (126 vs 41.9 mg/l). This might indicate that the particulate COD is hydrolyzed to a much higher degree in the simulation than in the experimental system.

4.3 Calibration of MLSS concentrations in the tanks

Regarding the sludge production and MLSS concentrations in the reactors, Rieger et al. (2012) suggests that the X_I influent parameter should be the first parameter to be investigated as it is often the most sensitive for MLSS concentration. Compared to other literature studies presented in Table 4.2, the X_I estimated in this study is quite high (25% vs 9% and 1.5%). Based on this comparison, and trial-and-error for fitting the MLSS concentration, the fraction of X_I was set to 16% (Hocaoglu et al., 2010).

This corresponds to a f_{BOD} = 0.3. This value is somewhat higher than recommended by the STOWA protocol (0.2). However, that recommendation is based on municipal wastewater. There is reason to suggest that the synthetic greywater mix contains a higher fraction of biodegradable COD than is estimated for municipal wastewater due to fact that it does not travel through the sewer system and suffer degradation before treatment.

Biofilm growth in the inflow pipe to the anaerobic tank was also observed during the experiment. Due to this observation, the soluble COD fraction was assumed reduced by 10%.

According to these assumptions, the new fractionation of the influent is presented in Table 4.4 and the result of the steady state simulation is presented in Table 4.5.

Table 4.4 - Influent fractionation after fitting MLSS concentrations

Parameter name	Influent variable	Calibrated influent values	Fractions of COD_{tot}
Soluble biodegradable COD	$S_S = S_A + S_F$	274	57 %
Soluble inert COD	S_I	18.2	4 %
Particulate biodegradable COD	X_S	114.2	24 %
Particulate inert COD	X_I	77.8	22 %
Orthophosphate	S_{PO}	0.7	-

Table 4.5 - Comparison between experimental results and steady state model simulation after fitting MLSS concentration

		Anaerobic		Anoxic		Aerobic		Effluent	
Parameter	**Units**	**Exp**	**Sim**	**Exp**	**Sim**	**Exp**	**Sim**	**Exp**	**Sim**
COD_{tot}	mg/l	-	4191	-	7252	-	8614	*18.2*	18.7
$COD_{soluble}$	mg/l	*41.9*	115	*27.7*	22.5	*18.4*	18.7	*18.2*	18.7
MLSS	mg SS/l	*3680 ± 395*	3380	*5658 ± 311*	6128	*6456 ± 279*	7355	*0*	0
Tot-$P_{soluble}$	mg P/l	*22.9*	27.6	*1.9*	15.3	*0.246*	0.13	*0.07*	0.13
Tot-$N_{soluble}$	mg N/l	*4.79*	6.3	*1.8*	2.3	*2.07*	1.34	*<1*	1.34
NH_4-N	mg N/l	*2.92*	5.2	*0.88*	2.0	*0.07*	0.57	*0.04*	0.57
NO_3-N	mg N/l	*0.14*	0.0	*0.17*	0.02	*0.52*	0.58	*1.64*	0.58

As can be observed in Table 4.5, the MLSS concentration for the anaerobic, anoxic and aerobic tank is reduced compared to the preliminary steady state simulation. However, the anoxic and aerobic MLSS is still overestimated by 8% and 14% respectively. The phosphorus distribution profile over the tanks is not affected by the adjustment of the influent X_I. The soluble COD in the anaerobic tank is still heavily overestimated (> 170%).

4.4 PAO kinetics of the pilot plant

The anaerobic P release and anoxic/aerobic P uptake was measured at the end of the measurement period. The results are shown in Table 4.6. The results, together with the P distribution profile in the tanks (Table 4.5), indicate that the denitrifying PAO

organisms is the dominant P removal mechanism. Typically, the anoxic P uptake have been observed to be less than the aerobic P uptake (García-Usach et al., 2010; Henze et al., 2008; Makinia et al., 2006).

Even though the ASM2d includes processes for denitrification by PAO organisms, it is difficult for ASM2d to model dominant anoxic P uptake due to the way these processes are implemented. The processes are the same as for aerobic P uptake with the same kinetic and stoichiometric parameters except for a reduction factor, $\eta_{NO3,PAO}$. This factor reduces the anoxic growth of PAO and polyphosphate storage by 60% with default ASM2d parameters. It is therefore likely that it will be difficult to find a parameter set for the ASM2d model that will correctly describe the P distribution and the aerobic/anoxic P uptake. However, it is reason to believe that a reasonable estimation of the P distribution will be obtained.

Table 4.6 - PAO kinetics at the end of the measurement period

	Process rate µg P/mg MLSS·h
Anaerobic P release	3.76
Anoxic P uptake	2.78
Aerobic P uptake	0.32

4.5 Sensitivity analysis

A separate sensitivity analysis was carried out for anaerobic and anoxic soluble phosphorus concentration. The sensitivity analysis included all the kinetic and stoichiometric parameters defined in the ASM2d model. The variation range of the kinetic and stoichiometric parameters was based on earlier literature reviews for sensitivity analysis (Brun et al., 2002; Cosenza et al., 2013; Hauduc et al., 2011) and is shown in Table 4.7 and Table 4.8. The composition factors and the Arrhenius temperature correction factors were not included in the sensitivity analysis as they have been found to be stable in many modeling studies (Rieger et al., 2012).

A description of the different parameters for ASM2d can be found in Appendix B – ASM2d Parameters and in Henze et al. (1999). The reference value for anaerobic and anoxic phosphorus concentration were 22.9 and 1.9 mg P/L respectively.

Table 4.7 - Kinetic parameter variation for sensitivity analysis

Symbol	Default 20 ^{O}C	Min	Max	Units
Hydrolysis of particulate substrate: X_S				
K_h	3.00	1.5	4.5	d^{-1}
$\eta_{NO3,HYD}$	0.60	0.4	0.8	-
η_{fe}	0.40	0.2	0.6	-
$K_{O2,HYD}$	0.20	0.1	0.3	g O_2/m^3
$K_{NO3,HYD}$	0.50	0.375	0.625	g N/m^3
K_X	0.10	0.05	0.15	g X_S/g X_H
Heterotrophic organisms: X_H				
μ_H	6.00	0.6	13.2	g X_S/g X_H*d
q_{fe}	3.00	1.5	4.5	g S_F/g X_H*d
$\eta_{NO3,H}$	0.80	0.6	1	-
$\eta_{NO3,H,d}$	0.5	0.3	0.7	-
b_H	0.40	0.05	1.6	d^{-1}
$K_{O2,H}$	0.2	0.1	1	g O_2/m^3
K_F	4.00	2	6	g COD/m^3
K_{fe}	4.00	2	6	g COD/m^3
$K_{A,H}$	4.00	2	6	g COD/m^3
$K_{NO3,H}$	0.50	0.1	0.625	g N/m^3
$K_{NH4,H}$	0.05	0.02	2	g N/m^3
$K_{P,H}$	0.01	0.005	0.015	g P/m^3
$K_{ALK,H}$	0.10	0.05	0.15	mole HCO_3^-/m^3
Phosphorus-accumulating organisms: X_{PAO}				
q_{PHA}	3.00	0.3	5.7	g X_{PHA}/g X_{PAO}*d
q_{PP}	1.50	0	3.3	g X_{PP}/g X_{PAO}*d
μ_{PAO}	1.00	0.5	1.5	d^{-1}
$\eta_{NO3,PAO}$	0.60	0.45	0.75	-
$\eta_{NO3,P,d}$	0.33	0.1	0.5	-
b_{PAO}	0.20	0.1	0.25	d^{-1}
b_{PP}	0.20	0.1	0.25	d^{-1}
b_{PHA}	0.20	0.1	0.25	d^{-1}
$K_{O2,PAO}$	0.20	0.1	0.3	g O_2/m^3
$K_{NO3,PAO}$	0.50	0.375	0.625	g N/m^3
$K_{A,PAO}$	4.00	2	6	g COD/m^3
$K_{NH4,PAO}$	0.05	0.025	0.075	g N/m^3
K_{PS}	0.20	0.1	0.3	g P/m^3
$K_{P,PAO}$	0.01	0.005	0.015	g P/m^3
$K_{ALK,PAO}$	0.10	0.05	0.15	mole HCO_3^-/m^3
K_{PP}	0.01	0.005	0.015	g X_{PP}/g X_{PAO}
K_{MAX}	0.34	0.2	0.51	g X_{PP}/g X_{PAO}
K_{iPP}	0.02	0.01	0.03	g X_{PP}/g X_{PAO}
K_{PHA}	0.01	0.005	0.015	g X_{PHA}/g X_{PAO}
Nitrifying organisms (autotrophic organisms): X_{AUT}				
μ_{AUT}	1.00	0.2	1.2	d^{-1}
$\eta_{NO3,AUT,d}$	0.33	0.1	0.5	-
b_{AUT}	0.15	0.04	0.16	d^{-1}
$K_{O2,AUT}$	0.50	0.1	2	g O_2/m^3
$K_{NH4,AUT}$	1.00	0.5	1.5	g N/m^3
$K_{P,AUT}$	0.50	0.005	0.015	g P/m^3
$K_{ALK,AUT}$	0.01	0.25	0.75	mole HCO_3^-/m^3

Table 4.8 - Stoichiometric parameter variation for sensitivity analysis

Symbol	Default (20 °C)	Min	Max	Units
Hydrolysis				
f_{XI}	0.10	0.05	0.4	g COD/g COD
Heterotrophic organisms: X_H				
Y_H	0.625	0.38	0.75	g COD/g COD
Phosphorus-accumulating organisms: X_{PAO}				
Y_{PAO}	0.625	0.42	0.78	g COD/g COD
Y_{PO4}	0.40	0.38	0.42	g P/g COD
Y_{PHA}	0.20	0.19	0.21	g COD/g P
Nitrifying organisms (autotrophic organisms): X_{AUT}				
Y_A	0.24	0.23	0.25	g COD/g N

The 30 parameters with the highest absolute value of SRC are shown for anaerobic and anoxic bulk concentration in Figure 4.2 and Figure 4.3. It was decided to base the calibration on parameters with an absolute value of SRC above 0.10. These parameters are highlighted on the figures.

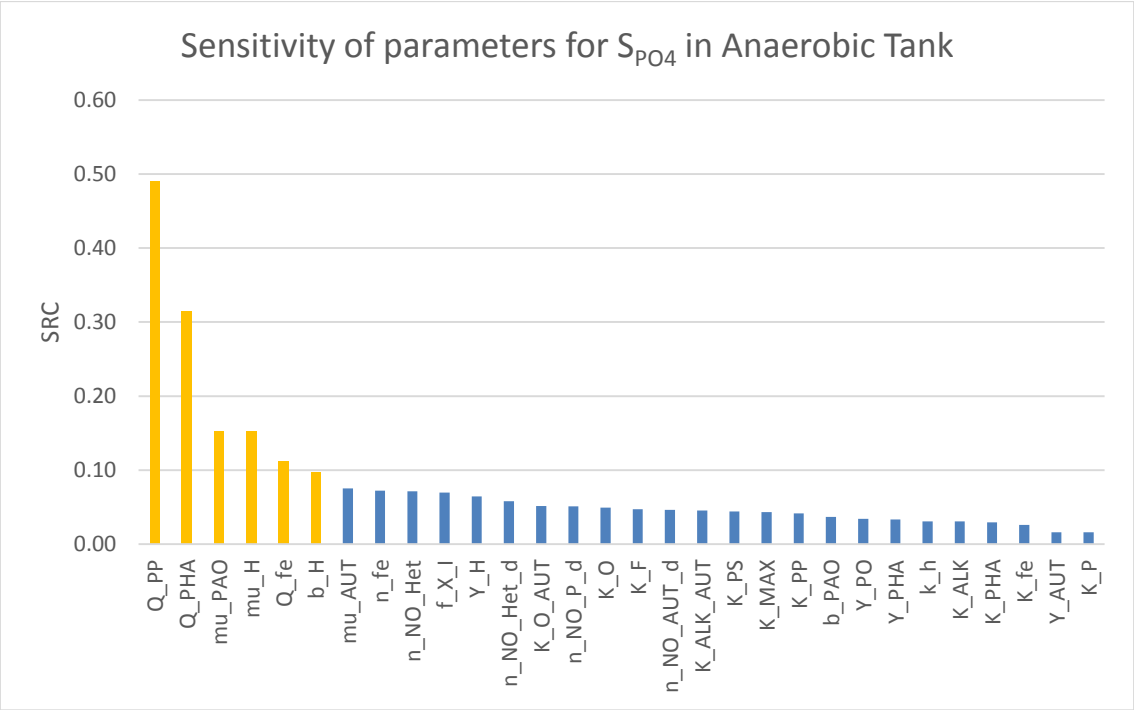

Figure 4.2 - SRCs for parameters for S_{PO4} in the anaerobic tank

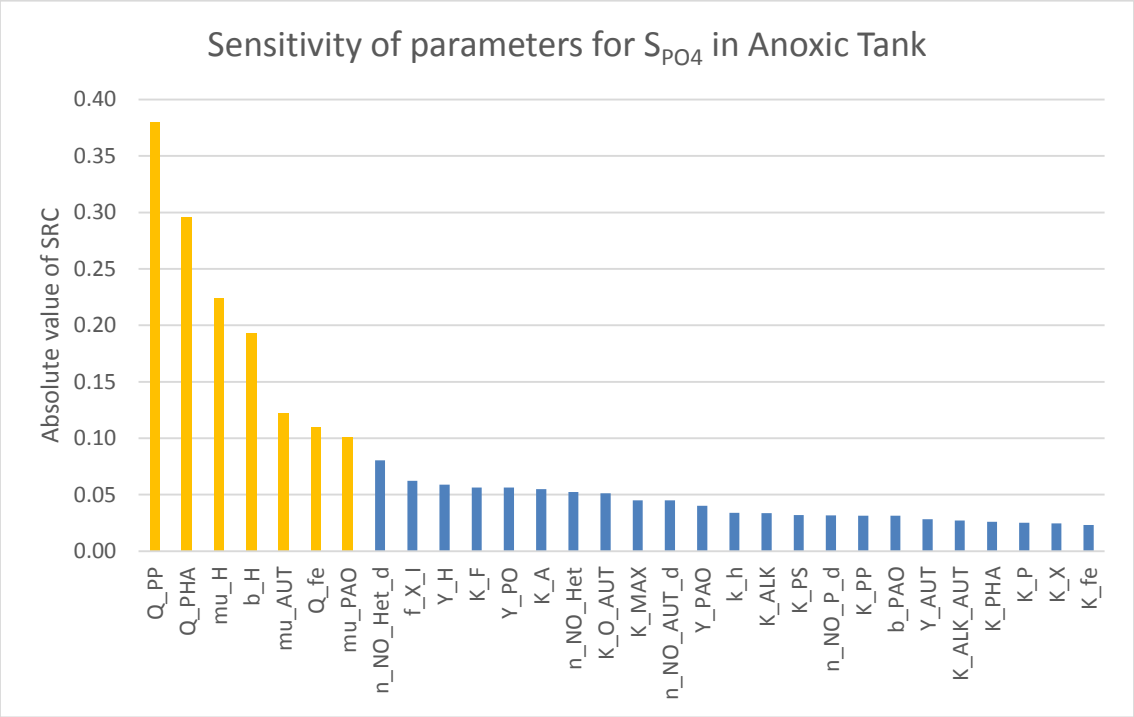

Figure 4.3 - SRCs for parameters for S_{PO4} in the anoxic tank

4.6 Calibration of kinetic/stoichiometric parameters

The calibration procedure used the soluble COD concentration in the aerobic tank and the phosphorus profile in the anaerobic, anoxic and aerobic tank for optimization. The

most sensitive parameters for both the anaerobic and anoxic P concentration that were found in the sensitivity analysis were subject to optimization.. An optimized parameter set was found, as shown in Table 4.9 and the steady-state simulation results is shown in Table 4.10. The optimal μ_{AUT} was set to the default ASM2d value.

Table 4.9 - Optimized parameter set

Parameter	Default value	Optimized value	Unit
q_{PP}	1.5	2.5	g X_{PP}/g X_{PAO}*d
q_{PHA}	3.0	3.6	g X_{PHA}/g X_{PAO}*d
q_{fe}	3.0	2.2	g S_F/g X_H*d
b_H	0.4	0.83	d^{-1}
μ_{PAO}	1	0.58	d^{-1}
μ_H	6	2.2	d^{-1}

The parameters q_{PP} and q_{PHA} were increased compared to default values, which represents the ability of PAO organisms to store polyphosphate and PHA. The parameters μ_{PAO} and μ_H were reduced which indicates a lower maximum growth rate for heterotrophic and PAO organisms. The parameter b_H represents the rate constant for lysis and decay of heterotrophic organisms and was significantly increased in the calibration. Therefore, the calibrated parameters suggests that heterotrophs grow slower and decay faster in the greywater treatment system than in a municipal WWTP. Furthermore, the PAO organisms store

The parameter $q_{fe,}$ which represents the fermentation rate by heterotrophic organisms, was reduced slightly. This is somewhat surprising because this parameter affects the hydrolysis of soluble organic matter and VFA production in the anaerobic tank and is essential for PAO growth. The VFA was assumed negligible in influent, and therefore fermentation by heterotrophs is essential for the PAO organisms. However, the default parameters are based on municipal wastewater and the greywater in this study contained a much higher soluble biodegradable COD fraction than typically found in municipal wastewater (Table 4.2). Therefore, even with a lower fermentation rate, a sufficient VFA production can be obtained.

However, even though the calibration was restricted to six parameters, most likely other parameter sets can also provide reasonable simulation results. This is illustrates the challenge for calibrating ASM models, which are overparameterized. For a more accurate calibration, it would have been desirable to perform off-line laboratory batch experiments to estimate the values of parameters such as μ_{PAO} and μ_H.

Table 4.10 - Comparison between experimental results and steady state model simulation after calibration.

		Anaerobic		Anoxic		Aerobic		Effluent	
Parameter	**Units**	**Exp**	**Sim**	**Exp**	**Sim**	**Exp**	**Sim**	**Exp**	**Sim**
COD_{tot}	mg/l	-	3992	-	7074	-	8399	*18.2*	33.3
$COD_{soluble}$	mg/l	*41.9*	119	*27.7*	42.9	*18.4*	33.3	*18.2*	33.3
MLSS	mg SS/l	*3680 ± 395*	3218	*5658 ± 311*	5828	*6456 ± 279*	6968	*0*	0
Tot-$P_{soluble}$	mg P/l	*22.9*	22.7	*1.9*	6.42	*0.246*	0.16	*0.07*	0.16
Tot-$N_{soluble}$	mg N/l	*4.79*	7.04	*1.8*	3.66	*2.07*	2.8	*<1*	2.8
NH_4-N	mg N/l	*2.92*	3.9	*0.88*	2.74	*0.07*	1.56	*0.04*	1.56
NO_3-N	mg N/l	*0.14*	0.0	*0.17*	0.04	*0.52*	0.66	*1.64*	0.66

The results of the steady-state simulation with the optimized parameter shows that the MLSS concentrations are within reasonable range of the experimental values. A much better fit is obtained for the P concentrations in the different tanks; however, there is still a disagreement for the anoxic P concentration (1.9 vs 6.2). The calibrated model also overestimates the prediction of P removal. However, this difference is very small because the pilot plant have a very high P removal (> 98%).

The pilot plant have a PAO culture that is capable of a high anoxic P uptake. The ASM2d model does not include separate yield coefficients for anoxic and aerobic PAO growth and P uptake ($Y_{PAO,}$ Y_{PHA}), and therefore is not be able to correctly simulate BNR systems with a high fraction of denitrifying PAO.

One possible modification to ASM2d for better simulation of the difference between the aerobic/anoxic P uptake is to implement different yield coefficients for aerobic and anoxic PAO growth and P uptake. García-Usach et al. (2010) applied a modified ASM2d model that included separate yield coefficients for anoxic and aerobic PAO growth and polyphosphate storage, and this resulted in a better modelling of the denitrifying PAO fraction. However, the pilot plant studied by García-Usach et al. (2010) did not contain a PAO culture with high anoxic P uptake, and this approach has yet to be tested for a system with dominating anoxic P uptake.

4.7 Optimization of operational parameters

4.7.1 Sensitivity analysis of operational parameters

The same sensitivity analysis procedure was used for the kinetic/stoichiometric parameters as was used for the operational parameters. The variation range of the operational parameters was based on values from the literature for UCT-MBR configuration (Metcalf & Eddy et al., 2013) and is presented in Table 4.11. The aerobic tank volume was not included due to software limitation. 1,000 Monte Carlo simulations was run for the sensitivity analysis, and the resulting SRCs for effluent concentrations of nitrate, TKN, COD and total P is presented in Figure 4.4.

Table 4.11 - Variation range for operational parameters for sensitivity analysis

Parameter	Unit	Min	Max
Nitrified Recycle	L/d	190 (2·Q)	665 (7·Q)
Anoxic Recycle	L/d	50 (0.5·Q)	380 (4·Q)
Anaerobic Volume	L	4 HRT: 1 h	16 HRT: 4 h
Anoxic Volume	L	4 HRT: 1 h	16 HRT: 4 h
Aeration	mg O_2/L	1	6

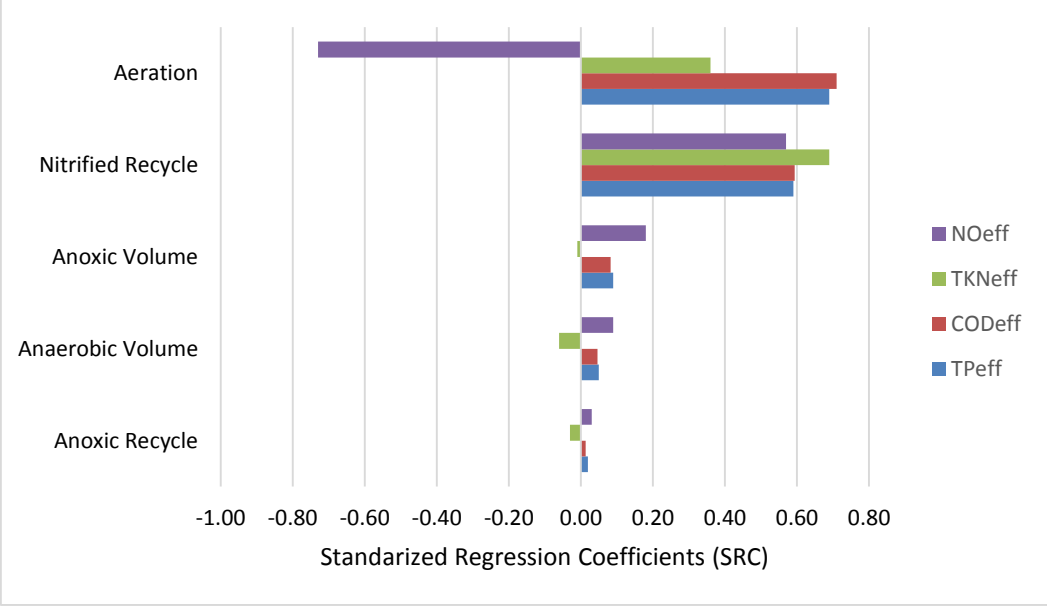

Figure 4.4 - SRC for operational parameters for phosphorus in the effluent

For COD, TP and nitrate, the oxygen concentration in the aerobic tank is the most sensitive parameter. Nitrate concentration increases in the effluent when the aeration

increases, therefore it is presented with a negative SRC. The most sensitive parameter for TKN is the size of the nitrified recycle flow.

From the SRC values, it seems like the anaerobic/anoxic volumes and the anoxic recycle are irrelevant compared to aeration and nitrified recycle. However, a wide range was chosen for aeration (1 – 6 mg O_2/L) and the nitrified recycle (2·Q – 7·Q), which might have affected the SRC calculations and given unreasonable high sensitivity to these parameters. Anyhow, it gives an indication that the anoxic and anaerobic volumes might be reduced without compromising the effluent quality.

4.7.2 Scenario analysis of operational parameters

To further investigate the system configuration a scenario analysis were performed over a set of predefined values shown in Table 4.12. The scenario analysis goes through all the different combinations of these parameters and thus results in 1296 ($3^4 \cdot 4^2$) simulations. The results of the simulations can be investigated in the attached Excel spreadsheet.

Table 4.12 - Operational parameter set for scenario analysis

Parameter	Units	Values			
Nitrified Recycle	L/d	200	477.7	600	
Anoxic Recycle	L/d	50	115.2	200	250
Aerobic Volume	L	15	20.8	25	30
Anaerobic Volume	L	5	12.7	15	
Anoxic Volume	L	5	10.34	15	
Aeration	mg O_2/L	1	3	5.5	

From the scenario analysis an optimized operational parameter set was found, and is shown in It is also important to be aware of that even though the steady state simulation shows a good effluent quality at this configuration, no safety factors have been applied to the operational parameters. Design of WWTP and greywater treatment systems employ various safety factors and the systems might be considered larger than necessary when compared to simulations of the system. However, the safety factors are important due to high uncertainty of inflows to the system.

Table 4.13. It was optimized with an higher priority given to reduced volume for the tanks, and low Tot-P and TKN concentrations. The internal recycle streams and wastage rate were maintained at the same flows used in the pilot plant. With a reduced total volume the SRT was decreased to 10 days. A lower SRT was also investigated, however it led to a deterioration of the phosphorus effluent quality. For this given configuration it suggests that SRT of 10 days is the lower SRT limit for

satisfying phosphorus removal. The aeration setting was reduced to be maintained at 2 mg O_2/L. This is quite a low oxygen concentration for an IFAS reactor, and might not be feasible for an IFAS reactor because the aeration is also responsible for the mixing and there is a need for a high oxygen concentration for penetration of the biofilm.

It is also important to be aware of that even though the steady state simulation shows a good effluent quality at this configuration, no safety factors have been applied to the operational parameters. Design of WWTP and greywater treatment systems employ various safety factors and the systems might be considered larger than necessary when compared to simulations of the system. However, the safety factors are important due to high uncertainty of inflows to the system.

Table 4.13 - Optimized operational parameter set based on scenario analysis

Parameter	Value	Unit	Effluent parameter	Value[a]	Comparison[b]	Unit
Anaerobic Vol	15	L	COD	26.5 (95%)	33.3	mg/l
Anoxic Vol	10.34	L	Tot-N	1.98 (90%)	2.8	mg N/l
Aerobic Vol	5	L	TKN	1.66	2.14	mg N/l
Total Vol	30.34	L	Nitrate	0.32	0.66	mg N/l
Nitrified Recycle	475.2	L/d	NH_4-N	1.24	1.56	mg N/l
Anoxic Recycle	115.2	L/d	Tot-P	0.11 (98%)	0.16	mg P/l
Aeration	2	mg O_2/L	PO_4-P	0.03	0.01	mg P/l
Wastage	2.5	L/d				
SRT	10	d				

a Values in parenthesis is the percentage removal with respect to the influent.

b Values from simulation with calibrated kinetic/stoichiometric parameters.

4.8 Success of the model

The preliminary steady state simulation (Table 4.3) were able to predict the effluent quality parameters COD, Tot-N, and Tot-P with a high degree of accuracy. This indicates that even though the parameters are based on municipal wastewater, that optimization and investigation of greywater systems with BNR can be done with an unmodified ASM2d model. Even a configuration with IFAS can be simulated reasonably well.

The model was calibrated to the operational data, and used for sensitivity analysis and optimization of operational parameters. This is a great advantage compared to pilot studies, as it would be very time consuming to explore the sensitivity and optimization of various operational parameters in a pilot study.

4.9 Limitations of the model

The model utilized a slightly modified ASM2d model, however it did not include any biofilm processes. This might lead to erroneous results, as the anoxic and aerobic tank was run with an IFAS configuration. Most likely this will affect the simulation of the nitrogen cycle in the pilot plant, because nitrifiers are able to proliferate in a biofilm. Thus, the simulation of nitrogen species (nitrate, ammonium, and organic nitrogen) should be used with care.

The model was calibrated with the X_I parameter in the influent, and subsequently a group of kinetic parameters were adjusted to fit the anaerobic/anoxic/aerobic P concentrations. The parameters were not outside any range previously used in the literature, however the calibration were based on operational measurements from a steady state period. Preferable, the adjustment of kinetic/stoichiometric parameter should have been based on off-line experimental procedure (e.g. determining the maximum growth rate for heterotrophs and PAOs).

The steady-state model is set up based on values from an analysis period of 31 days. The SRT of the system was set to 14 days, and thus the analysis period represent about two times the system SRT. This might be considered as a short analysis period compared to other modelling studies utilizing MBR for greywater treatment which typically analyze a pilot running over at least 3 months (Friedler et al., 2008; Hocaoglu et al., 2013; Jabornig and Rauch, 2015). However, the pilot had already been running for several months and the synthetic greywater mix was fed at a constant rate, so the system was maintained in a steady state. The system did not suffer dynamic fluctuations in the biomass or effluent quality, so the system can be assumed to be in steady state.

The model was unsuccessful in simulating the soluble COD in the anaerobic tank (119 vs. 41.9). For the modelling of COD removal in the system as a whole, this aspect is not essential. However, this influences the growth of PAO organisms and heterotrophs in the anaerobic tank, and might lead to incorrect results.

The model has not been validated with a separate independent dataset, due to the lack of such dataset. This is a typical problem for ASM models due to the fact that it is hard to gather sufficient data to set up a model, and therefore the available data is used for calibration purposes (Rieger et al., 2012). It would have been favorable to have a dynamic inflow analysis period that could be used as a validation dataset to gain better confidence in the calibrated parameter set.

5 Conclusion

In this thesis, the modelling of a novel greywater treatment system (IFAS-EBNR-MBR) was achieved by WEST modelling software and the ASM2d model. Various simplifications and assumptions were made for applying the model to an IFAS configuration with MBR. The model was successful in prediction of the effluent quality, however calibration was needed to fitting the model to the measurements of various components in the different tanks (MLSS, soluble COD, phosphorus and nitrogen).

Firstly, the influent characterization was examined closer and adjusted for a better fit with the MLSS concentration. For further calibration, the number of kinetic/stoichiometric parameters needed for calibration was reduced to six parameters due to sensitivity analysis. An automatic parameter estimation algorithm (Simplex) was used for calibration, where the variation range of the parameters were based on literature values. The parameter were slightly adjusted after the automatic calibration. After the calibration the phosphorus distribution in the different tanks were better predicted. However, the model was not able to successfully simulate the anoxic P uptake in the pilot plant. The pilot plant had a dominating anoxic P uptake, and the ASM2d model most likely needs to be modified to be able to simulate systems with a dominant anoxic P uptake.

The calibrated model was used further for sensitivity analysis of operational parameters. Aeration and the nitrified internal recycle were found to be the most sensitive operational parameters with respect to all effluent quality variables (COD, nitrogen and phosphorus). The aerobic volume and the wastage rate was not included in the sensitivity analysis.

Finally, scenario analysis was used to investigate many different combinations of operational parameters. An optimized parameter set was found and presented based on low total volume of the configuration and high P and N removal.

This thesis have for the first time applied a popular activated sludge model for BNR systems to a IFAS-EBNR-MBR configuration for greywater treatment. It is not without challenges and limitations, and the model fails at certain aspects. However, it is still a valuable tool to investigate and optimize different operational parameters of the process.

6 Further work

1. The model has difficulties at correctly describing the orthophosphate concentration in the anoxic tank. One possible explanation for this is that the ASM2d model does not have different yield coefficients for PAO organisms under aerobic and anoxic conditions. The model could therefore be extended to include the different growth yield for PAO under these conditions and investigate the improvement in predictability of anoxic P uptake.

2. Greywater treatment systems in real applications experience a wide range of fluctuations in flows and characteristics. In this thesis, a steady-state simulation was used to investigate the system, but to further investigate the operation of such a system in a real application it is necessary to do a dynamic simulation. The dynamic inflow pattern is dependent on where greywater treatment system would be implemented. For example for a system used for a household or a high-story building it would be interesting to investigate the consequence of the high morning/evening inflow in the greywater treatment system. A vacation scenario where zero inflow is expected for a long period of time (one month) should also be investigated.

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Appendix A – Matrix for ASM2d

The full ASM2d matrix can be found in the attached Excel spreadsheet “ASM2d WEST matrix”. This Excel sheet is based on Hauduc et al. (2010). The processes rate equations are presented here.

j	Process	Process rate equation $\rho_j > 0$
Hydrolysis processes		
1	Aerobic Hydrolysis	$K_{\mathrm{h}} \cdot \frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{X_{\mathrm{S}}/X_{\mathrm{H}}}{K_{\mathrm{X}} + X_{\mathrm{S}}/X_{\mathrm{H}}} \cdot X_{\mathrm{H}}$
2	Anoxic Hydrolysis	$K_{\mathrm{h}} \cdot \eta_{NO_3} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}} \cdot \frac{X_{\mathrm{S}}/X_{\mathrm{H}}}{K_{\mathrm{X}} + X_{\mathrm{S}}/X_{\mathrm{H}}} \cdot X_{\mathrm{H}}$
3	Anaerobic Hydrolysis	$K_{\mathrm{h}} \cdot \eta_{\mathrm{fe}} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{K_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}} \cdot \frac{X_{\mathrm{S}}/X_{\mathrm{H}}}{K_{\mathrm{X}} + X_{\mathrm{S}}/X_{\mathrm{H}}} \cdot X_{\mathrm{H}}$
Regular Heterotrophic Organisms X_H		
4	Aerobic growth on S_F	$\mu_{\mathrm{H}} \cdot \frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{F}}}{K_{\mathrm{F}} + S_{\mathrm{F}}} \cdot \frac{S_{\mathrm{F}}}{S_{\mathrm{F}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{NH_4}}}{K_{\mathrm{NH_4}} + S_{\mathrm{NH_4}}} \cdot \frac{S_{\mathrm{PO_4}}}{K_{\mathrm{P}} + S_{\mathrm{PO_4}}} \cdot \frac{S_{\mathrm{ALK}}}{K_{\mathrm{ALK}} + S_{\mathrm{ALK}}} \cdot X_{\mathrm{H}}$
5	Aerobic growth on S_A	$\mu_{\mathrm{H}} \cdot \frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{A}}}{K_{\mathrm{A}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{F}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{NH_4}}}{K_{\mathrm{NH_4}} + S_{\mathrm{NH_4}}} \cdot \frac{S_{\mathrm{PO_4}}}{K_{\mathrm{P}} + S_{\mathrm{PO_4}}} \cdot \frac{S_{\mathrm{ALK}}}{K_{\mathrm{ALK}} + S_{\mathrm{ALK}}} \cdot X_{\mathrm{H}}$
6	Anoxic growth on S_F	$\mu_{\mathrm{H}} \cdot \eta_{\mathrm{NO_3}} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{K_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}} \cdot \frac{S_{\mathrm{F}}}{K_{\mathrm{F}} + S_{\mathrm{F}}} \cdot \frac{S_{\mathrm{F}}}{S_{\mathrm{F}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{NH_4}}}{K_{\mathrm{NH_4}} + S_{\mathrm{NH_4}}} \cdot \frac{S_{\mathrm{PO_4}}}{K_{\mathrm{P}} + S_{\mathrm{PO_4}}} \cdot \frac{S_{\mathrm{ALK}}}{K_{\mathrm{ALK}} + S_{\mathrm{ALK}}} \cdot X_{\mathrm{H}}$
7	Anoxic growth on S_A, Denitrification	$\mu_{\mathrm{H}} \cdot \eta_{\mathrm{NO_3}} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{K_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}} \cdot \frac{S_{\mathrm{A}}}{K_{\mathrm{A}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{F}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{NH_4}}}{K_{\mathrm{NH_4}} + S_{\mathrm{NH_4}}} \cdot \frac{S_{\mathrm{PO_4}}}{K_{\mathrm{P}} + S_{\mathrm{PO_4}}} \cdot \frac{S_{\mathrm{ALK}}}{K_{\mathrm{ALK}} + S_{\mathrm{ALK}}} \cdot X_{\mathrm{H}}$
8	Fermentation	$q_{\mathrm{fe}} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{K_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}} \cdot \frac{S_{\mathrm{F}}}{K_{\mathrm{F}} + S_{\mathrm{F}}} \cdot \frac{S_{\mathrm{ALK}}}{K_{\mathrm{ALK}} + S_{\mathrm{ALK}}} \cdot X_{\mathrm{H}}$
9	Lysis	$b_{\mathrm{H}} \cdot (\frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} + \eta_{\mathrm{NO_3},H,d} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}}) \cdot X_{\mathrm{H}}$
Phosphorus-accumulating organisms X_{PAO}		
10	Storage of X_{PHA}	$q_{\mathrm{PHA}} \cdot \frac{S_{\mathrm{A}}}{K_{\mathrm{A}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{ALK}}}{K_{\mathrm{ALK}} + S_{\mathrm{ALK}}} \cdot \frac{X_{\mathrm{PP}}/X_{\mathrm{PAO}}}{K_{\mathrm{PP}} + X_{\mathrm{PP}}/X_{\mathrm{PAO}}} \cdot X_{\mathrm{PAO}}$
11	Aerobic storage of X_{PP}	$q_{\mathrm{PP}} \cdot \frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{PO_4}}}{K_{\mathrm{PS}} + S_{\mathrm{PO_4}}} \cdot \frac{X_{\mathrm{PHA}}/X_{\mathrm{PAO}}}{K_{\mathrm{PHA}} + X_{\mathrm{PHA}}/X_{\mathrm{PAO}}} \cdot \frac{K_{\mathrm{MAX}} - X_{\mathrm{PP}}/X_{\mathrm{PAO}}}{K_{\mathrm{PP}} + K_{\mathrm{MAX}} - X_{\mathrm{PP}}/X_{\mathrm{PAO}}} \cdot X_{\mathrm{PAO}}$
12	Anoxic storage of X_{PP}	$\rho_{12} = \rho_{11} \cdot \eta_{\mathrm{NO_3}} \cdot \frac{K_{\mathrm{O_2}}}{S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}}$
13	Aerobic growth of X_{PAO}	$\mu_{\mathrm{PAO}} \cdot \frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NH_4}}}{K_{\mathrm{NH_4}} + S_{\mathrm{NH_4}}} \cdot \frac{S_{\mathrm{PO_4}}}{K_{\mathrm{P}} + S_{\mathrm{PO_4}}} \cdot \frac{S_{\mathrm{ALK}}}{K_{\mathrm{ALK}} + S_{\mathrm{ALK}}} \cdot \frac{X_{\mathrm{PHA}}/X_{\mathrm{PAO}}}{K_{\mathrm{PHA}} + X_{\mathrm{PHA}}/X_{\mathrm{PAO}}} \cdot X_{\mathrm{PAO}}$
14	Anoxic growth of X_{PAO}	$\rho_{14} = \rho_{13} \cdot \eta_{\mathrm{NO_3}} \cdot \frac{K_{\mathrm{O_2}}}{S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}}$
15	Lysis of X_{PAO}	$b_{\mathrm{PAO}} \cdot (\frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} + \eta_{\mathrm{NO_3},P,d} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}}) \cdot X_{\mathrm{PAO}} \cdot S_{\mathrm{ALK}}/(K_{\mathrm{ALK}} + S_{\mathrm{ALK}})$
16	Lysis of X_{PP}	$b_{\mathrm{PP}} \cdot (\frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} + \eta_{\mathrm{NO_3},P,d} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}}) \cdot X_{\mathrm{PP}} \cdot S_{\mathrm{ALK}}/(K_{\mathrm{ALK}} + S_{\mathrm{ALK}})$
17	Lysis of X_{PHA}	$b_{\mathrm{PHA}} \cdot (\frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} + \eta_{\mathrm{NO_3},P,d} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}}) \cdot X_{\mathrm{PHA}} \cdot S_{\mathrm{ALK}}/(K_{\mathrm{ALK}} + S_{\mathrm{ALK}})$
Autotrophic Nitrifying Organisms X_A		
18	Aerobic growth of X_{AUT}	$\mu_{\mathrm{AUT}} \cdot \frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NH_4}}}{K_{\mathrm{NH_4}} + S_{\mathrm{NH_4}}} \cdot \frac{S_{\mathrm{PO_4}}}{K_{\mathrm{P}} + S_{\mathrm{PO_4}}} \cdot \frac{S_{\mathrm{ALK}}}{K_{\mathrm{ALK}} + S_{\mathrm{ALK}}} \cdot X_{\mathrm{AUT}}$
19	Lysis	$b_{\mathrm{AUT}} \cdot (\frac{S_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} + \eta_{\mathrm{NO_3},AUT,d} \cdot \frac{K_{\mathrm{O_2}}}{K_{\mathrm{O_2}} + S_{\mathrm{O_2}}} \cdot \frac{S_{\mathrm{NO_3}}}{K_{\mathrm{NO_3}} + S_{\mathrm{NO_3}}}) \cdot X_{\mathrm{AUT}}$

Appendix B – ASM2d Parameters

Composition factors

Symbol	Description	20 °C	Units
Nitrogen:			
$i_{N,SF}$	N content of S_F	0.03	g N/g COD
$i_{N,SI}$	N content of S_I	0.01	g N/g COD
$i_{N,XI}$	N content of X_I	0.02	g N/g COD
$i_{N,XS}$	N content of X_S	0.04	g N/g COD
$i_{N,BM}$	N content of biomass (X_H, X_{PAO}, X_{AUT})	0.07	g N/g COD
Phosphorus:			
$i_{P,SF}$	P content of S_F	0.01	g P/g COD
$i_{P,SI}$	P content of S_I	0.00	g P/g COD
$i_{P,XI}$	P content of X_I	0.01	g P/g COD
$i_{P,XS}$	P content of X_S	0.01	g P/g COD
$i_{P,BM}$	P content of biomass (X_H, X_{PAO}, X_{AUT})	0.02	g P/g COD
Total suspended solids TSS:			
$i_{TSS,XI}$	Conversion factor X_I in TSS	0.75	g TSS/g COD
$i_{TSS,XS}$	Conversion factor X_S in TSS	0.75	g TSS/g COD
$i_{TSS,XPHA}$	Conversion factor $X_{PAO,PHA}$ in TSS	3	g TSS/g COD
$i_{TSS,BM}$	Conversion factor biomass (X_H, X_{PAO}, X_{AUT}) in TSS	0.90	g TSS/g COD
$i_{TSS,XPP}$	Conversion factor $X_{PAO,PP}$ in TSS	3.23	g TSS/g P

Stoichiometric parameters

Symbol	**Description**	**20 °C**	**Units**
Hydrolysis			
f_{SI}	Fraction of inert COD generated in hydrolysis	0	g COD/g COD
f_{XI}	Fraction of X_I generated in biomass decay	0.10	g COD/g COD
Heterotrophic organisms: X_H			
Y_H	Yield for X_H growth	0.625	g COD/g COD
Phosphorus-accumulating organisms: X_{PAO}			
Y_{PAO}	Yield for X_{PAO} growth per X_{PHA}	0.625	g COD/g COD
Y_{PO4}	Yield for X_{PP} requirement (S_{PO4} release) per X_{PHA} stored (S_A utilized)	0.40	g P/g COD
Y_{PHA}	Yield for X_{PP} storage (S_{PO4} uptake) per X_{PHA} utilized	0.20	g COD/g P
Nitrifying organisms (autotrophic organisms): X_{AUT}			
Y_A	Yield of X_{AUT} growth per S_{NO3}	0.24	g COD/g N

Kinetic parameters

Symbol	Description	20 °C	Units
Hydrolysis of particulate substrate: X_S			
K_h	Maximum specific hydrolysis rate	3.00	d^{-1}
$\eta_{NO3,HYD}$	Correction for hydrolysis under anoxic conditions	0.60	-
η_{fe}	Correction for hydrolysis under anaerobic conditions	0.40	-
$K_{O2,HYD}$	Half saturation/inhibition parameter for S_{O2}	0.20	g O_2/m^3
$K_{NO3,HYD}$	Half saturation/inhibition parameter for S_{NO}	0.50	g N/m^3
K_X	Half saturation parameter for X_S/X_H	0.10	g X_S/g X_H
Heterotrophic organisms: X_H			
μ_H	Maximum growth rate of X_H	6.00	g X_S/g X_H*d
q_{fe}	Maximum specific fermentation growth rate	3.00	g S_F/g X_H*d
$\eta_{NO3,H}$	Reduction factor for anoxic growth of X_H	0.80	-
$\eta_{NO3,H,d}$	Reduction factor for anoxic lysis of X_H	0.5	-
b_H	Decay rate for X_H	0.40	d^{-1}
$K_{O2,H}$	Half saturation parameter for S_{O2}	0.2	g O_2/m^3
K_F	Half saturation parameter for S_F	4.00	g COD/m^3
K_{fe}	Half saturation parameter for fermentation of S_F	4.00	g COD/m^3
$K_{A,H}$	Half saturation parameter for S_A	4.00	g COD/m^3
$K_{NO3,H}$	Half saturation parameter for S_{NO}	0.50	g N/m^3
$K_{NH4,H}$	Half saturation parameter for S_{NH}	0.05	g N/m^3
$K_{P,H}$	Half saturation parameter for S_{PO4}	0.01	g P/m^3
$K_{ALK,H}$	Half saturation parameter for S_{Alk}	0.10	mole HCO_3^-/m^3
Phosphorus-accumulating organisms: X_{PAO}			
q_{PHA}	Rate constant for S_A uptake rate (X_{PHA} storage)	3.00	g X_{PHA}/g X_{PAO}*d
q_{PP}	Rate constant for storage of X_{PP}	1.50	g X_{PP}/g X_{PAO}*d
μ_{PAO}	Maximum growth rate of X_{PAO}	1.00	d^{-1}
$\eta_{NO3,PAO}$	Reduction factor for anoxic growth of X_{PAO}	0.60	-
$\eta_{NO3,P,d}$	Reduction factor for anoxic lysis of X_{PAO}, X_{PP} and X_{PHA}	0.33	-
b_{PAO}	Endogenous respiration rate of X_{PAO}	0.20	d^{-1}
b_{PP}	Rate constant for Lysis of X_{PP}	0.20	d^{-1}
b_{PHA}	Rate constant for respiration of X_{PHA}	0.20	d^{-1}
$K_{O2,PAO}$	Half saturation parameter for S_{O2}	0.20	g O_2/m^3
$K_{NO3,PAO}$	Half saturation parameter for S_{NO}	0.50	g N/m^3
$K_{A,PAO}$	Half saturation parameter for S_A	4.00	g COD/m^3
$K_{NH4,PAO}$	Half saturation parameter for S_{NH}	0.05	g N/m^3
K_{PS}	Half saturation parameter for S_{PO4} uptake (X_{PP} storage)	0.20	g P/m^3
$K_{P,PAO}$	Half saturation parameter for S_{PO4} as nutrient (X_{PAO} growth)	0.01	g P/m^3
$K_{ALK,PAO}$	Half saturation parameter for S_{Alk}	0.10	mole HCO_3^-/m^3
K_{PP}	Half saturation parameter for X_{PP}/X_{PAO}	0.01	g X_{PP}/g X_{PAO}
K_{MAX}	Maximum ratio of $X_{PAO,PP}/X_{PAO}$	0.34	g X_{PP}/g X_{PAO}
K_{iPP}	Half Inhibition parameter for X_{PP}/X_{PAO}	0.02	g X_{PP}/g X_{PAO}
K_{PHA}	Saturation constant for X_{PHA}/X_{PAO}	0.01	g X_{PHA}/g X_{PAO}
Nitrifying organisms (autotrophic organisms): X_{AUT}			
μ_{AUT}	Maximum growth rate of X_{AUT}	1.00	d^{-1}
$\eta_{NO3,AUT,d}$	Reduction factor for anoxic lysis of X_{AUT}	0.33	-
b_{AUT}	Decay rate for X_{AUT}	0.15	d^{-1}
$K_{O2,AUT}$	Half saturation parameter for S_{O2}	0.50	g O_2/m^3
$K_{NH4,AUT}$	Half saturation parameter for S_{NHx}	1.00	g N/m^3
$K_{P,AUT}$	Half saturation parameter for S_{PO4}	0.50	g P/m^3
$K_{ALK,AUT}$	Half saturation parameter for S_{Alk}	0.01	mole HCO_3^-/m^3

Arrhenius temperature correction factors

A modified Arrhenius temperature correction equation is used for adjusting the kinetic parameters from the value for 20 °C to the specified temperature in the model.

$$k = k_{20} \cdot \theta^{(T-20)}$$

Symbol	20 °C
Hydrolysis of particulate substrate: X_S	
K_h	1.041
K_X	0.896
Heterotrophic organisms: X_H	
μ_H	1.072
q_{fe}	1.072
b_H	1.072
Phosphorus-accumulating organisms: X_{PAO}	
q_{PHA}	1.041
q_{PP}	1.041
μ_{PAO}	1.041
b_{PAO}	1.072
b_{PP}	1.072
b_{PHA}	1.072
Nitrifying organisms (autotrophic organisms): X_{AUT}	
μ_{AUT}	1.111
b_{AUT}	1.116