Computer-aided Framework for Synthesis, Design and Retrofit of Wastewater Treatment Plants

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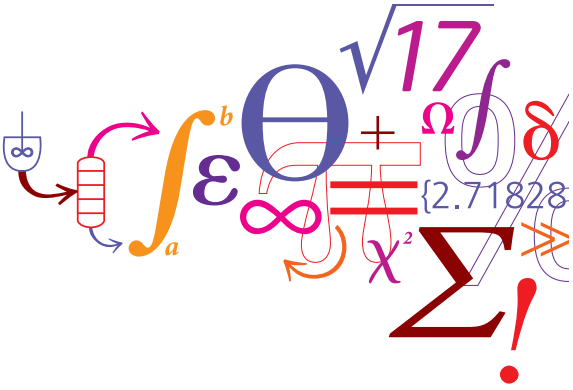

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Ph.D. Thesis
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DTU Chemical Engineering
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PhD Thesis

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Preface

This thesis is submitted as partial fulfillment of the requirements for the Doctor of Philosophy (PhD) degree at the Technical University of Denmark. The PhD project was carried out at the Computer Aided Process Engineering Center (CAPEC) at the Department of Chemical and Biochemical Engineering from December 2011 to February 2015 under the supervision of Associate Professor Gürkan Sin as the main supervisor and Professor Krist V. Gernaey as the co-supervisor. Moreover, an external research stay had been carried out at the Environmental Biotechnology Group at the Technical University of Delft, hosted by Professor Mark C.M. van Loosdrecht.

First of all I would like to thank to my supervisors Gürkan Sin and Krist V. Gernaey for their unlimited support, valuable criticism and guidance. I am grateful for all the discussions and their endless patience during this study. I would also like to thank to Mark van Loosdrecht and the researchers in Environmental Biotechnology Group at TU Delft for their time, valuable ideas and collaboration during and after the research stay.

I would specially like to thank to Alberto Quaglia and Peam Cheali for their valuable contributions, advices and time; without their presence and guidance this work could not be finalized.

I started my journey in Denmark three years ago and met many great people on the way. Looking back, I realize that we have shared many wonderful memories in and outside of DTU. For that, I would like to thank to all the current and past CAPEC and PROCESS members as well as friends and colleagues. Thank you for making me feel like belonging to a big 'Danish' family.

For the past three years, despite being thousands of kilometers away from home, I could always feel the support and encouragement from so many beautiful people from Turkey. Thank you for everything and especially for always being there (sometimes even in Copenhagen) when I needed.

Finally, I would like to thank to my parents, my grandmother and Baran. I owe them a lot for their support, patience and love that I could always feel and be grateful for.

Hande Bozkurt
Ankara, February, 2015

...to my big family

Abstract

Water is used for several purposes in houses and industrial applications, which results in the generation of considerable amounts of wastewater. Wastewater should be handled appropriately which is required from legal, environmental as well as economic and societal perspectives.

Wastewater treatment plant (WWTP) design is a formidable challenge. One of the key steps involved is the process synthesis - defined as the selection of treatment processes as a combination of unit operations and processes to create the process flow diagram.

As a consequence of the emerging technological developments and resulting increase in the number of alternative wastewater treatment technologies, as well as stricter effluent limit values imposed by regulations; it became increasingly harder to identify the most feasible decision regarding the WWTP network design. Retrofitting of existing treatment plants can also be formulated as a process synthesis challenge in the sense that a new task can be added to the existing treatment line or one or several existing processes can be changed as a result of the emerging needs. Existing plants need retrofitting due to a number of reasons such as: change in the wastewater flow and composition, change in the effluent limitations, as well as changes in the wastewater treatment trends, e.g. from nutrient removal to nutrient recovery. Similarly, recovery possibilities for clean water, energy and materials shifted the perception about wastewater towards being a valuable resource rather than being a waste. While the regulations change to impose stricter effluent limit values for the contaminants, the increasing population and the size of the cities put a barrier on the expansion of the existing WWTPs. Therefore, the retrofitting task has become a complex integrated decision making problem where a number of aspects have to be accounted for in the early stage decision making. WWTP layouts are currently developed based on expert and experience based designs. However as a result of the above-mentioned considerations, it is evident that making the most feasible decision with this experience-based approach will be increasingly difficult if not subjective. In this study, a systematic framework based on mathematical programming is proposed to handle the complex process synthesis problem by a superstructure optimization approach to generate a novel and optimal WWTP process selection for treatment of domestic wastewaters. The framework has been implemented as a tool which consists of the superstructure covering all relevant treatment alternatives and a database storing design parameters and performances for each alternative technology. The solution of the optimization problem provides an optimal process selection and the optimal flows through the selected network.

Finally, the framework is applied to two case studies constituting typical examples for the different scales of wastewater treatment design (BSM2) and retrofitting studies (Lynetten WWTP of 750,000 PE, and Avedøre WWTP of 265,000 PE) in order to highlight and validate the use of the developed methodology and database.

Resumé på dansk

Vand anvendes til vores daglige formål i huse og industri, hvilket resulterer i betydelige mængder spildevand. Spildevand skal håndteres på bedste vis i overensstemmelse med juridiske, miljømæssige, økonomiske og samfundsmæssige perspektiver.
Design af renseanlæg udgør en enorm udfordring. Et af de vigtigste trin er processyntese - defineret som valget af behandlingsprocesser som en kombination af enhedsoperationer og processer, der til sammen udgør procesdiagrammet.
Som følge af den teknologiske udvikling, og dermed et stigende antal af alternative spildevandsrensningsteknologier samt indførelse af strengere grænseværdier for afløbet fra renseanlæg, bliver det stadig vanskeligere at identificere den bedste løsning vedrørende renseanlægs netværksdesign. Opgradering af eksisterende renseanlæg kan også formuleres som en processynteseopgave i den forstand, at en ny funktion kan føjes til den eksisterende proces, eller et eller flere eksisterende processer kan ændres som følge af de nye behov. Eksisterende anlæg behøver opgradering på grund af en række årsager såsom: ændring i mængde og sammensætning af spildevandsstrømmen der skal behandles, ændring i afløbsgrænseværdier, samt generelle ændringer i teknikkerne inden for spildevandsrensning (f.eks. fra næringsstoffjernelse til udvinding af næringsstoffer).
Ligeledes, har muligheden for udvinding af rent vand, energi og materialer flyttet opfattelsen om spildevand i retning af at være en værdifuld ressource i stedet for at være et spildprodukt. Mens reglerne ændres til strengere grænseværdier af forurenende stoffer i afløbet kombineret med et stigende befolkningstal og størrelsen af byerne, sættes en barriere på udvidelse af eksisterende renseanlæg. Derfor er opgraderingsopgaven blevet et komplekst, integreret beslutningstagningsproblem, hvor der skal tages højde for en række aspekter i det tidlige stadie i beslutningsprocessen. Layouts af rensningsanlæg bliver i øjeblikket udviklet baseret på ekspert- og erfaringsbaseret design, men som følge af de ovennævnte betragtninger er det indlysende, at identificering af den mest eftertragtede beslutning ang. renseanlægsdesign baseret på erfaring bliver fortsat vanskeligere, hvis ikke, subjektivt.
I dette projekt, foreslås en systematisk metode baseret på matematisk programmering til at håndtere det komplekse processynteseproblem via en superstruktur-optimeringsfremgangsmåde til at generere et nyt og optimalt renseanlæg til behandling af husholdningsspildevand. Metoden er implementeret som et værktøj, der består af en superstruktur, der dækker alle relevante behandlingsalternativer samt en database til opbevaring af designparametre og -evaluering for hver alternativ teknologi. Løsningen af optimeringsproblemet resulterer i et optimal procesnetværk og de optimale strømme igennem det valgte netværk.
Endelig, anvendes strukturen på to casestudier, som udgør typiske eksempler i forskellige størrelsesordener for spildevandsrensning; design- (BSM2) og opgraderingsstudier (Lynetten rensningsanlæg på 750.000 PE og Avedøre på 265.000 PE), for at fremhæve og validere anvendelsen af den udviklede metode og database.

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1 INTRODUCTION

The first chapter, *Introduction*, constitutes a general overview of the PhD project. The definitions of common concepts used within this document are given together with a brief introduction to wastewater treatment plant design, and the development stages of treatment concepts and technologies. The motivation and objectives of the study are also presented in this chapter along with the overall structure of the thesis. Finally, dissemination activities of the results and main achievements are given.

One of the most challenging steps in wastewater treatment plant design is the selection of the treatment technologies, defined as a combination of unit operations and processes capable of meeting effluent permit requirements (Tchobanoglous, 2003). This particular task is referred to as *Wastewater treatment process synthesis* in the context of this study and defined as:

> "Wastewater treatment process synthesis is the step in the design or retrofitting of a wastewater treatment plant (WWTP) where the design engineer selects unit processes (separation and/or reaction including physical, chemical and biological processes) from numerous alternatives and interconnects them to create the process flow diagram."

Hence, the objective of process synthesis is to find the best process flow diagram, among numerous alternatives, for treating a given influent wastewater with its flow rate and composition to meet predefined performance criteria including effluent permit requirements as well as cost and technical requirements.
The number of alternative processes to choose from has been increasing steadily since the beginning of the 20th century, where many wastewater treatment processes and technologies have been developed to meet increasingly stringent performance demands (Henze et al., 2008). Moreover, recently the WWTP process selection and network design problem has evolved from being a simple technical design problem to a complex integrated decision making task, mainly because of the many aspects being considered in the early decision making stage (Hamouda et al., 2009).
The current phase of development in municipal wastewater treatment technologies was initiated with the stricter effluent limit values imposed by both emission and immission based regulations for controlling the quality of effluent streams as well as the receiving bodies. In EU, for instance, the Water Framework Directive (Directive 2000/60/EC) regulates the ecosystem by setting quality objectives for receiving environments and the urban effluent wastewater quality is controlled by the Urban Wastewater Treatment Directive (91/271/EEC). A wide range of parameters were included in several different regulations covering both water and sludge disposal, i.e. organics, nutrients, pathogens, heavy metals, emerging contaminants etc. This resulted in development of new treatment technologies as well as new process flow diagrams for WWTPs.
Process synthesis is also performed during retrofitting studies in the sense that a new task can be added to the existing treatment line or one or several processes can be changed as a result of emerging needs. For instance, increasing nitrogen limitation in the regulations for the WWTP effluents gave rise to development of innovative nitrogen removal technologies which are mostly used for water streams rich in nitrogen resulting from sludge treatment (Lackner et al., 2014). Similarly, recovery possibilities for clean water, energy and materials shifted the perception about wastewater being a valuable resource

rather than being a waste; and brought new technology advancements and design approaches as well.

Eventually, the number of available technologies using physical, chemical and biological means of treatment has increased considerably in order to satisfy the efficiency requirements by the stricter regulations and developing needs.

The fact that the number of alternative wastewater treatment technologies is growing steadily increases the importance of early-stage decision making in WWTP design and retrofitting problems. When the design procedure is divided into different stages as stated in the development funnel approach, which is illustrated in Figure 1.1 (Quaglia, 2013), the first stage of the funnel – the early decision making stage – corresponds to the design stage where a variety of concepts and ideas are generated and a high number of alternatives are evaluated in a less detailed / simplified manner. The alternatives that are proven to satisfy the criteria needed by the designer can move further through the funnel to be investigated in more detail.

When considering a WWTP design / retrofit case, early stage decision making is mainly about:

- Which treatment unit and processes to select for a particular wastewater treatment problem,
- How to define the interconnections between the treatment technologies and,
- How to verify the rationale and ensure engineering optimality of the decision.

Often – if not always – such decisions are multi-objective and multi-criteria based considering economics, environmental, legal and social constraints.

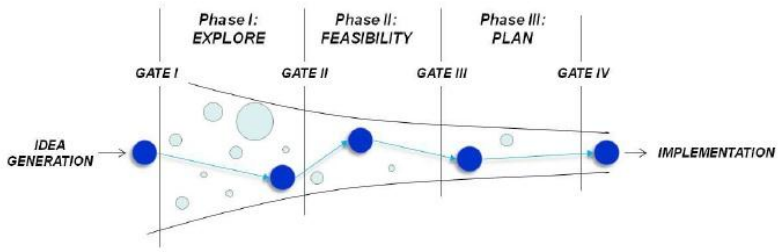


Figure 1.1 Illustration of the development funnel approach, where the number of feasible process options is gradually reduced from left to right (Quaglia, 2013)

Currently, the early stage decision making for WWTP design and retrofit is mainly based on expert decisions and previous experiences (Tchobanoglous, 2003). This approach takes values like environmental issues, water reuse, by-product recovery and impacts of the selected treatment technologies on the surrounding population into account and identifies the alternatives based on experiences, similar existing solutions and brainstorming to come up with the most viable WWTP network (Daigger, 2005). However, with the increased complexity of the technologies for wastewater treatment and

the stricter limit values for effluents, it is evident that the capacity to make the most feasible decision using this approach is limited.

An alternative approach is to cast the decision making problem using mathematical programming which has been an active research area in chemical process synthesis (Grossmann, 2005); but has also seen various applications in the wastewater treatment field in several studies such as Rigopoulos and Linke (2002), Vidal et al., (2002), and Alasino et al. (2007, 2010). While these studies provided valuable insights and showed the promising potential of the optimization based approaches for plant design, their scope was however rather limited and focused on either optimizing a given treatment process or selecting the best candidate process from a limited number of alternatives. Moreover, the knowledge-based decision support systems developed for conceptual WWTP design have been presented in the literature covering many different aspects of early stage design including technical, economic, environmental and social considerations; however, these approaches do not cover the optimization step for the process synthesis (Comas et al., 2003; Garrido-Baserba et al., 2012).

1.1 Motivation of the study

In order to realize the full potential of the process synthesis approach and its use in a wastewater treatment context, there are a number of barriers that need to be tackled and overcome, including the representation of the increasing number of unit operations and processes being used in wastewater treatment as well as tackling the resulting multi-disciplinary complexity of the optimization problem, which requires both competences and methods from optimization together with wastewater engineering disciplines. In particular, for formulating a realistic wastewater treatment design problem (i.e. a large number of alternatives representing the market together with their feasible combinations as well as necessary constraints that should be taken into account), the complexity of the mixed integer nonlinear programming problem (MINLP) can grow exponentially, which needs an effective formulation and analysis method, which is the focus of this study.

Therefore, in this study, a superstructure based optimization framework based on mathematical programming is proposed to manage the complexity of the WWTP design and retrofitting problems and to generate and identify novel and optimal process selection and interconnections to create a process flow diagram (i.e. Wastewater treatment process synthesis) for design and retrofit of WWTPs. The purpose of the framework is to support and complement the expertise of the design engineers / specialists in the process of making early stage design decisions by allowing them to compare several different treatment technologies at their optimality with respect to many different criteria. The framework contains a superstructure method for representing the design space, and a systematic method for modelling and data collection to constitute the database covering design data for individual treatment technologies. The framework also includes a generic and effective formulation of a mixed integer nonlinear programming problem to address the wastewater treatment process synthesis problem.

1.2 Objectives of the study

On the basis of the current status of the wastewater treatment plant design / retrofitting and the motivation of the study presented above, the determined objectives of the PhD study are listed below in this section.

- To modify and adapt the superstructure based optimization framework proposed by Quaglia (2013), which has been used for various network design problems, in the context of WWTP design and retrofitting problems. The main aim is to fill the gap between optimization-based design methods and wastewater engineering.
- To represent the design space, which includes high number of treatment alternatives as well as feasible network designs – well-known as well as innovative combinations –, with the novel superstructure approach.
- To develop and use a generic process interval, which is capable of performing as any treatment unit or process in a WWTP by encompassing several phenomena in one interval such as: mixing, reaction, separation etc.
- To use simple yet representative design / optimization models (i.e. optimal design at steady state by fixing design parameters for treatment technologies and mass input-output type of optimization model) in order to cover a large design space and to be able to solve the design problem under several different scenarios.
- To perform uncertainty and sensitivity analysis in order to comment on the robustness of the optimal solution and to further generate more robust solutions.
- To formulate and solve different case studies in order to highlight the applicability of the methodology.

1.3 Structure of the Thesis

This PhD thesis consists of six chapters and covers the following aspects of the subject. The current chapter – Chapter 1 – constitutes a general introduction into the wastewater treatment plant design, its development stages and specifically the importance of early decision making stage of the design studies. It also presents the motivation and objectives of the PhD study and the dissemination activities.

The second chapter – Chapter 2 mainly contains a literature review about the theoretical background of wastewater treatment process developments, recent concerns contributing to the development of innovative technologies and approaches, process synthesis and its applications together with mathematical programming in the wastewater treatment context as well as decision support systems, which in all respects constitute a detailed background for the motivation of this study.

Chapter 3 summarizes the superstructure based optimization methodology which is presented as the steps of the proposed framework. The framework is presented here in six steps covering the stages of the design approach used in this study from problem definition to identifying the optimal solution and its analysis.

Chapter 4 presents the details of the mathematical models used in this study for designing the individual treatment technologies as well as generation of the database for generic process interval models (i.e. converting the design outputs into parameters that are further used by the optimizer).

In Chapter 5, the use of the developed methodology is highlighted using several case studies constituting examples for the different scales of wastewater treatment design and retrofit problems (i.e. small, medium and large scale in terms of the volume of wastewater treated).

The last chapter – Chapter 6 – is the conclusion chapter where the main conclusions are drawn, the achievements of the PhD study are summarized and the future perspectives and suggestions are given.

1.4 Dissemination activities

The optimization based approach for early stage design and retrofitting of WWTPs, including the developed methodology and results obtained in different case study applications during this PhD study, have been presented in five conferences as listed below.

- 2nd IWA Specialized Conference on Eco-Technologies for Sewage Treatment Plants – EcoSTP2014, June 2014, Verona, Italy (oral presentation).
- ESCAPE24 Conference, June 2014, Budapest, Hungary (oral presentation).
- 4th IWA/WEF Wastewater Treatment Modelling Seminar – WWTMod2014, March 2014, Spa, Belgium (poster presentation).
- 11th IWA Conference on Instrumentation Control and Automation – ICA2013, September 2013, Narbonne, France (poster presentation).
- IWA Conference on Asset Management for Enhancing Energy Efficiency in Water and Wastewater Systems, April 2013, Marbella, Spain (oral presentation).

Moreover, the detailed explanation of the framework for synthesis, design and retrofit of WWTP layouts, the data collection and design methodology developed within the framework and several case study applications have been published in scientific journals and peer reviewed conference proceedings as listed below.

- Bozkurt H., van Loosdrecht M.C.M., Gernaey K.V., Sin G. (2015). Optimal WWTP process selection for treatment of domestic wastewater – a realistic full-scale retrofitting study. Water Research (submitted).
- Bozkurt H., Gernaey K.V., Sin G. (2015). Optimization-based methodology for wastewater treatment plant synthesis – a full scale retrofitting case study. Computer Aided Process Engineering (in press).
- Bozkurt, H., Quaglia A., Gernaey K.V., Sin, G. (2015). A mathematical programming framework for early stage design of wastewater treatment plants. Environmental Modelling & Software, 64, 164 – 176.
- Bozkurt, H., Quaglia A., Gernaey K.V., Sin, G. (2014). Superstructure development and optimization under uncertainty for design and retrofit of municipal wastewater treatment plants. Computer Aided Chemical Engineering, 33, 37 – 42.
- Bozkurt H., Quaglia A., Gernaey K.V. Sin G. (2014). An optimization based framework for design and retrofit of municipal wastewater treatment plants: Case study on side-stream nitrogen removal technologies. 2nd IWA Specialized Conference on Eco-technologies for Sewage Treatment Plants-EcoSTP2014. 23-25 June, 2014. Verona, Italy.
- Bozkurt H., Quaglia A., Gernaey K.V. Sin G. (2014). Early-stage design of municipal wastewater treatment plants – presentation and discussion of an

optimization based concept. 4th IWA/WEF Wastewater Treatment Modelling Seminar – WWTMod2014. 30 March – 2 April, 2014. Spa, Belgium.

- Bozkurt H., Quaglia A., Gernaey K.V. Sin G. (2013). Superstructure development and optimization for design/retrofit of municipal wastewater treatment plants. 11th IWA Conference on Instrumentation Control and Automation – ICA2013. 18-20 September, 2013. Narbonne, France.
- Bozkurt H., Quaglia A., Gernaey K.V. Sin G. (2013). Design of future municipal wastewater treatment plants: A mathematical programming approach to manage complexity and identify optimal solutions. IWA Conference on Asset Management for Enhancing Energy Efficiency in Water and Wastewater Systems. 24-26 April, 2013. Marbella, Spain.

2 LITERATURE REVIEW

The *Literature Review* chapter provides a detailed overview about the theoretical background of the wastewater treatment process selection / synthesis problem. It starts by giving the historical development of wastewater treatment approaches and technologies and concludes by describing the importance of early stage design decisions during WWTP design studies, which is referred to as wastewater treatment process selection / synthesis, and by giving examples from the literature of different approaches dealing with this problem.

2.1 Wastewater treatment history and development

As a result of the massive use of water for a variety of purposes in households and industrial applications; considerable amounts of wastewater are produced. The major contaminants in wastewater which lead to nuisance conditions are:

- Organic matter which results in the consumption of oxygen in the surrounding environment and production of noxious gases,
- Pathogenic microorganisms that have negative health effects for different living organisms including humans, and
- Nutrients, which after entering the ecosystem, can promote the growth of aquatic plants and alter the balance between species in the ecosystem.

Considering all the above mentioned reasons, it is clear that wastewater should be collected, treated and subsequently reused or discharged to the environment for the sake of public health and the environment (Tchobanoglous, 2003).

2.1.1 Early stages of WWTP development

Development of wastewater treatment technologies received increasing attention in the 20th century due to potential health risks of wastewater and the nuisance that it caused in the urban areas (Henze et al., 2008). In London, for instance, thousands of people died as a result of several diseases like cholera, typhoid, plague and pestilence until it was realized that these diseases were caused by the city's own wastes (Lens and Lettinga, 2001).

In the early years of the Ancient Greeks and the Romans (300 BC to 500 AD), wastewater had generally been used for agricultural purposes. It was collected and conveyed to agricultural fields to serve as fertilizer for crops (Lens and Lettinga, 2001; Henze et al., 2008). However, with the rapid increase in the growth rate of the population, in the early 19th century, wastewater had become a major problem since the increase in the death rates experienced at that time was associated with water and waste borne diseases (Lens and Lettinga, 2001). In the beginning of the 1900s, the cities increased in size resulting in an increasing amount of wastewater and difficulties to find sufficient nearby land to dispose of the wastewater. Consequently, the idea of treating the wastewater by biological means came into the picture; and the activated sludge process was invented in the UK after performing experimental studies on an early draw-fill type of reactors (Ardern and Lockett, 1914; Henze et al., 2008).

Starting from the early 1900s until the 1970s, wastewater treatment was shaped in order to remove three major pollutant groups: (1) suspended material of mostly colloidal size, (2) biodegradable organics and (3) pathogenic organisms (Tchobanoglous, 2003). Moreover, the water bodies that receive wastewater discharges were taken into account while developing strategies for wastewater treatment; because, the dissolved oxygen (DO) concentration was found to fall below an acceptable level after wastewater was discharged into a receiving water environment (Henze et al., 2008). This was one of the

key concerns and the driving force behind the increase in the number of studies aimed at developing new wastewater treatment technologies for decreasing the organic load.
While most of the attention was on the removal of organics, a new problem appeared in the 1960s. As a result of the increase in the discharge of urban and industrial wastewater to surface water bodies as well as the increasing agricultural activity, eutrophication emerged. Eutrophication can be defined as the nutrient enrichment (mainly with nitrogen and phosphorus) in the surface waters resulting in a growing population of algae and other water plants (Henze et al., 2008; Andersen and Conley, 2009). Since eutrophication had deteriorated many aquatic environments in the second half of the 1900s, research in wastewater treatment technology development found a new direction; i.e. to decrease the nitrogen and phosphorus content of the treated wastewater to be discharged.
Anaerobic treatment appeared to be the next big step in the wastewater treatment process development area. Considering the energy related problems of the late 1900s; anaerobic treatment became a popular alternative for treatment of wastewater for several reasons: (1) it requires less energy for operation mainly because of lack of aeration; (2) it produces less sludge; (3) as a result of the anaerobic destruction of the organic material methane is produced which is a potential energy source; and, (4) it can be operated in smaller reactors (McCarty, 1964).

2.1.2 Contemporary phase of development

The contemporary phase of development was initiated with the stricter effluent limit values put forth by both emission and immission based regulations in the USA and EU. For example, in the European Union (EU), the Water Framework Directive (Directive 2000/60/EC) regulates the ecosystem by setting quality objectives, while the effluent urban wastewater quality is controlled by the Urban Wastewater Treatment Directive (91/271/EEC). A wide range of parameters were included in different regulations covering both water and sludge disposal, i.e. organics, nutrients (total nitrogen content of the effluent wastewater should be as low as 10 mg N/L while this value is 1 mg P/L for total phosphorus as regulated in 91/271/EEC), pathogens, heavy metals, emerging contaminants etc. This resulted in the development of new treatment technologies as well as new process flow diagrams for WWTPs.
The number of available alternative technologies using physical, chemical and biological means of treatment has thus increased considerably in order to satisfy the high removal efficiencies required by the stricter regulations. Several configurations of different biological processes (Bardenpho, UCT, A2O, etc. with more than 10 configurations most commonly used in Europe (Benedetti, 2006)) and other processes like UASB, MBR etc. are increasingly used.

2.1.3 Recent developments and innovative approaches

Current trends are often used to shape the possible future conditions. In that sense, it has been more noticeable that the wastewater industry faces many new challenges such as

increasing energy costs, presence of trace organics which has become more critically investigated, depletion of the resources, water conservation as well as more stringent regulations (Reardon et al., 2013). As a result, domestic wastewater is now being considered more as a resource than as a waste with the recovery possibilities for clean water, energy and various materials (primarily nitrogen and phosphorus as plant fertilizers) satisfied by novel approaches and emerging technological developments (McCarty et al., 2011).

Economics, i.e. mainly operational and capital cost for the treatment facilities, has always been a key parameter when making decisions on which treatment methods and technologies to be applied. As a consequence of the fact that wastewater treatment plants are significant energy consumers, principally for aeration, mixing, pumping, sludge disposal etc., together with the rising energy costs and concerns and restrictions on emissions of greenhouse gases; wastewater specialists focus more on effective energy management and alternative energy strategies. Current initiatives include increasing the biogas production (e.g. Yadvika et al., 2004; Weiland, 2010), managing oxygen demand by controlling oxygen concentration (e.g. Åmand et al., 2013) or by decreasing the oxygen demand of the microbial activities (e.g. Partial nitritation described in Hellinga et al., 1998 and anaerobic ammonium oxidation described in Mulder et al., 1995) as well as controlling the equipment for efficient power use (Reardon et al., 2013). Moreover, the increasing construction cost and decreasing space availability stimulated the development and use of more compact systems which require less footprint (for instance, biological aerated filters (Mendoza-Espinoza and Stephenson, 1999) and granular activated sludge (de Kreuk et al., 2005; Giesen et al., 2013)).

A major necessity in wastewater treatment is the removal of nutrients – especially nitrogen and phosphorus – to acceptable limits prior to discharge. For instance, increased nitrogen limitation in the regulations for the WWTP effluents gave rise to development of innovative nitrogen removal technologies mostly used for nitrogen rich streams resulting from sludge treatment (Lackner et al., 2014). On the other hand, there are also recent developments for recovering phosphorus in the form of struvite (Le Corre et al., 2009) and research is still going on for assimilating excess nutrients by making use of microalgae as well (Cai et al., 2013).

Hence both the multi-criteria nature of the decision-making process and the large number of alternatives of wastewater treatment technologies bring us to the question ‘How do we take strategic decisions on the wastewater treatment technologies and process networks to choose for a given wastewater treatment project?’

2.1.4 Mathematical programming in a wastewater engineering context

Mathematical models have been used in the wastewater treatment area for the purpose of design, control and research. In wastewater treatment plants, one of the most widely used treatment technologies is the activated sludge (AS) process. Recently, the AS process has developed into a more complex process by expanding from AS for removal of organics

to AS including nitrification, denitrification and phosphorus removal (Tchobanoglous, 2003). These reactions are carried out by different microorganism groups, which function under different environmental conditions, with different reaction rates, oxygen/nitrate consumptions and sludge productions. Moreover, wastewater is known to be a complex medium containing many different components which can be divided into soluble, particulate, biodegradable and non-biodegradable fractions. In that sense, mathematical modeling provides a useful tool to deal with a large number of components and reactions as well as varying environmental conditions (i.e. oxygen concentration, pH, temperature etc.). The Activated Sludge Models (ASM1, ASM2, ASM2d and ASM3) were developed by the IWA Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment and they deal with the simulation of AS type of processes (Henze et al., 2000). ASM1 is the first developed model and it incorporates carbon oxidation, nitrification and denitrification through modelling the activities of the heterotrophic and autotrophic microorganisms. ASM2 and ASM2d constitute a comprehensive mathematical model for dynamic simulation of combined biological processes for organics, nitrogen and phosphorus removal with many more components and reactions defined and some modifications made in addition to ASM1. In an effort to build further on the ASM1, the ASM3 was developed by the same task group to incorporate more mechanistic knowledge about microbial growth and storage of intracellular products, among others.

Recently, the wastewater treatment modelling community has focused on extending the activated sludge models and their benchmarking applications (e.g. Benchmark Simulation Model no. 1 and 2 – BSM1 and BSM2 (Gernaey et al., 2014)) by the addition of different phenomena such as formation of N_2O (Hiatt and Grady 2008) and occurrence and fate of micropollutants (Snip et al., 2014) in activated sludge systems. While the activated sludge models are used for suspended growth biological treatment processes; biofilm type of systems were also modeled with a different approach where space is introduced as an independent variable (Wanner et al., 2006; Vangsgaard, 2013).

Activated sludge models can be used to simulate a wide range of treatment configurations of the AS type; furthermore, mathematical modelling is also used to simulate other types of technologies. For instance the Anaerobic Digestion Model no.1 (ADM1) is a simulation model to cover the biochemical and physicochemical processes in anaerobic digesters (Batstone et al., 2002) and a dynamic model to represent the clarification-thickening processes was developed by Takacs et al. (1991).

Besides the effective use of current mathematical models in the wastewater engineering area, there is a need for simpler models when using mathematical programming for optimization purposes. This is especially relevant when the size of the optimization problem is large, which is determined by the number of alternative technologies, components, reactions etc. It is important that the resulting optimization problem can handle the complexity of the treatment unit models. In that sense it is necessary to develop

and use simpler models; an example can be the steady state mass input-output type of models, which is the type also developed and used within the context of this study.
To conclude, with all the recent developments in the wastewater modelling area, today's models can be considered as important tools for researchers and design engineers not only to consider many different design aspects (e.g. different phenomena, many components, effect of time, temperature, pH etc.) at the same time, but also to save time and money in the frame of the development of improved wastewater treatment options.

2.2 Wastewater treatment process selection and synthesis

2.2.1 Importance of process selection and synthesis

The process selection procedure is a collective effort of many parties evaluating various factors. The stakeholders are individuals and groups such as wastewater engineers, plant operators as well as the community that will be served by the treatment services; and they clearly play an essential role, directly or indirectly, in process selection (Daigger, 2005). They have interests in different aspects of the decision making procedure; for example they can either be the financers of the project or the planners of the WWTP; they can as well be the governmental authorities defining the related regulation, companies supplying their products for the construction and operation of the WWTP, or the public to be served with the planned WWTP. While the financers try to keep the subsidies at a minimum level and users demand for low user fees; the authorities takes mostly the side of implementing Best Available Techniques (BAT) (Starkl and Brunner, 2004). Therefore, despite the conflicting priorities among the involved parties; the selected process network alternative should be acceptable for all the parties in terms of legislative, environmental, social and economic aspects.

As stated in the previous section, the perception of wastewater treatment has always been influenced by health and environmental concerns. In the course of wastewater treatment development, the objectives of the overall treatment system have shifted from hygienic concerns to environmental protection; the latter then further widened to include the aim of environmental impact minimization (Starkl and Brunner, 2004).

When the receiving surface water bodies were integrated to the overall wastewater treatment system, the concerns regarding their quality started to shape the wastewater treatment processes. The low DO concentrations and risk of eutrophication in the surface waters led the way to development of new wastewater treatment processes so as to decrease the C, N and P content of the wastewater to the desired levels. Moreover, more recently, due to problems like global warming, acidification, ozone layer depletion, occurrence of micro-organic pollutants as well as the reduction of important resources like phosphorus, potassium and fossil fuels; a new insight was added to wastewater treatment process developments (Jenssen et al., 2007). The establishment of energy producing processes on the WWTP and the possibility of resource recovery from industrial and domestic wastewaters are now more and more on the agenda.

All the above mentioned concerns resulted in a considerable number of available wastewater treatment processes. The biological processes mostly result in efficient removal of organic matter. They are designed also to remove nitrogen to a great extent. Phosphorus removal results in phosphorus rich solids, but there are also technologies to recover it from sludge. The compact systems enable reductions in the construction costs significantly whereas the burdens of operational costs are reduced by the use of energy producing processes.

The treatment processes of physical, biological and chemical nature should be chosen and the network of processes should be determined carefully so that the resulting WWTP process network would not only be able to treat the wastewater to the desired quality but also would adequately take the sustainability related considerations into account. This brings us to the importance of early stage decision making while attempting to select the most suitable WWTP configuration for a given wastewater composition.

2.2.2 Different approaches for wastewater treatment process selection and synthesis

Currently, the early stage decision making for WWTP design is mainly based on expert decisions and previous experiences (Tchobanoglous, 2003). This approach takes values like environmental issues, water reuse, by-product recovery (if possible) and public impacts into account and identifies the alternatives based on experience, similar existing solutions and brainstorming to come up with the most viable WWTP network (Daigger, 2005). However, with the increased complexity of the technologies and stricter limit values for effluents, making the most feasible decision using this approach is expected to become harder and harder.

An alternative approach is to cast the decision problem using mathematical programming which has been an active research area in chemical process synthesis (Grossmann, 2005). There are numerous studies using this approach in water network design problems in different industries as well as design of combined water networks and wastewater networks (e.g. Takama et al., 1980; Bagajewicz and Faria, 2009; Karuppiah and Grossmann, 2006). This approach has also been used for applications in the wastewater treatment field. For example, Galán and Grossmann (2011) formulated a MINLP problem to select among the BATs for a given set of contaminants mostly of industrial origin. The goal of their study was to select a subset of BATs in the design space and the consequent distribution of the flow rates in order to efficiently treat the wastewater with respect to several criteria such as: minimum flow rate through BATs and minimum cost. It is noted as well, however, that the aforementioned study used a fictitious and rather simple definition of the industrial wastewater characteristics and treatment options. Rigopoulos and Linke (2002) and Linke and Kokossis (2003) applied the stochastic optimization for activated sludge process design by applying the optimization-based synthesis technology for reaction/separation networks where they aimed at minimizing the carbon and nitrogen in the effluent stream. A conceptual design methodology combining a hierarchical design procedure with mathematical modelling was studied by Vidal et. al. (2002) where alternative WWTP designs were evaluated with respect to a set of criteria using mathematical modelling. In another study, process configuration and equipment dimensions of activated sludge systems with simultaneous carbon and nitrogen removal (Alasino et. al., 2007) and carbon, nitrogen and phosphorus removal (Alasino et. al., 2010) were optimized where they formulated the problem as a nonlinear programming problem (NLP) and solved by using GAMS. All of the studies have either focused on

optimizing a given treatment process or selecting from a limited number of alternative candidates. Hence these studies have not dealt with the increasing number of processes and unit operations in wastewater treatment processes. This in turn limits their applicability for early stage decision making on industrially relevant and realistic problem formulations which is the scope of this thesis. Among others one needs a systematic approach to manage the database and the resulting complexity of the MINLP problem formulation, its solution and analysis under uncertainties.

3 FRAMEWORK FOR SYNTHESIS, DESIGN AND RETROFIT OF WWTP LAYOUTS

In this chapter, the superstructure optimization based framework for synthesis, design and retrofit of WWTP layouts is presented. The framework consists of six steps, which are explained generically below along this chapter. The first three steps of the framework constitute the base formulation of the problem, where the problem is defined, the superstructure (i.e. the design space) is generated and the data collection and model generation is done. In the second part, the optimization problem is solved under deterministic conditions and uncertainty prior to a detailed design of the optimum process network. The developed framework together with different example case studies was presented in Bozkurt et al., (2014) and Bozkurt et al., (2015a).

A superstructure based optimization framework was developed and evaluated successfully for various network design problems including soybean oil processing, biorefineries, oil refinery wastewater treatment etc. (Quaglia, 2013). In this chapter, the individual steps of the framework, which has been modified, adapted and used in this study in the context of WWTP design and retrofit problems, are presented. The framework is illustrated in Figure 3.1. The framework consists of six steps and results in the optimal solution for the network design. It contains a superstructure method for representing the design space and a systematic method for data collection and modelling of the treatment alternatives, which further enables effective formulation and solution of a MI(N)LP problem under both deterministic conditions and uncertainty.

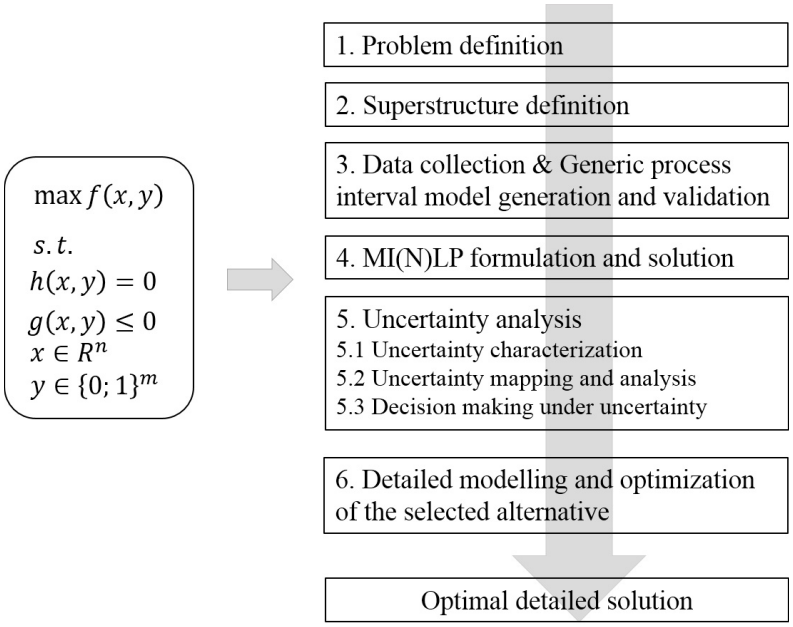


Figure 3.1 Framework for the superstructure based optimization methodology

3.1 Step 1. Problem definition

The first step in the framework is where the scope of the problem is defined. In this step, the boundaries of the design problem are defined such that the wastewater characterization and the effluent limit definitions are made. Additionally, the objective function of the optimization problem is selected. In this step of the framework, the principal factors to be considered while designing and/or retrofitting a WWTP are identified. In other words, the main expected outcomes of the project have to be listed. Generally, the objective of a design project is to treat the wastewater with the lowest possible cost while satisfying the effluent limitations for individual contaminants. In addition to that, several aspects might be considered on top of that during early stage design studies prior to process selection. With the recent changes in the wastewater treatment trends, designing a treatment plant with lower energy consumption, higher efficiency in terms of particularly nutrient removal, higher potential of nutrient and energy recovery and lower greenhouse gas emissions has become significantly more important. Therefore, at this stage all these considerations, which affect the solution of the problem, are investigated in order to be further modelled and added into the optimization problem as constraints or in the objective function formulation. Moreover, at this stage, the problem is identified being either a design or a retrofitting problem.

3.2 Step 2. Superstructure definition

The second step comprises the definition of a superstructure consisting of different wastewater sources, tasks for water and sludge treatment together with sinks and process alternatives for the defined tasks. A superstructure, as shown in Figure 3.2, is a compact representation of different process alternatives (i.e. treatment technologies in the wastewater treatment case). Process steps, which are represented in the columns of the superstructure, comprise wastewater sources and sinks for the effluent streams (effluent water, sludge, by-products etc.) as well as different tasks to be carried out throughout the network in order to establish the wastewater and sludge treatment network in between sources and sinks. In each process step, in the rows of the superstructure, alternative treatment process intervals (e.g. separation – primary clarifier, secondary clarifier, membrane reactor etc; or reaction – activated sludge for C, N and P removal, anammox, anaerobic digestion etc.) responsible for a specific task are placed. The superstructure definition is finalized by defining the feasible connection streams between treatment tasks.

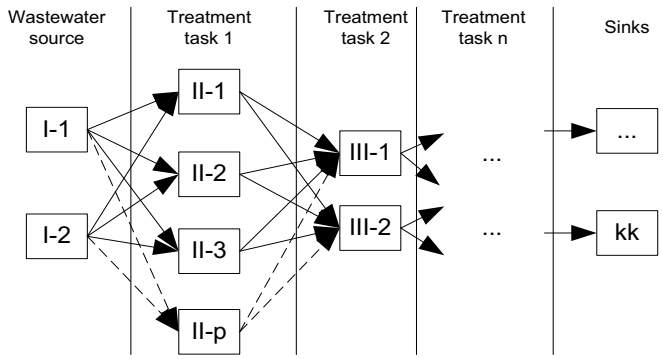


Figure 3.2 A representative superstructure for wastewater treatment networks

There are three different ways of constructing a superstructure. One of the methods is *alternative collection*, in which all known WWTP network configurations are arranged in a superstructure representation. The resulting superstructure includes the known configurations and enables only to screen among the known candidates, which does not allow the selection of innovative technologies or configurations. The second approach is the *method of combinatorial synthesis*. In this approach, the superstructure is composed of all treatment technologies placed under the relevant task connected to the others in every possible connection way (Figure 3.2 is an example of a full combinatorial superstructure). This approach results in a very large search space and might contain redundant configurations. A third approach is called the *insight-based approach*, which

is used in this study. The latter approach takes into account expert knowledge to include the well-known configurations together with the innovative technologies and configurations in the superstructure, as well as eliminating the unfeasible and non-convenient alternatives and connections (Quaglia et al., 2014). At this point, the selection of technologies to be placed in the superstructure and the connections between the alternatives are defined by design experts with a prior screening procedure.

3.3 Step 3. Data collection & Generic process interval model generation and validation

3.3.1 Data collection and design of individual treatment technologies

The purpose of this step of the framework is collecting the necessary design data for the treatment technologies to be placed in the superstructure. To this end, a systematic data collection and design procedure is used which is illustrated in Figure 3.3.

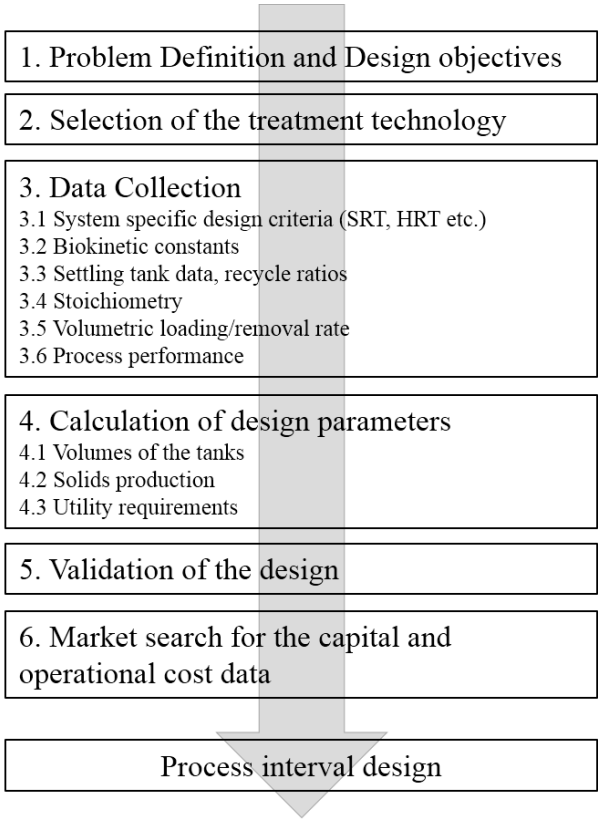


Figure 3.3 Illustration of the systematic data collection and design procedure

After defining the characteristics of the wastewater or sludge stream to be treated, the target concentrations to be achieved in the effluent and the design temperature are determined. This comprises the first step in the workflow and is followed by the selection of the treatment technology to be further designed. The next phase is the collection of system specific data and information about the specified treatment technology such as; sludge retention time (SRT) and hydraulic retention time (HRT), temperature dependent biokinetic constants, settling data and recycle ratios if applicable, stoichiometry information for the reactions together with volumetric loading and/or removal rates and

process performances in terms of removal efficiencies of the key contaminants. Here, the treatment technologies are designed at fixed temperature, at their optimality and at steady state by fixing the design parameters (SRT, HRT, efficiencies etc.) rather than optimizing them; later in a second step, more rigorous models can be used for optimization once the number of alternative technologies is reduced. This two-tiered approach for optimization is chosen on purpose to manage the complexity of the optimization problem which becomes otherwise intractable. The output from the design includes volumes of the units, utility consumption (electricity, chemicals, aeration etc.) and sludge production data which are used to calculate the capital and operational costs. The design algorithms were implemented in Matlab® scripts to automate this step and ensure consistency and reproducibility. An example Matlab® script for design of biological nutrient removal (BNR) systems is given in Appendix 2. The procedure is iterative; i.e. the SRT and HRT, which are reported as a range in the literature, are modified until converging to a solution satisfying all constraints (effluent requirements, minimum capital and operational cost etc.). When the steady state design is finalized, the design parameters and performance values are compared with the steady state results obtained from a simulation carried out using a rigorous model. For this purpose, Activated Sludge Model No.1 (ASM1) is used (Henze et al., 2000). In this way, the design for treatment alternatives is considered to be validated against a more rigorous model. Finally, the cost data for utilities, electricity, products and construction of the treatment units are collected from the open literature. The data collection and design methodology for individual treatment alternatives is detailed in section 4.1.

3.3.2 Generic process interval model generation and validation

Each process interval in the superstructure is structured using a generic model which is illustrated in Figure 3.4.

The generic model is composed of a number of phenomena namely: mixing of all the flows entering the interval and the utilities added, reaction, flow separation, waste separation and phase separation. Thus, the process interval can perform as a combination of different units (reaction and separation with external and internal recycle flows) as well as a simple reactor with one inlet and one outlet.

Using the generic model, the treatment alternatives are described based on input-output mass balances. The flow of components is represented in mass flux units (M/t) whereas the total flow rate of the stream is given in volumetric flow rate units (L^3/t). Below, the definition of all the phenomena existing within the generic process interval and the associated mathematical model are explained. Moreover, the logical model and economic models are described. It is important first to explain the indexes used in the mathematical formulation; their definitions are given in Table 3.1.

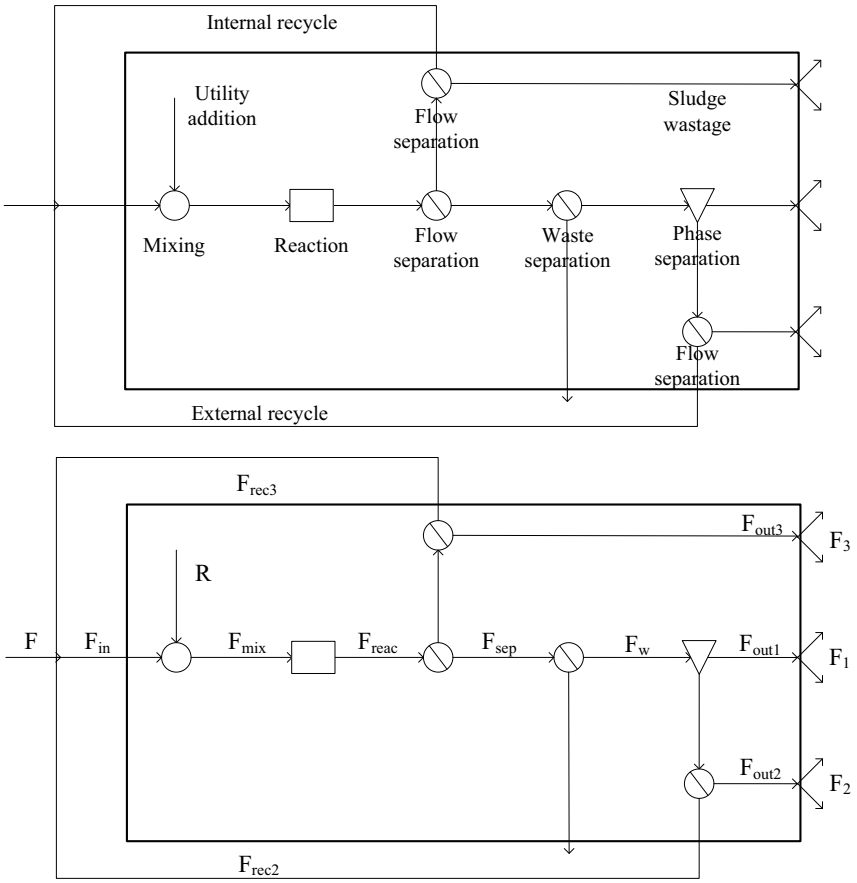


Figure 3.4 Generic process interval structure: definition of phenomena (above), flow definitions of mass input-output model (below)

Table 3.1 Index definitions

Index	Definition
i, ii	Component index
k, kk	Process interval index
rr	Reaction index
react	Reactant index

Mixing

First, the streams entering the process interval are mixed together with the utilities added. Equation 3.1 represents the mixing of all different influent flows originating from the previous process intervals (*k*) to the process interval of interest (*kk*) - $F_{i,k,kk}$ as well as the internal and external recycle streams $F_{i,kk}^{rec2}$ and $F_{i,kk}^{rec3}$. Then the sum of influent flows - $F_{i,kk}^{in}$ is mixed with the utility added - $R_{i,kk}$ to give the flow after mixing - $F_{i,kk}^{mix}$ in equation 3.2 (where $0 \leq \alpha_{i,kk} \leq 1$).

$$F_{i,kk}^{in} = \sum_k F_{i,k,kk} + F_{i,kk}^{rec2} + F_{i,kk}^{rec3} \quad 3.1$$

$$F_{i,kk}^{mix} = F_{i,kk}^{in} + \alpha_{i,kk} * R_{i,kk} \quad 3.2$$

Utility addition

The utility flow - $R_{i,kk}$ is calculated by equation 3.3 where $\mu_{i,ii,kk}$ is given as daily mass of utility added divided by the mass flow of the corresponding component entering the process interval.

$$R_{i,kk} = \sum_{ii}\left(\mu_{i,ii,kk} * F_{ii,kk}^{in}\right) \quad 3.3$$

Reaction

The reaction in the generic process interval is defined so that the key reactant(s) is/are converted to the other components with a given conversion efficiency by using the utilities added, while maintaining the overall mass balance within the boundaries of the process interval. The reaction equation (3.4) calculates the flow after reaction - $F_{i,kk}^{reac}$; the key reactant(s) is/are removed with the specified conversion efficiency - $\theta_{react,kk,rr}$ and the other components are produced or removed according to the defined stoichiometry - $\gamma_{i,kk,rr}$.

$$F_{i,kk}^{reac} = F_{i,kk}^{mix} + \sum_{rr,react}\left(\gamma_{i,kk,rr} * \theta_{react,kk,rr} * F_{react,kk}^{mix}\right) \quad 3.4$$

Flow separation

This type of separation is implemented in several parts of the generic process interval. It represents the separation of the stream into two different streams of the same composition. It is employed for three different purposes (represented by equations 3.5, 3.6 and 3.7): separation of the flow for internal recycle, sludge wastage (provided that the sludge is wasted from the reactor) and separation of the settler underflow stream for external

recycle. In the below equations SP_1, SP_2 and SP_3 are separation fractions and are fixed to have a value between 0 and 1.

$$F_{i,kk}^{sep} = F_{i,kk}^{reac} * SP_{kk}^{1} \quad 3.5$$

$$F_{i,kk}^{rec3} = \left(F_{i,kk}^{reac} - F_{i,kk}^{sep}\right) * SP_{kk}^{2} \quad 3.6$$

$$F_{i,kk}^{rec2} = \left(F_{i,kk}^{w} - F_{i,kk}^{out1}\right) * SP_{kk}^{3} \quad 3.7$$

Waste separation

In the case of generation of an unwanted component after reaction, it can be sent out of the system by waste separation (given in equation 3.8). This stream is not directed to any other process interval. This separation can also be used to represent the release of the gases produced in the reactor in open systems. The parameter $W_{i,kk}$ defines the fraction of the corresponding component to be wasted with the $F_{i,kk}^{w}$ stream.

$$F_{i,kk}^{w} = F_{i,kk}^{sep} * W_{i,kk} \quad 3.8$$

Phase separation

Phase separation functions as a separation unit (e.g. sedimentation, membrane separation). Here the flow is separated into two different streams of different composition. The parameter $split_{i,kk}$ is defined individually for every component *i* and has a value between 0 and 1.

$$F_{i,kk}^{out1} = F_{i,kk}^{w} * split_{i,kk} \quad 3.9$$

Once the outlet streams - $F_{i,kk}^{outX}$ are defined (X: 1, 2, 3; representing three different outlet streams), the flow is directed to the next process interval(s) by equation 3.10. The direction of the flow leaving the process interval is determined by the parameter $S_{k,kk}$ which contains superstructure information and is defined before in the superstructure development step. Its value is equal to 1 if the connection between two process intervals (*k* and *kk*) is present and 0 otherwise.

$$FX_{i,k,kk} \leq F_{i,kk}^{outX} * S_{k,kk} \quad 3.10$$

Activation and logical constraints

If a process interval is selected by the optimizer, then the binary variable assigned to it - y_{kk} is equal to 1, if it is not selected then it is equal to 0. This is only possible by defining activation and logical constraints shown in equations 3.11 and 3.12, respectively. The

activation constraint defines the upper and lower boundaries for a variable - x_k and the equation satisfies that if the specific process interval is selected the variable is bounded by the specified boundaries. If the process interval is not selected, the value of the variable is assigned as 0. The logical constraint on the other hand represents the selection of the process intervals. Accordingly, among the process intervals belonging to the same task, only one can be selected and the others are eliminated from the solution.

$$y_{kk} * x_k^{LO} \leq x_k \leq y_{kk} * x_k^{UP} \quad 3.11$$

$$\sum_{kk} y_{kk} \leq 1 \quad 3.12$$

Definition of the wastewater characterization

The mass flow rates of the components in the influent are assigned into the corresponding process interval placed in the sources column by the following equation, where $\phi_{i,kk}$ is the matrix containing wastewater characterization information. This equation is coupled with a condition that it is only valid for the process intervals placed at the sources column.

$$F_{i,kk}^{w} = \phi_{i,kk} * y_{kk} \quad 3.13$$

Effluent limit definition

The equation 3.14 ensures that the effluent limits are satisfied in the sink intervals for defined components. $Lim_{i,kk}$ is the limit value defined for the component *i*. Similar to the previous equation, the limit definition is only valid for the specified process intervals placed at the sinks column.

$$Lim_{i,kk} \geq \sum_f F_{i,kk}^{in} \quad 3.14$$

Economic models

The objective function, which is to be minimized, is defined as the total annualized cost (TAC) and comprises the operational costs (OPEX) and capital cost (CAPEX) of the treatment units. Below, in the equations from 3.15 to 3.19, formulations of different components of OPEX and CAPEX are shown together with the objective function in equation 3.20.

$$OPEX = U_{cost} + S_{cost} - P_{cost} \quad 3.15$$

$$U_{cost} = \sum_i P2_i \sum_{kk} R_{i,kk} \quad 3.16$$

$$S_{cost} = P3_{kk} \sum_i F_{i,kk}^{in} \quad 3.17$$

$$P_{cost} = P3_{kk} * F_{i,kk}^{reac} \quad 3.18$$

$$CAPEX = \sum_k V_k * P1_k * y_k \quad 3.19$$

$$OBJ = OPEX + \frac{CAPEX}{t} \quad 3.20$$

Where; U_{cost} is the utility cost, S_{cost} is the cost related to the sink intervals, P_{cost} is the product cost, V_k is the volume of the unit, t is the project lifetime and *P1*, *P2* and *P3* are the parameters representing the related unit cost for the components or process intervals. One of the most challenging steps in optimization based approaches is the resulting mathematical complexity of formulating and solving the optimization problem. In order to manage this complexity and facilitate effective formulation and analysis of the problem, a separation principle was used that separates the database needed for model parameters from the MI(N)LP formulation and solution in GAMS. The procedure is as follows:

Once the data have been collected for all the process intervals, they are stored as matrices in an MS Excel based structure. The data in the matrices are sent to GAMS by using GDX (GAMS Data Exchange) utilities. GDXXRW is used in this respect, which is the utility responsible for reading from and writing to an MS Excel spreadsheet. Once the data are transferred to GAMS, the formulated MI(N)LP problem, consisting of the generic equations defined above, is solved. Note that when a new problem is defined, only the database needs to be changed, while the generic MI(N)LP model can still be used. The data flow and problem formulation (partly as a screenshot) can be seen in Figure 3.5.

The generation of the optimization problem parameters and their structuring prior to be sent to the optimizer are explained in more detail in section 4.2.

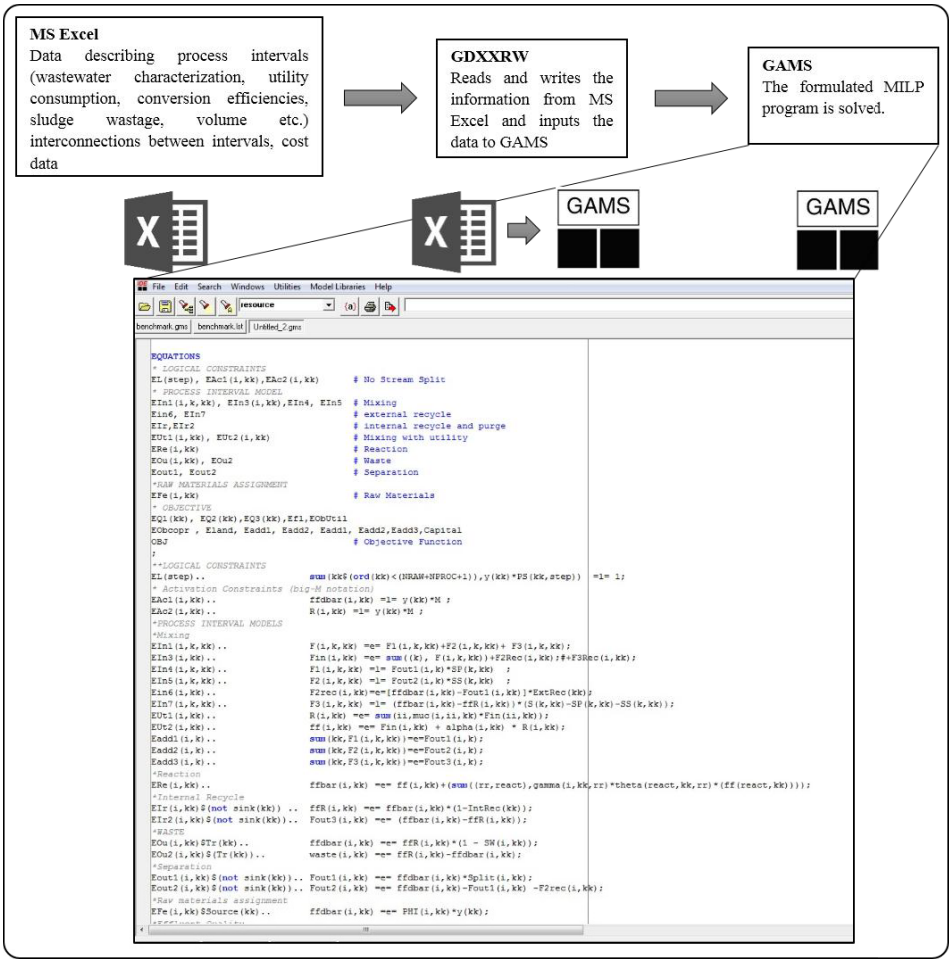


Figure 3.5 Illustration of the generic and reusable MI(N)LP formulation in GAMS

3.4 Step 4. MI(N)LP formulation and solution

The superstructure optimization problem is formulated as a Mixed Integer (non)Linear Programming (MI(N)LP) problem as shown in equations 3.21 – 3.26.

$$min_{x,y}\ f(x,y) \tag{3.21}$$

subject to;

$$g(x,y)\ \geq 0 \tag{3.22}$$

$$h(x,y) = 0 \tag{3.23}$$

$$x\ \in X \tag{3.24}$$

$$x_{LO} \leq x \leq x_{UP} \tag{3.25}$$

$$y \in \{0;1\}^n \tag{3.26}$$

The formulation of the MI(N)LP problem and its deterministic solution take place in the fourth step of the synthesis, design and retrofit framework. The solution of the optimization problem results in the optimal network, the fate of pollutants/components throughout the selected treatment network and the value of the objective function together with the cost breakdown into the components of the objective function (i.e. utility cost, product cost, capital cost etc.). With respect to the nature of the problem, the optimization problem can result in a linear (MILP) or non-linear (MINLP) formulation.
In this step, the MI(N)LP problem is formulated and solved. The models represent the mass input-output model for each treatment technology (i.e. each process interval in the superstructure), process constraints, structural constraints, effluent limit constraints, and economic models together with the objective function. The adapted MI(N)LP formulation for the specific case of a WWTP design/retrofit study is described below with the equations 3.27 – 3.30.

$$\text{Min } OBJ = \sum_{kk} OPEX_{kk} + \frac{CAPEX_{kk}}{t} \tag{3.27}$$

subject to;

$$h\left(\alpha_{i,kk}, \mu_{i,ii,kk}, \gamma_{i,kk,rr}, \theta_{react,kk,rr}, W_{i,kk}, Split_{i,kk}, rec_{kk}\right) = 0 \tag{3.28}$$

$$g\left(S_{k,kk}\right) \leq 0 \tag{3.29}$$

$$\sum_{kk} y_{kk} \leq 1 \quad \text{where} \quad y \in \{0;1\}^n \tag{3.30}$$

3.5 Step 5. Uncertainty analysis

Uncertainty analysis is performed in order to be able to comment on the robustness of the deterministic solution and further to generate more robust solutions, if needed. It is also important to show that the selected network is feasible over the whole uncertain domain defined with respect to uncertain input parameters. In wastewater treatment plant design studies, there are a number of uncertain parameters that have to be taken into account. The common practice is to lump the individual uncertainty sources into safety factors, which often results in overly conservative designs (Belia et al., 2009). In order to maximize efficiency and avoid excessively sized plant designs, different individual sources of uncertainty are evaluated in uncertainty analysis, moving away from lumped safety factors. This is only possible by evaluating the design/retrofit problem under uncertainty. The uncertainty analysis is performed in three different steps, which are defined in detail below.

3.5.1 Uncertainty characterization

Selecting the uncertain data

This step is where the design expert, among all the input data of the superstructure optimization problem, selects the uncertain data and identifies their uncertainty domain. Input data in wastewater treatment plant design studies are highly uncertain especially due to two reasons: (1) Wastewater is produced as a result of daily domestic and industrial activities, and therefore the amount and composition is highly variable; (2) WWTPs are designed for long operating time horizons (years) which results in the change of many parameter values, especially the market values over the design lifetime. More specifically for instance, the composition of the wastewater - ratio of COD and nitrogen fractionations, flow rate etc. - is highly uncertain over time (daily and seasonally) and this uncertainty has to be taken into account during design studies. Similarly, the effect of changing temperature on kinetics, cost data (i.e. electricity price, landfill tax etc.), equipment performances (for instance, oxygen transfer efficiency due to diffuser performance) over the lifetime of the project and limit values for the effluent concentrations of specific contaminants might also be examples for sources of uncertainty in WWTP design/retrofit studies. This selection is highly subjective and depends on the users'/experts' priorities.

Defining the uncertain domain

In this step, the domain of uncertainty is defined with respect to the uncertain parameters. After selecting the probability density function for the distribution of the individual uncertain parameters – normal distribution, uniform distribution etc. - their probability

distribution is defined with their minimum, maximum and mean values recorded in the database. If there is a correlation between the uncertain parameters, it is defined in terms of covariance between the probability distributions and stored in the database as well.

Sampling the uncertain domain

The uncertain domain defined in the previous step is sampled to perform Monte Carlo simulations. By means of sampling the uncertain domain, a selected number of future scenarios are generated assuming different realizations of uncertain parameters. The sampling technique used in this step is Latin Hypercube Sampling (LHS) (Iman and Conover, 1982) with its effective coverage of the uncertain domain.

3.5.2 Uncertainty mapping and analysis

This step covers the deterministic mathematical formulation of the optimization problem solved for the realization of the uncertain future scenarios. In other words, the data sets for the uncertain scenarios created in the previous step as a result of the sampling procedure are given to the deterministic optimization problem (formulated in step 4) as input data and the solution is repeated for the number of future scenarios defined. Therefore, the result is a distribution of outputs; i.e. selected networks, objective function values etc.

These results reveal, for each different future scenario, the resulting topology and other related information about the treatment plant network such as: annual operational cost, capital cost and effluent water characterization. Therefore, this analysis is important to understand the effect of uncertainty on the problem solution by showing the user how the outputs can vary in the future with the possible realization of a change in the input conditions.

3.5.3 Decision making under uncertainty

In the final step of the uncertainty analysis, the optimization problem is formulated as shown below in equations 3.31 – 3.38. Here, the optimization problem is formulated as a two stage stochastic programming problem and the indexes *I* and *II* correspond to the objective function components related to the first and the second stage. While in the first stage, exact values (i.e. realization) of the uncertain data is unknown, in the second stage it is known and corrective actions are taken accordingly in order to find a network and operation conditions, which are feasible over the whole uncertain domain (Quaglia, 2013). In the equations below, Θ represents the uncertain data and $E_{\Theta}\left(f_{II}(x_I, x_{II}, y, \Theta)\right)$ represents the expected value of the objective function within the uncertain domain.

The expected value of the objective function is calculated by solving it using the sample average approximation (SAA) technique (Birge and Louveaux, 1997). While formulating SAA, the constraints are converted into a number of equations which is determined by

the number of uncertain scenarios defined previously (i.e. NS- number of samples), which consequently increases the size of the optimization problem, thus its complexity. Consequently, the objective function value is calculated by averaging the sum of all the values obtained for different uncertain scenarios.

$$min_{x,y} f_I(x_I, y) + E_\Theta\big(f_{II}(x_I, x_{II}, y, \Theta)\big) \quad 3.31$$

subject to;

$$g(x_{II}, y, \Theta) \geq 0 \quad 3.32$$

$$h(x_{II}, y, \Theta) = 0 \quad 3.33$$

$$p(x_I, x_{II}, y, \Theta) \geq 0 \quad 3.34$$

$$q(x_I, x_{II}, y, \Theta) = 0 \quad 3.35$$

$$x_{LO} \leq x \leq x_{UP} \quad 3.36$$

$$y \in \{0; 1\}^n \quad 3.37$$

$$\Theta \in [\Theta_{LO}, \Theta_{UP}] \quad 3.38$$

In order to summarize the results of the uncertainty analysis, several indicators are defined (Birge and Louveaux, 1997; Quaglia, 2013): Expected value of perfect information (EVPI), value of stochastic solution (VSS) and uncertainty price (UP).

The EVPI represents the expected increase in the objective function resulting from uncertainty. When the EVPI is large (as compared to the value of the deterministic objective function), the designer is expected to work more on the design phase; a low EVPI, on the other hand, indicates that the current design can move further the project development stages. The formulation of EVPI is shown in equation 3.39.

$$EVPI = min\Big(E_\theta\big(f(x, y, \theta)\big)\Big) - E_\theta\Big(min\big(f(x, y, \theta)\big)\Big) \quad 3.39$$

In the VSS calculation, the difference between the performance of the selected network (in the deterministic solution) under uncertainty conditions (i.e. solution of uncertainty mapping step by fixing the binary variables with the deterministic network selection) and the solution of the problem under uncertainty is calculated. This indicator shows the possible gain from solving the stochastic optimization problem and is formulated as shown in equation 3.40.

$$VSS = E_\theta\big(f(x_{det}, y_{det}, \theta)\big) - min\Big(E_\theta\big(f(x, y, \theta)\big)\Big) \quad 3.40$$

Finally, the UP, as shown in equation 3.41, indicates the cost of uncertainty by calculating the difference between the objective function values of the solution under uncertainty and the deterministic solution.

$$UP = min\left(E_\theta\big(f(x,y,\theta)\big)\right) - min\big(f(x,y)\big) \quad 3.41$$

3.6 Step 6. Detailed modeling and optimization of the selected alternative

The last step of the framework is where the detailed design of the selected alternative is done through modeling and optimization. It was mentioned earlier that in the context of the optimization based solution approach for the early stage design/retrofitting problem, to allow the user to consider many alternatives at the same time, simple mass input-output models have been used together with steady state design of individual technologies at fixed temperature, at their optimality at steady state by fixing the design parameters. This approach facilitates not only to manage the complex decision making problem but also to cover a large design space. Therefore, in a separate step of the framework, once the optimal network selection is done by the optimizer; the selected network is designed in a more detailed manner. This can be done through optimizing the design parameters as well as by making use of commercial wastewater treatment simulators such as WEST etc. When the selected network is designed and its effectiveness is validated, it can move further through the project development stages.

4 DATA COLLECTION, DESIGN AND GENERIC PROCESS INTERVAL MODEL GENERATION

In the fourth chapter, Step 3 of the framework, which was briefly introduced in Chapter 3, is explained in more detail. In the first part, the design models for treatment technologies developed within this study or collected from the literature, are presented. The second part gives the details of the procedure, where the output of the design models are converted into the parameters of the optimization problem and sent to the optimizer. Bozkurt et al., (2015a) explains the details of the systematic data collection and design procedure by following an example case study application.

4.1 Design of individual treatment technologies

In this section, the design models that have been used with the purpose of designing the individual treatment technologies are presented. Some of the models employed are well-established, known and approved models by the wastewater community while some others are developed by bringing together the commonly accepted design procedures. This section is divided into four different sub-sections depending on the type of treatment: (1) activated sludge type of wastewater treatment systems, (2) sludge treatment alternatives, (3) sludge reject water stream treatment alternatives, and (4) separation units. The treatment technologies of the first category are responsible for the removal of organic matter and nitrogen from the wastewater stream of municipal origin by means of nitrification-denitrification in a pre-denitrification sequence. Sludge treatment consists of different means of biological sludge stabilization. Different configurations of partial nitritation – anammox treatment processes are modeled for the treatment of the reject water stream resulting from the sludge treatment. The models for various separation units in the water and sludge treatment line are given under the fourth category.

4.1.1 Models for activated sludge type of wastewater treatment processes

The activated sludge process is classified as a suspended growth treatment process in which a reactor, where the microorganisms responsible for treatment are kept in suspension, is coupled with a separation unit (i.e. settler) to separate two phases: liquid and solids. The most characteristic component of the system, which also gives its name to the treatment technology, is the recycle stream carrying the solids/microorganisms (i.e. active sludge) from the bottom of the settler to the reactor (Tchobanoglous, 2003). Different design configurations of the process exist with different mechanisms employed. For instance, with the increased interest in nutrient removal, staged reactors – anaerobic, anoxic and aerated reactors put into series – are developed with the possible use of several internal recycle flows.

In this study, two design models for pre-denitrification type of activated sludge processes (as shown in Figure 4.1) are developed by using the commonly accepted design procedures given by ATV design standards (2000), Tchobanoglous (2003), WEF WWTP design manuals (2010) and Henze et al. (2008). These models are steady state models which are based on (1) kinetics and (2) fixed removal efficiencies for the two proposed models, respectively. Moreover, for the purpose of validating the proposed design models, the design parameters and performance values for a number of cases (changing SRT, HRT, anoxic/aerobic volume ratio as well as wastewater characteristics) are compared with the steady state results obtained from a simulation carried out using a rigorous model, i.e. Activated Sludge Model no. 1 (ASM1). The simulation with the rigorous model was performed in Matlab/Simulink®. The definition of the models used and the results of the validation procedure are presented below.

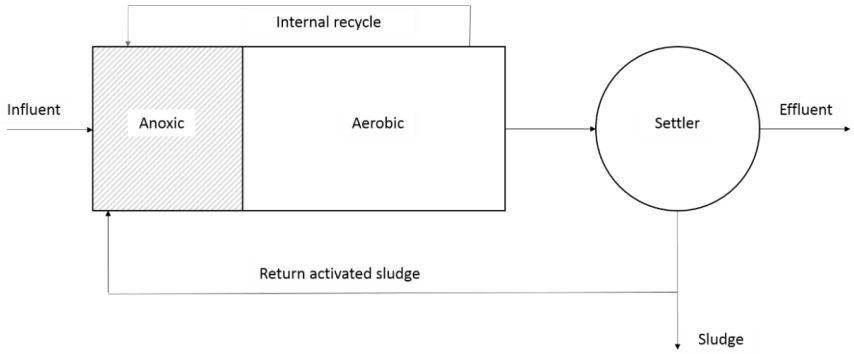


Figure 4.1 A representative configuration of a pre-denitrification type of activated sludge process for organic matter and nitrogen removal

4.1.1.1 Activated sludge model no.1 (ASM1)

ASM1 describes the concepts of carbon oxidation, nitrification and denitrification together with the simultaneous growth and decay of heterotrophic and autotrophic microorganisms. It uses a matrix notation in which, the components (i.e. pollutants, microorganisms, oxygen and alkalinity), processes (growth, decay, hydrolysis etc.), process rate equations and stoichiometry are presented (Henze et al., 2000).
The components in the ASM1 matrix are defined in a unique way. They are listed together with their definitions in Table 4.1. The components given with the symbol S are the soluble components, whereas the symbol X refers to particulate components.

Table 4.1 Component list for ASM1 matrix (Henze et al., 2000)

Component	Description	Unit
S_I	Soluble inert organic matter	M COD/L^3
S_S	Readily biodegradable substrate	M COD/L^3
X_I	Particulate inert organic matter	M COD/L^3
X_S	Slowly biodegradable substrate	M COD/L^3
$X_{B,H}$	Active heterotrophic biomass	M COD/L^3
$X_{B,A}$	Active autotrophic biomass	M COD/L^3
X_P	Particulate products arising from biomass decay	M COD/L^3
S_O	Oxygen	M -COD/L^3
S_{NO}	Nitrate and nitrite nitrogen	M N/L^3
S_{NH}	$NH_4^+ + NH_3$ nitrogen	M N/L^3
S_{ND}	Soluble biodegradable organic nitrogen	M N/L^3
X_{ND}	Particulate biodegradable organic nitrogen	M N/L^3
S_{ALK}	Alkalinity	molar units

Organic matter is divided into two main fractions in terms of its biodegradability (Figure 4.2): non-biodegradable organic matter and biodegradable organic matter. There are two fractions of non-biodegradable organic matter depending on their physical state which are soluble non-biodegradable (i.e. inert) - S_I and particulate non-biodegradable - X_I organic matter. The biodegradable fraction of the organic matter is also divided into two parts: readily biodegradable - S_S and slowly biodegradable X_S. Nitrogenous matter is similarly divided into two categories with regard to its biodegradability. The particulate non-biodegradable fraction is incorporated into non-biodegradable particulate COD and the soluble non-biodegradable fraction is assumed negligible. The biodegradable nitrogen compounds are described within three components: Ammonia – S_{NH}, soluble organic nitrogen – S_{ND} and particulate organic nitrogen – X_{ND}. Moreover, the sum of nitrate and nitrite nitrogen is referred to as S_{NO}.
The two groups of microorganisms presented in ASM1, which are active in organic matter degradation, nitrification and denitrification, are heterotrophic biomass - X_{BH} and autotrophic biomass - X_{BA}.

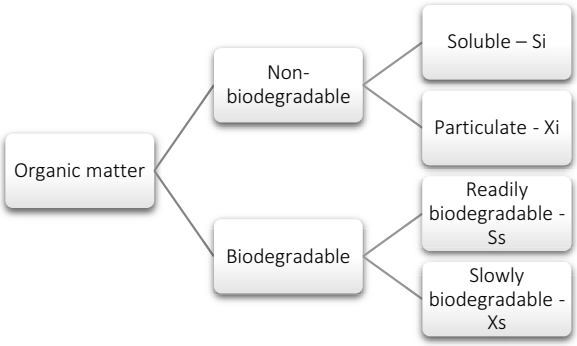


Figure 4.2 Organic matter fractionation

There are 8 different processes defined in ASM1. In Table 4.2, the processes are given with their rate equations. The complete kinetics and stoichiometry matrix can be seen in Appendix 2.

Table 4.2 Process rate equations defined in ASM1

Process	Rate equation (M/L^3T) - ρ_j
Aerobic growth of heterotrophs	$\mu_h \left(\frac{S_S}{K_s + S_S}\right)\left(\frac{S_O}{K_{OH} + S_O}\right) X_{BH}$
Anoxic growth of heterotrophs	$\mu_h \left(\frac{S_S}{K_s + S_S}\right)\left(\frac{K_{OH}}{K_{OH} + S_O}\right) * \left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right) \eta_g X_{BH}$
Aerobic growth of autotrophs	$\mu_a \left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right) \left(\frac{S_O}{K_{OA} + S_O}\right) X_{BA}$
Decay of heterotrophs	$b_H X_{BH}$
Decay of autotrophs	$b_A X_{BA}$
Ammonification of soluble organic nitrogen	$k_a S_{ND} X_{BH}$
Hydrolysis of entrapped organics	$k_h \frac{X_S/X_{BH}}{K_X + (X_S/X_{BH})} \left[\left(\frac{S_O}{K_{OH} + S_O}\right) + \eta_h \left(\frac{K_{OH}}{K_{OH} + S_O}\right)\left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right) \right] X_{BH}$
Hydrolysis of entrapped organic nitrogen	$\rho_7 (X_{ND}/X_S)$

Within the ASM1 matrix, the stoichiometric coefficients are placed. They define the mass relationships between the compounds. The matrix representation makes writing the mass balance equations easier. A generic mass balance equation can be defined as in equation 4.1. By using the ASM1 matrix the *Reaction* term can be calculated easily. For a component *i* the reaction term r_i is obtained by summing the products of the stoichiometric coefficients ν_{ij} and process rate expression ρ_j as given in equation 4.2.

$$Accumulation = Input - Output + Reaction \quad 4.1$$

$$r_i = \sum_j \upsilon_{ij} \rho_j \quad 4.2$$

The stoichiometric and kinetic parameters used to establish the model are given in Table 4.3. To constitute an example, the temperature depended parameter values are given for 15°C. Different values for the parameters at different temperatures can be found elsewhere (Henze et al., 2000).

Table 4.3 ASM1 stoichiometric and kinetic parameters at 15°C

Symbol	Unit	Value
Y_A	g cell COD formed/(g N oxidized)	0.24
Y_H	g cell COD formed/(g COD oxidized)	0.67
f_P	dimensionless	0.08
i_{XB}	g N/(g COD) in biomass	0.08
i_{XP}	g N/(g COD) in particulate products	0.06
μ_H	1/d	4.0
K_S	g COD/m^3	10.0
K_{OH}	g (-COD)/m^3	0.2
K_{NO}	g NO_3-N/m^3	0.5
b_H	1/d	0.3
η_g	dimensionless	0.8
η_h	dimensionless	0.8
k_h	g slowly biodegradable COD/(g cell COD . d)	3.0
K_X	g slowly biodegradable COD/(g cell COD)	0.1
μ_A	1/d	0.5
K_{NH}	g NH_3-N/m^3	1.0
b_A	1/d	0.05
K_{OA}	g (-COD)/m^3	0.4
k_a	m^3/(g COD . d)	0.05

4.1.1.2 Design model no.1

As mentioned earlier, the first design model developed in this study for designing the pre-denitrification type of activated sludge processes is based on process kinetics. This model is established by bringing together the commonly accepted design procedures given by ATV design standards (2000), Tchobanoglous (2003), WEF WWTP design manuals (2010) and Henze et al. (2008). While creating the model, a systematic procedure has been followed, which was presented earlier under section 3.3 as the systematic data collection and design procedure. The design model no.1 is detailed here by following the steps of the proposed methodology (Figure 3.3).

Model step 1. In the first step, the wastewater composition is defined. The influent and effluent streams are characterized in terms of ASM1 components; however, in the model, use of lumped contaminant concentrations (COD, BOD, TKN etc.) is necessary. Therefore, a conversion is made prior to model equations as shown below, where f_{Xi} is the non-biodegradable fraction of the biomass and DO_{SP} is the dissolved oxygen set point value inserted into the equation for the condition in which oxygen enters the system with

the internal and external recycle streams. Together with the influent characterization, effluent limit definitions should be made at this step. Moreover, the user should specify the temperature, since the design parameters to be further selected are highly temperature dependent.

$$COD_b^{in} = S_S^{in} + X_S^{in} + (1 - f_{Xi})\left(X_{BH}^{in} + X_{BA}^{in}\right) - DO_{SP} \quad 4.3$$

$$TKN_{in} = S_{NH}^{in} + S_{ND}^{in} + X_{ND}^{in} \quad 4.4$$

Model step 2. In the second step of the systematic data collection and design procedure, the treatment technology to be designed is selected. This design model is developed for the design of pre-denitrification type of activated sludge processes.

Model step 3. In the third step, the system specific data are collected from the open literature for the selected treatment technology. For the data given as a range, the necessary assumptions are made. System SRT, HRT, anoxic/aerobic volume ratio, and external recycle ratio are selected together with stoichiometric and kinetic parameters.

Model step 4. After selecting the design parameters, in this step, the design is done following the steps below. The parameters/variables used in the equations are described below, unless they are defined in Table 4.1 or 4.3.

- The sizing of the reactor is done based on the selected HRT of the system and the influent flow rate - Q_{in}. Different compartments of the system (anoxic compartment - V_{an} and aerobic compartment - V_{ae}) are sized separately by using the selected anoxic/aerobic volume ratio.

  $$V_{an} = HRT_{an} * Q_{in} \quad 4.5$$

  $$V_{ae} = HRT_{ae} * Q_{in} \quad 4.6$$

- Effluent biodegradable COD and ammonium nitrogen are calculated based on the following equations. It is assumed that all the incoming biodegradable COD is used for denitrification in the anoxic compartment; therefore the growth of anoxic heterotrophic organisms occurs only in this compartment. Similarly, the organisms responsible for nitrification (aerobic autotrophic organisms) grow solely in the aerobic compartment. It is furthermore assumed that, all the organisms go through decay in the entire reactor volume.

$$COD_b^{out} = \frac{K_S(1+b_H SRT)}{SRT\left(\mu_H\left(\frac{V_{an}}{V_T}\right)-b_H\right)-1} \quad 4.7$$

$$S_{NH}^{out} = \frac{K_{NH}(1+b_A SRT)}{SRT\left(\mu_A\left(\frac{V_{ae}}{V_T}\right)-b_A\right)-1} \quad 4.8$$

- The solids production in the system is determined by calculating the production / accumulation of different fractions of solids as shown below (all given in concentration units M/L^3). Here, *CN* represents the sum of NH_4-N that is nitrified in the aerobic compartment and assimilated into the biomass, where N_S is the nitrogen content of the biomass.

$$X_{BH} = \frac{SRT}{HRT}\left[\frac{Y_H\left(COD_b^{in}-COD_b^{out}\right)}{1+b_H SRT}\right] \quad 4.9$$

$$N_S = \frac{i_{XB} X_{BH} HRT}{SRT} \quad 4.10$$

$$CN = TKN_{in} - S_{NH}^{out} - N_S \quad 4.11$$

$$X_{BA} = \frac{SRT}{HRT}\left[\frac{Y_A CN}{1+b_A SRT}\right] \quad 4.12$$

$$X_P = [(f_P b_H X_{BH}) + (f_P b_A X_{BA})]\, SRT \quad 4.13$$

$$X_I = X_I^{in}\frac{SRT}{HRT} \quad 4.14$$

$$X_T = X_{BH} + X_{BA} + X_P + X_I \quad 4.15$$

- The oxygen is consumed for cell decay - RO_b and nitrification - RO_n. The oxygen for COD degradation is excluded here based on the assumption that biodegradable COD is fully consumed in denitrification. (*MX$_{BH}$* and *MX$_{BA}$* refers to mass units – *M*).

$$RO_b = \left[(1-f_P) b_H MX_{BH}\frac{V_{ae}}{V_T} + (1-f_P) b_A MX_{BA}\frac{V_{ae}}{V_T}\right] \quad 4.16$$

$$RO_n = 4.57 * Q * CN \quad 4.17$$

- The flow rate of the sludge wastage stream - Q_W, which is assumed to be wasted from the reaction tank is calculated as follows.

$$Q_W = \frac{V_T}{SRT} \quad 4.18$$

- In order to find the effluent nitrate concentration, the denitrification potential (DP) is calculated by using the following equations where K_2 refers to denitrification rate (Henze et al., 2008). DP_1, DP_2 and DP_3 represent the denitrification potentials with respect to readily biodegradable COD, slowly biodegradable COD and biomass respiration, respectively.

$$DP_1 = \frac{S_S^{in} \frac{1}{Y_H}}{2.86} \quad 4.19$$

$$DP_2 = \frac{K_2\left(X_S^{in} - COD_b^{out}\right) Y_H \, SRT}{1+(b_H \, SRT)} \quad 4.20$$

$$DP_3 = \frac{(1-f_P) b_H M X_{BH}\left(\frac{V_{an}}{V_T}\right)}{2.86 \, Q} \quad 4.21$$

$$DP = DP_1 + DP_2 + DP_3 \quad 4.22$$

$$S_{NO}^{out} = CN - DP \quad 4.23$$

- Finally, the concentration of particulate biodegradable nitrogen - X_{ND} is calculated from stoichiometry.

$$X_{ND} = i_{XB}(X_{BH} + X_{BA}) + i_{XP} \, X_P \quad 4.24$$

- Once all the concentrations are calculated, the results are assigned to related ASM1 components as shown in Table 4.4. The concentration of inert soluble organics does not changed after reaction. The remaining biodegradable COD is assumed to be all in slowly biodegradable form - X_S and therefore the readily biodegradable organics - S_S concentration is assumed to be 0. Moreover, the soluble nitrogen is assumed to be in S_{NH} and S_{NO} form and not in S_{ND} form which is taken as 0 as well.

Table 4.4 Concentrations of components after reaction for Design model no.1

ASM1 Component	Concentration (M/L^3) / Model representation	Related equation
S_I	S_I^{in}	-
S_S	0	-
X_I	X_I	4.14
X_S	COD_b^{out}	4.7
$X_{B,H}$	X_{BH}	4.9
$X_{B,A}$	X_{BA}	4.12
X_P	X_P	4.13
S_O	DO_{SP}	-
S_{NO}	S_{NO}^{out}	4.23
S_{NH}	S_{NH}^{out}	4.8
S_{ND}	0	-
X_{ND}	X_{ND}	4.24

4.1.1.3 Design model no.2

The second design model developed within the context of this study is based on fixed removal efficiencies for organics and nitrogen compounds. This model is also created by the use of previously mentioned design procedures together with the reported removal efficiencies for pollutants in the applications of specified technologies at different scales (laboratory, pilot or full-scale). The model development, similar to the first design model, follows the steps of the systematic data collection and design procedure (Figure 3.3).

Model step 1. The first step of the model is where the wastewater characterization is made. Similar to the first design model, the wastewater is characterized in terms of ASM1 components and the concentrations of organic components and nitrogen components are converted to lumped contaminant concentration parameters as shown previously in equations 4.3 and 4.4.

Model step 2. The design model is proposed to be used for design of a pre-denitrification type of activated sludge processes.

Model step 3. In this step, the system specific data (SRT, HRT etc.) are collected; as well as the performance data for the treatment technology to be designed in terms of % removal efficiencies of the contaminants. Moreover, the stoichiometric and kinetic parameters are defined with respect to the selected design temperature.

Model step 4. The fixed removal efficiency based design of the treatment technology is done following the steps below.

- The reactor volume is calculated by using the specified HRT of the system and the influent flow rate.

$$V = HRT * Q_{in} \quad 4.25$$

- Removed biodegradable COD - COD_b^{rem} is calculated next, by using the COD_b removal efficiency - η_{COD}. Here, the efficiency includes the removal both by COD oxidation and denitrification mechanisms.

$$COD_b^{rem} = COD_b^{in} * \eta_{COD} \quad 4.26$$

$$COD_b^{out} = COD_b^{in} - COD_b^{rem} \quad 4.27$$

- The heterotrophic biomass production as a result of COD degradation is calculated by equation 4.28; and equation 4.29 gives the oxygen consumption provided that all the COD is removed by oxidation, which is subject to correction in later steps.

$$X_{BH} = \frac{SRT}{HRT}\left[\frac{Y_H\, COD_b^{rem}}{1+b_H SRT}\right] \quad 4.28$$

$$RO_b = [(1 - Y_H)\, Q_{in}\, COD_b^{rem}] + [(1 - f_P) b_H\, MX_{BH}] \quad 4.29$$

- Next in the workflow, comes the calculation of nitrogen removal by means of nitrification and denitrification. Nitrification and denitrification efficiencies are represented as η_{Snh} and η_{Sno} respectively.

$$S_{NH}^{rem} = S_{NH}^{in} * \eta_{Snh} \quad 4.30$$

$$S_{NH}^{out} = S_{NH}^{in} - S_{NH}^{rem} \quad 4.31$$

$$CN = S_{NH}^{rem} - N_S \quad 4.32$$

$$S_{NO}^{rem} = CN * \eta_{Sno} \quad 4.33$$

$$S_{NO}^{out} = CN - S_{NO}^{rem} \quad 4.34$$

- Previously, all the biodegradable COD was assumed to be degraded by oxidation - COD_b^{oxid}. However; after calculating the amount of nitrate removed by denitrification, the COD amount used during this process is calculated -

COD_b^{denit}. An oxygen consumption correction is done as well. Accordingly, equation 4.29 is updated as seen in equation 4.37. Oxygen consumption for nitrification is calculated as shown previously in equation 4.17.

$$COD_b^{denit} = \frac{S_{NO}^{rem}\ 2.86}{1-Y_H} \quad 4.35$$

$$COD_b^{oxid} = COD_b^{rem} - COD_b^{denit} \quad 4.36$$

$$RO_b = \left[(1-Y_H)\ Q_{in}\ COD_b^{oxid}\right] + \left[(1-f_P) b_H\ MX_{BH}\right] \quad 4.37$$

- The remaining fractions of particulate material (i.e. solids) are calculated by using equations 4.12 – 4.14. Similarly, the wastage flow rate is assumed to be done from the aeration tank and calculated by equation 4.18.
- The final step, where the calculated concentrations of the components are assigned to ASM1 components, is done similar to the first design model as shown in Table 4.4.

4.1.1.4 Validation of Design model no.1 and Design model no.2

In order to validate the systematic data collection procedure through the validation of proposed design models (Design model no.1 & Design model no.2), system performances in terms of removal of three key contaminants – COD, Total-N and suspended solids, obtained using steady-state design models are compared with the steady state results obtained from a simulation carried out using a rigorous model, i.e. ASM1. The simulation with the rigorous ASM1 model was performed in Matlab/Simulink®. The results are summarized in Table 4.5.

The design parameters (HRT, SRT, volume ratio etc.) are kept constant for three different models; as well as the influent wastewater characterization. The results indicate that the differences between the estimated removal efficiencies for COD, total-N and suspended solids by the rigorous model (ASM1) and the steady-state design models developed in this study were quite small. The average relative error is less than 1.5 %, 5 % and 1.5 % for three key contaminants, respectively. Therefore, it is concluded that with the same design values selected, the estimated system performance results in terms of removal efficiencies are in agreement with each other and therefore the systematic data collection and design procedure, and thus the Design model no.1 & 2, are considered to be validated against the more rigorous model. A more detailed analysis has been made with changing system conditions and wastewater characteristics and the results of this analysis are presented in Appendix 2.

Table 4.5 Validation for systematic data collection procedure

Parameter	ASM1	Design model no.1	Design model no.2
Corresponding technology	Pre-denitrification activated sludge		
Temperature (°C)		15	
HRT (hour)		12	
SRT (days)		14	
Anoxic / Aerobic volume ratio		0.6	
TKN/COD ratio		0.13	
COD (g COD / m^3)			
Influent	381.19	381.19	381.19
Effluent	46.29	44.15	41.35
Reduction (%)	**87.85**	**88.42**	**89.15**
Nitrogen (g N / m^3)			
Total-N influent	54.43	54.43	54.43
S_{NO} effluent	11.50	13.48	10.69
S_{NH} effluent	0.36	0.64	0.47
Total-N effluent	13.61	15.71	12.47
Reduction (%)	**75.00**	**71.13**	**77.09**
Suspended Solids (g COD / m^3)			
Influent	211.27	211.27	211.27
Effluent	11.67	10.61	8.59
Reduction (%)	**94.47**	**94.97**	**95.93**

4.1.2 Models for sludge stabilization units

The solids resulting from wastewater treatment operations and processes are referred to as sludge and they have to be treated in order to satisfy some conditions prior to be discharged. Characteristics of sludge which affect their final use are listed as organics content, nutrients, pathogens, metals and toxic organics. In that respect one of the important elements of sludge treatment is sludge stabilization; it is mainly responsible for reduction of the organic matter content and removal of pathogens.

In the context of this study, two types of sludge stabilization units have been modeled: anaerobic sludge stabilization and aerobic sludge stabilization. Anaerobic stabilization is described as the conversion of organic matter into carbon dioxide and methane at elevated

temperatures in the absence of oxygen; whereas, aerobic digestion refers to conversion of organic matter in the presence of oxygen (Tchobanoglous, 2003).

4.1.2.1 Steady state model for anaerobic digestion of sludge

In this study, the steady state anaerobic digestion (AD) model proposed by Sötemann et al. (2005) is used in order to predict the COD removal and methane production during anaerobic digestion of sludge. Moreover, the release of ammonia/ammonium nitrogen is calculated based on a mass balance analysis. The definition of the model is given below.

- First, the sludge characterization is defined. The ASM1 components are converted into the representation of components given by the proposed model (Sötemann et al., 2005) as shown below in equations 4.38 – 4.41 where S_{bsf} is the readily biodegradable soluble COD, S_{bp} is the particulate biodegradable COD, S_{up} represents the unbiodegradable particulate COD and S_{us} is unbiodegradable soluble COD.

$$S_{bsf}^{in} = S_S^{in} \quad 4.38$$

$$S_{bp}^{in} = X_S^{in} + (1 - f_P)\left(X_{BH}^{in} + X_{BA}^{in}\right) - 2.86\, S_{NO}^{in} - S_O^{in} \quad 4.39$$

$$S_{up}^{in} = X_I^{in} + X_P^{in} \quad 4.40$$

$$S_{us}^{in} = S_I^{in} \quad 4.41$$

- In order to calculate the residual biodegradable particulate organics – S_{bp}, acidogen biomass concentration – Z_{AD}, unbiodegradable organics concentration – S_{up} and methane production – S_m; the following model is used based on Monod kinetics.

  - Hydrolysis rate - r_h (g COD/L.d) is calculated by equation 4.42 where; K_m=*3.34 g COD organics/g COD biomass.d* and K_s=*6.76 g COD/L*.

$$r_h = \frac{K_m S_{bp}}{(K_s + S_{bp})} Z_{AD} \quad 4.42$$

  - Equation 4.43 determines the residual biodegradable organics concentration – S_{bp} *(g COD/L)* where *R* is the retention time of the system, b_{AD} is the decay coefficient and Y_{AD} is the yield coefficient. The values for b_{AD} and Y_{AD} are taken as *0.041 1/d* and *0.113 g COD biomass/g COD organics*, respectively.

$$S_{bp} = \frac{K_S(1/R + b_{AD})}{Y_{AD}\, K_m - (1/R + b_{AD})} \quad 4.43$$

- By equation 4.44, the acidogen biomass concentration – Z_{AD} (g COD/L) is calculated.

$$Z_{AD} = \frac{Y_{AD}\left(S_{bp}^{in} - S_{bp}\right)}{[1 + b_{AD}\, R(1 - Y_{AD})]} \quad 4.44$$

- The unbiodegradable organics concentration does not change in the reactor:

$$S_{up} = S_{up}^{in} \quad 4.45$$

- Finally, the methane production – S_m (g COD/L) is determined by equation 4.46.

$$S_m = (1 - Y_{AD}) R\, r_h \quad 4.46$$

- The calculated concentrations are assigned to ASM1 components as summarized in Table 4.6. The calculated acidogen biomass concentration - Z_{AD} is assigned to components X_S and X_P as shown below and it is assumed that there is no remaining heterotrophic and autotrophic biomass in the system (i.e. X_{BH} and X_{BA}, respectively)

$$X_S = S_{bp} + (1 - f_P) Z_{AD} \quad 4.47$$

$$X_p = X_P^{in} + f_P\, Z_{AD} \quad 4.48$$

- Once the ASM1 components are determined for COD components, the nitrogen release in the digester is calculated from a nitrogen mass balance as shown in equations 4.49 – 4.51. Nitrogen is assumed to be released in ammonia/ammonium nitrogen form and nitrite/nitrate nitrogen together with soluble organic nitrogen fractions are assumed to be 0. The concentrations of nitrogen components after reaction are summarized in Table 4.6 as well.

$$TN_{in} = i_{XB}\left(X_{BH}^{in} + X_{BA}^{in}\right) + i_{XP}\, X_P^{in} \quad 4.49$$

$$TN_{out} = i_{XB}(Z_{AD}) + i_{XP}\, X_P \quad 4.50$$

$$S_{NH} = TN_{in} - TN_{out} + S_{NH}^{in} \quad 4.51$$

$$X_{ND} = TN_{out} \quad 4.52$$

Table 4.6 Concentrations of components after reaction for the anaerobic digester model

ASM1 Component	Concentration (M/L^3) / Model representation	Related equation
S_I	S_{us}^{in}	4.41
S_S	0	-
X_I	X_I^{in}	-
X_S	X_S	4.47
$X_{B,H}$	0	-
$X_{B,A}$	0	-
X_P	X_P	4.48
S_O	0	-
S_{NO}	0	-
S_{NH}	S_{NH}	4.51
S_{ND}	0	-
X_{ND}	X_{ND}	4.52

4.1.2.2 Steady state model for aerobic digestion of sludge

The model used for aerobic digestion of sludge was proposed by Marais and Ekama (1976). For the purpose of this study, the model for a single completely mixed reactor has been chosen in order to describe COD destruction and nitrification. The model is explained in the following steps.

- The three types of solid masses (g COD/L) considered in the model are active solids - X_a, endogenous residuals – X_e and inert solids – X_i. The influent sludge, which is characterized in terms of ASM1 components, is converted into the model components by equations 4.53 – 4.55.

$$X_a^{in} = X_S^{in} + X_{BH}^{in} + X_{BA}^{in} \quad 4.53$$

$$X_e^{in} = X_P^{in} \quad 4.54$$

$$X_i^{in} = X_I^{in} \quad 4.55$$

- Steady state masses of the solid components in the digester are calculated by the following equations where; *b* is the decay coefficient (*1/d*), *R* is the residence time in days and *f* represents the ratio of endogenous residue solids to active solids. The mass of inert compounds is not affected in the digester.

$$X_a = \frac{X_a^{in}}{1+b\,R} \quad 4.56$$

$$X_e = f\left(X_a^{in} - X_a\right) \quad 4.57$$

$$X_i = X_i^{in} \quad 4.58$$

- The production of nitrite/nitrate nitrogen - S_{NO} in the digester is assumed to be the sum of S_{NO} resulting from the complete nitrification of incoming ammonia/ammonium nitrogen - S_{NH} and nitrification of released TKN during COD destruction. In equation 4.59, f_n refers to the nitrogen content of the active solids. Moreover, the particulate biodegradable organic nitrogen concentration is calculated as shown in equation 4.60.

$$S_{NO} = S_{NH}^{in} + \left[\left(X_a^{in} - X_a\right)(1-f) f_n\right] \quad 4.59$$

$$X_{ND} = i_{XB}(X_a) + i_{XP}\,X_e \quad 4.60$$

- The oxygen is consumed in the digester in two different processes: (1) oxidation of the carbonaceous material – *MO* and (2) nitrification - MO_n.

$$MO = (1-f)\,b\,MX_a \quad 4.61$$

$$MO_n = (4.6\,f_n\,(1-f)\,b\,MX_a) + (4.6\,MS_{NH}) \quad 4.62$$

- The final step covers assigning the calculated concentrations which are given in terms of model components, into ASM1 components as shown in Table 4.7. The assumptions made here can be listed as: (1) all the biodegradable COD (i.e. S_S and X_S) is destructed and thus reported as 0, (2) the concentration of soluble and particulate inert COD does not change and (3) all the active particulates are in the heterotrophic microorganisms form.

Table 4.7 Concentrations of components after reaction for anaerobic digester model

ASM1 Component	Concentration (M/L^3) / Model representation	Related equation
S_I	S_I^{in}	-
S_S	0	-
X_I	X_I^{in}	-
X_S	0	-
$X_{B,H}$	X_a	4.56
$X_{B,A}$	0	-
X_P	X_e	4.57
S_O	DO_{SP}	-
S_{NO}	S_{NO}	4.59
S_{NH}	0	-
S_{ND}	0	-
X_{ND}	X_{ND}	4.60

4.1.3 Models for sludge reject water stream treatment units

The sludge reject water stream, in other words return water from sludge thickening and/or drying units, which is characterized with its high nitrogen load, low flow rates and high temperature (20 – 35 °C), is recycled to the inlet of the wastewater treatment units. This stream accounts for 10 – 30 % of the total nitrogen load entering the treatment plant; therefore, removing nitrogen at this point by means of physical or biological processes can result in improvements in the overall plant nitrogen removal efficiency (Henze et al., 2008).

Biological techniques for the removal of nitrogen from wastewater streams has been widely used with proven effectiveness. The nitrification/denitrification route (NH_4 → NO_2 → NO_3 → N_2), which can be seen in Figure 4.3 around the circle, requires addition of oxygen for the route of NH_4 to NO_3, and addition of carbon to convert NO_3 to N_2. Therefore, it is distinguished to be energy intensive due to aeration and costly because of the possible addition of external carbon. Therefore, in the recent years more sustainable and innovative ways of nitrogen removal have been explored resulting in several treatment approaches.

One of them employs the conversion of NH_4 to NO_2 by ammonium oxidizing bacteria (AOB); reducing the aeration requirements by almost 25 % as compared to conventional nitrification route (NH_4 → NO_3) as well as reducing the sludge production. By means of subsequent denitritation with the use of 40 % less organic matter, this approach reduces the cost of operation significantly. The technology which operates with the nitritation/denitritation route is named as Single reactor High activity Ammonia Removal

over Nitrite – or shortly SHARON (Hellinga et al., 1998). Moreover, a new pathway was discovered for removal of NH_4 with less oxygen requirement and without the need for organic matter; this discovery is called Anaerobic Ammonium Oxidation or shortly Anammox (Mulder et al., 1995). This route is shown inside the circle in Figure 4.3 where NH_4 and NO_2 are converted to nitrogen gas under anaerobic conditions following partial nitritation where 50 % of the NH_4 is converted to NO_2. By means of a combined partial nitritation-anammox (PN/A) process, low effluent nitrogen concentrations can be achieved with aeration savings up to 63 % and completely omitting the need for external organic matter sources (Volcke, 2006).

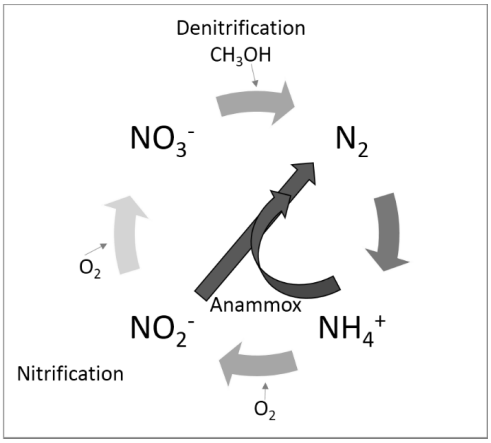


Figure 4.3 Nitrogen cycle

By 2012, the full scale applications of about 30 side-stream treatment processes consisting of four plants, which were using spatially separated PN/A reactors (i.e. two-stage reactor where PN and anammox occur in separate reactors) and the rest were using single stage systems (i.e. PN and anammox occur in the same reactor) (Vlaeminck et al., 2012). Currently, the PN/A system is used in many full-scale applications, majority of which are located in Europe with an increasing interest for side-stream treatment in North America. In early stages of the applications, mainly for better control of nitritation, two-stage systems were favored; however with more experience, the applications shifted towards single stage (Lackner et al., 2014).

Within the context of this study, two different mechanisms have been modelled: (1) Nitritation/denitritation and (2) Partial nitritation/anammox. The details of the models are given in this section.

4.1.3.1 Modeling nitritation and denitritation

As mentioned previously, the sludge reject water stream is characterized by its high temperature. When the microorganisms operate at high temperatures their growth rates are so high that a biological reactor can be run without any sludge retention required. Moreover, another advantage of high temperature is that nitrite oxidizers (NOB) grow faster as compared to ammonium oxidizers (AOB) at low temperatures; however, the opposite is true for high temperatures. This means, NOB can be eliminated from the system which allows nitritation rather than nitrification (Hellinga et al., 1998).
The model for the nitritation/denitritation mechanism includes sizing of the reactor by using SRT/HRT of the system, estimating the utility addition requirements from stoichiometry, definition of the process performance in terms of removal efficiencies from the reported applications of the system and calculating the sludge production by using yields. The step-by-step definition of the design model is given below.

- Since the system can be operated without any need for sludge retention, the SRT is controlled by HRT; in other words the SRT of the system is equal to its HRT. Therefore, by choosing the HRT of the system the volume of the reactor is simply calculated by the following equation.

  $$V = Q * HRT \tag{4.63}$$

- The two-step nitritation/denitritation stoichiometry is given below (Notenboom et al., 2002). As a result of the first reaction, the pH of the system decreases significantly with the produced H^+. For almost 50% of this can be neutralized by the bicarbonate existing in the sludge reject water stream. However, in order to deal with the rest of it there should be either base addition into the system or the denitritation route should be followed. Methanol addition (i.e. to initiate the denitritation route) is less costly than base addition; therefore, denitrification has been chosen for our model. In this step, as mentioned earlier, the utility addition requirements are calculated with the stoichiometry given in equations 4.64 and 4.65. Accordingly, for each gram of NH_4-N, 3.43 gram of oxygen should be supplied. Similarly, for every 1 gram of NH_4-N entering the system, approximately 1 gram of methanol should be added (Hellinga et al., 1998).

  $$NH_4^+ + 1.5\ O_2 \rightarrow NO_2^- + H_2O + 2H^+ \tag{4.64}$$

  $$NO_2^- + 0.5CH_3OH + 0.5CO_2 \rightarrow 0.5N_2 + HCO_3^- + 0.5H_2O \tag{4.65}$$

- In literature, the efficiency of nitritation/denitritation systems is given as % removal of NH_4-N and/or % removal of Total-N. At this step, by using the

reported removal efficiencies, the performance of a reactor, which is operating at its optimum, is estimated.

- Finally the sludge production is calculated by using the yield values and the estimated nitrogen removal in the system. Production of AOB microorganisms is calculated by equation 4.66 where Y_{AOB} equals *0.15 g COD/g NH_4-N* and similarly nitrite denitrifiers are produced by removal of nitrite according to Y_{denit} which is given as *0.55 g COD/g NO_2-N* (Hellinga et al., 1999).

$$X_{AOB} = NH_4^{rem} * Y_{AOB} \quad 4.66$$

$$X_{denit} = NO_2^{rem} * Y_{denit} \quad 4.67$$

4.1.3.2 Modeling partial nitritation/anammox

Partial nitritation/anammox is a two-step mechanism, where each step occurs in different conditions in terms of presence of oxygen in the medium. Anammox is the acronym for ANaerobic AMMonia Oxidation, and as the name implies it occurs in anaerobic conditions. On the other hand, partial nitritation occurs under aerobic conditions where ammonia is partially oxidized to nitrite with oxygen. Considering the nature of the mechanism, convenient medium conditions should be satisfied for both microorganism groups (ammonia oxidizing bacteria – AOB and anammox bacteria).

One way of establishing this is by performing the reactions in two different reactors; one of which is aerated and the other one is kept under anaerobic conditions. This system is referred to as two-stage reactor (e.g. van Dongen et al., 2001; van der Star et al., 2007). Another approach is combining the partial nitritation and anammox reactions in one reactor (i.e. single stage reactor). This is only possible by providing biomass immobilization. For this purpose, sludge is retained in biofilm or granular conditions under oxygen limitation (Henze et al., 2008). In the literature, the single stage partial nitritation/anammox application has been given several different acronyms (Hu et al., 2013).

In the context of this study, a model is developed in order to (1) determine the size of the reactor(s) by using either HRT/SRT of the system or volumetric loading/removal rates reported in the literature for different application scales, (2) estimate the utility addition requirements from stoichiometry, (3) calculate the process performance from reported efficiencies, and (4) calculate the sludge production from yield values. The details are given below.

- The sizing of the system differs with respect to the reactor type selected. When the two-stage reactor configuration is modeled; the first reactor, in which the partial nitritation takes place is sized based on the selected HRT/SRT of the system (the system runs without any sludge retention therefore SRT of the system

is equal to its HRT as mentioned earlier for the nitritation/denitritation reactor model) as shown in equation 4.63. The second reactor on the other hand, is sized based on the reported volumetric loading - q_{load} or removal rate - q_{rem} values (in *kg N/m^3.d*) from the literature. Similarly, the sizing of a single stage reactor is done by the use of volumetric loading or removal rate values with respect to nitrogen.

$$V = \frac{M\,Tot_N^{in}}{q_{load}} \quad 4.68$$

$$V = \frac{M\,Tot_N^{rem}}{q_{rem}} \quad 4.69$$

- The two-step stoichiometry for the partial nitritation/anammox mechanism is shown below in equations 4.70 and 4.71 (van Dongen et al., 2001). In the partial nitritation reaction, the ammonium entering the system is oxidized to nitrite with the supplied oxygen. This reaction is maintained to run with 50% efficiency in order to supply sufficient ammonium and nitrate mixture for the second reaction, which is anammox. In this reaction, ammonium and nitrite are converted together to give nitrogen gas.

$$NH_4^+ + HCO_3^- + 0.75O_2 \rightarrow 0.5NH_4^+ + 0.5NO_2^- + CO_2 + 1.5H_2O \quad 4.70$$

$$NH_4^+ + NO_2^- \rightarrow N_2 + 2H_2O \quad 4.71$$

- By using the reported values of efficiencies for partial nitritation/anammox systems in terms of % removal of NH_4-N and/or % removal of Total-N, the performance of the reactor(s) is/are estimated.

- In the final step, the sludge production is calculated from yield values and the estimated nitrogen removal in the system. The production of AOB microorganisms are calculated according to equation 4.66. Similarly, production of anammox microorganisms is calculated by equation 4.72 where Y_{anAOB} equals *0.157 g COD/g NH_4-N* (van Dongen et al., 2001).

$$X_{anAOB} = NH_4^{rem} * Y_{anAOB} \quad 4.72$$

4.1.4 Models for separation units

The separation in WWTPs is usually employed in order to separate the water and sludge phases: in the wastewater treatment line to obtain a water stream with no or little particular materials and in the sludge treatment line for the purpose of dewatering the sludge prior to being stabilized and disposed of. For separation purposes, different units based on

different separation principles are used. For instance, in the wastewater line clarifiers, filters and air flotation units are commonly used; whereas, in the sludge treatment line, use of belt presses, centrifuges and gravity thickeners is widespread.
In the generic process interval model of this study, separation is incorporated into the process interval by defining a phase separation phenomenon (see Figure 3.4) and defined by equation 3.9. The parameter defining the phase separation is $split_{i,kk}$, which is assigned to each component – i in each process interval - k.

Modelling separation in the wastewater treatment line

Primary and secondary clarifiers are the two commonly used separation units in the wastewater treatment line. In order to define the separation factor for those two units, the non-settleable fraction of the particulate materials (f_{ns}) and the ratio of overflow (i.e. water effluent) to underflow (i.e. concentrated sludge stream) streams are estimated either by collecting information from the literature or on the basis of prior expert knowledge.
The sizing of the sedimentation units is done based on three parameters selected from the given ranges (Tchobanoglous, 2003 and WEF, 2010) which are: solids loading rate (*SLR*), surface overflow rate (*SOR*) and retention time (t_d). Therefore, the volume of the settler ($V_{settler}$) can be calculated from equations 4.73 – 4.75 where d is the depth of the tank and *MLSS* is the concentration of solids entering the tank (used especially for secondary settler sizing).

$$V_{settler} = \frac{Q}{SOR} * d \quad 4.73$$

$$V_{settler} = \frac{MLSS*Q}{SLR} * d \quad 4.74$$

$$V_{settler} = Q * t_d \quad 4.75$$

Similarly, for different type of filters, information regarding removal efficiencies for different contaminants is collected from the literature in order to define the phase separation parameter.

Modelling separation in the sludge treatment line

In order to define liquid/solid separation in the sludge treatment line, the models given by Gernaey et al. (2014) for designing sludge thickeners and dewatering units are used. Below, the details of the models are given and Figure 4.4 summarizes the model assumptions.

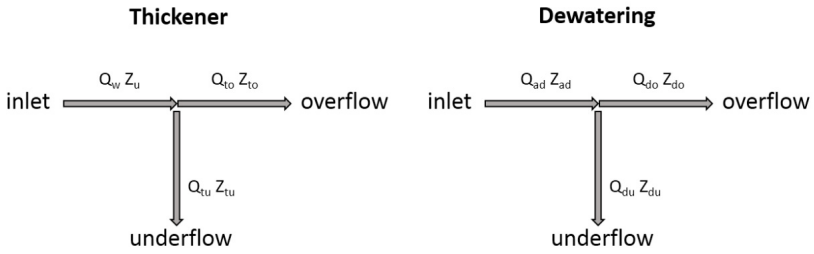


Figure 4.4 Model assumptions for thickener and dewatering design (Gernaey et al., 2014)

- In equations 4.76 – 4.78, TSS_{sc} represents the suspended solids concentration at the inlet of the thickener, p_{thick} is the percentage of suspended solids in the underflow and TSS_{rem} is the percentage of suspended solids removed. The thickening factor f_{thick} is calculated by equation 4.76 and the thinning factor f_{thin} is represented by equation 4.78. Moreover, equations 4.79 – 4.84 are used to calculate the model variables. A similar procedure is followed for the dewatering design, which is summarized through equations 4.85 - 4.93.

$$f_{thick} = p_{thick} \frac{10000}{TSS_{sc}} \quad 4.76$$

$$fq_{tu} = \frac{TSS_{rem}}{100\, f_{thick}} \quad 4.77$$

$$f_{thin} = \frac{1 - TSS_{rem}/100}{1 - fq_{tu}} \quad 4.78$$

For the underflow:

For particulate fractions: $Z_{tu} = Z_u \,.\, f_{thick}$ 4.79

For soluble fractions: $Z_{tu} = Z_u$ 4.80

Underflow rate: $Q_{tu} = Q_w \,.\, fq_{tu}$ 4.81

For the overflow:

For particulate fractions: $Z_{to} = Z_u \,.\, f_{thin}$ 4.82

For soluble fractions: $Z_{to} = Z_u$ 4.83

Overflow rate: $Q_{to} = Q_w \,.\, (1 - fq_{tu})$ 4.84

$$f_{dewat} = p_{dewat} \frac{10000}{TSS_{ad}} \quad 4.85$$

$$fq_{du} = \frac{TSS_{rem}}{100\, f_{dewat}} \quad 4.86$$

$$f_{thin} = \frac{1 - TSS_{rem}/100}{1 - fq_{du}} \quad 4.87$$

For the underflow:

For particulate fractions: $Z_{du} = Z_{ad} \cdot f_{dewat}$ 4.88

For soluble fractions: $Z_{du} = Z_{ad}$ 4.89

Underflow rate: $Q_{du} = Q_{ad} \cdot fq_{du}$ 4.90

For the overflow:

For particulate fractions: $Z_{do} = Z_{ad} \cdot f_{thin}$ 4.91

For soluble fractions: $Z_{do} = Z_{ad}$ 4.92

Overflow rate: $Q_{do} = Q_{ad} \cdot (1 - fq_{du})$ 4.93

4.2 Generation of generic process interval model

The information about the generated superstructure and the design of the treatment technologies, which are placed in the superstructure, has to be stored and sent to the optimizer. The optimization problem has a number of parameters defined, as previously shown in section *3.3.2*, and the values of these parameters are calculated based on the individual treatment unit designs employed, stored in matrices in an MS Excel based structure and finally sent to the optimizer for being used in the solution of the optimization problem (see Figure 3.5). In this section, the generation of the database (i.e. the parameters stored in the MS Excel based structure) is defined in detail.

Superstructure definition

The first thing that has to be defined in the database is the superstructure; this is done by defining the names of the process intervals (index *k*), their locations in the superstructure and the connection streams between the process intervals. Below, the structure is exemplified by illustrating it in two different matrices. In Table 4.8, a matrix showing the names of the process intervals and their locations under the tasks is illustrated. The names of the process intervals, which are shown on the left side column of the matrix constituting the index *k*; and their allocation under the tasks (from 1 to 4 on the top row) are further used in the optimization problem to constitute the logical cuts (i.e. selection of only one process interval from each task).

Table 4.8 Definition of process interval names (on the left) and locations under the tasks (on top 1-4)

	1	**2**	**3**	**4**
I-1	1			
I-2	1			
II-1		1		
II-2		1		
II-3		1		
III-1			1	
III-2			1	
IV-1				1
IV-2				1

In Table 4.9, the matrix used to define the possible connection streams between the process intervals is shown. The letters P, S and T stand for primary outlet, secondary outlet and tertiary outlet, respectively. When this matrix is generated by the user, three other similar matrices are generated automatically storing the same information defined in number form (0 - if the connection is not defined and 1 - if the connection is defined) for three different outlet streams. These matrices constitute the data associated to the parameter $S_{k,kk}$ shown in equation 3.10.

Table 4.9 Definition of connection streams between process intervals

	I-1	**I-2**	**II-1**	**II-2**	**II-3**	**III-1**	**III-2**	**IV-1**	**IV-2**
I-1			P	P	P				
I-2			P		P				
II-1						P	P		S
II-2						P	P		S
II-3						P			S
III-1			T	T	T			P	
III-2			T	T				P	
IV-1									
IV-2									

Definition of components, reactants and characterization of wastewater

One of the indexes used in the optimization problem is the component index *i*. Components of the optimization problem are constituted by (1) the flow rate (i.e. the water, sludge and gas streams in L^3/t), (2) the pollutants in the influent wastewater stream, (3) the utilities added in the treatment units, and (4) the components produced in the reactions such as: methane, nitrogen gas, carbon dioxide and various by-products. Therefore, while building the optimization problem, the component list should be created and stored in the database.

A subset of the component index, which is named as the *react* index, stores the list of key reactants and should be given as an input to the optimizer. A key reactant is simply a component, which is removed in a reaction with a known efficiency; moreover, as a result of its removal, other components are either consumed or produced with the specified stoichiometry (details of this step are presented below under *Definition of reaction* section). Each reaction has one key reactant; however, within one treatment unit, the user can define several reactions and thus several components can be assigned as the key reactant.

The matrix $\phi_{i,kk}$ is storing the data for the wastewater composition (see equation 3.13). An illustrative matrix, shown in Table 4.10, demonstrates the data stored in the database for parameter $\phi_{i,kk}$. This parameter assigns the mass flow rate of the pollutants/components, in M/t units, into the process intervals under the first column of the superstructure, which is designated for the wastewater sources.

Table 4.10 Definition of the wastewater characterization

$\phi_{i,kk}$	**I-1**	**I-2**	**…**
i_1	$\phi_{i1,I-1}$	$\phi_{i1,I-2}$	…
i_2	$\phi_{i2,I-1}$	…	…
…	…	…	…

Definition of utility addition

The utilities are any type of component or service that is added or used during the operation of a treatment unit. In this sense, as the oxygen addition is defined as a utility; the electricity consumption, external carbon dosage or chlorine addition are also considered as utility added by the stream *R* shown in Figure 3.4 and formulated by equation 3.3. As mentioned above, the utilities are listed together with all the other components with the index *i*. At this point, some additional definitions have to be made, which are (1) the amount of utility to be added into the system and (2) the fraction of it that is mixed with the main stream. The utility addition functions in two different ways. First, it supplies the utilities necessary for the reaction to proceed and also, the utility cost is calculated by using the stream *R*.

The parameter $\mu_{i,ii,kk}$ determines the amount of utility to be added and it is defined by a matrix which is shown in Table 4.11. The index *i* refers to the utilities; whereas the index *ii* refers to the full list of components as shown in the first two columns of the matrix. Since utility requirements of different treatment technologies might differ, the parameter also has the index *kk* which allows to define different values for different process intervals. Equation 4.94 shows how $\mu_{i,ii,kk}$ is calculated. It is basically the ratio of *the amount of utility i added* to *mass flow of component ii entering the interval kk*. While these values can be taken as the stoichiometric utility requirements (for instance, stoichiometric oxygen requirement for nitrification), they can also be taken from the open literature as common operational experiences (an example might be the necessary ozone dose to accomplish complete disinfection in terms of *mass of ozone/volume of wastewater treated*).

The parameter $\alpha_{i,kk}$ on the other hand, which is also illustrated in Table 4.11, defines the fraction of the utility added - *i* that is mixed with the main stream in the interval *kk*. This parameter therefore takes values between 0 and 1. For instance, when oxygen is added as the utility it has to mix with the main stream to further enter the reaction; on the contrary, if electricity is considered as the utility, it does not mix with the main stream.

Table 4.11 Definition of utility addition

$\mu_{i,ii,kk}$		kk_1	kk_2	…
u_1	i_1	$\mu_{u1,i1,kk1}$		
u_2	i_2		$\mu_{u2,i2,kk2}$	
…	…			

$\alpha_{i,kk}$	kk_1	kk_2	…
u_1			
u_2		$\alpha_{u2,kk2}$	
…			

$$\mu_{i,ii,kk} = \frac{amount\ of\ utility\ i\ added}{mass\ flow\ of\ component\ ii\ entering\ the\ process\ interval\ kk} \quad 4.94$$

Definition of reaction

In the direction of the flow, after mixing and utility addition, the generic process interval model proceeds with the reaction(s). As previously illustrated in equation 3.4, reaction is defined such that the key reactant is consumed with a given efficiency - $\theta_{react,kk,rr}$ and the other components are produced or consumed according to a stoichiometry which is stored in a stoichiometry matrix - $\gamma_{i,kk,rr}$.

The reaction efficiency is given as the reported/calculated removal efficiency of the key reactant. The key reactant is selected as a representative compound, whose removal efficiency can easily be calculated or found in the literature; as well as the other components can easily be related to its removal by stoichiometry. For instance, in partial nitritation, ammonium nitrogen is removed with 50% efficiency and nitrite nitrogen is produced and oxygen is consumed accordingly. Therefore, in this case ammonium nitrogen is selected as the key reactant. Another example could be as follows: in a high rate activated sludge treatment unit, COD is reduced by approximately 60% and accordingly biomass is produced and oxygen is consumed; thus, a biodegradable COD component (either X_S or S_S) can be selected as the key reactant.

The stoichiometry matrix is illustrated in Figure 4.5. There are two ways of calculating the stoichiometry data: (1) from a given reaction, using directly the reaction stoichiometry (e.g. partial nitritation/anammox reaction) or (2) from the known influent and effluent concentrations calculated by the design models by using equation 4.95. The resulting reaction/design data are converted into a matrix which the MI(N)LP routine can use.

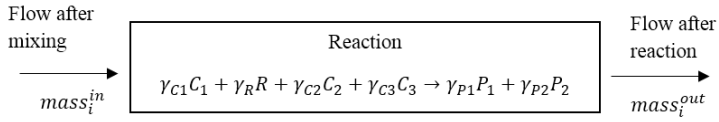


Figure 4.5 Illustration of reaction occurring in the process interval and its stoichiometry

$$\gamma_{i,kk,rr} = -\left(\frac{F_{i,kk}^{mix} - F_{i,kk}^{reac}}{F_{react,kk}^{mix} - F_{react,kk}^{reac}}\right) \quad 4.95$$

Definition of flow, waste and phase separation

In some treatment units, a fraction of the total flow is recycled to another compartment of the same unit (e.g. nitrate recirculation in pre-denitrification type activated sludge systems). Moreover, in some treatment plants, sludge wastage is done from the reactor rather than the secondary sedimentation underflow. In order to model internal recycle flow and sludge wastage flow, flow separation is defined within the generic process interval. It is also used to define the separation of sedimentation tank underflow into two streams (as shown in Figure 3.4): sludge wastage and sludge recycle flows. In this kind of separation, the composition of the flow in terms of concentration of the compounds does not change; it is separated into two fractions with the same composition. For this purpose three parameters are defined: SP_{kk}^1, SP_{kk}^2 and SP_{kk}^3. These parameters are specifically defined for the process intervals, and therefore they are stored in the database with the *kk* index. They take values between 0 and 1, which are calculated with respect to selected internal and external recycle ratios as well as the calculated sludge wastage flow rate from the system SRT (eq. 4.18).

Waste separation is identified as the separation of any type of waste components produced in the treatment unit from the main flow. In the wastewater treatment context, the most significant use of this flow is for the separation of gases that are produced in the open reactors. The parameter $W_{i,kk}$ is defined in order to formulate this kind of separation (as shown in equation 3.8). It is identified by two indexes – the component index and the process interval index, which means that different waste separation fractions can be defined for different components in different treatment units. The parameter takes values between 0 and 1 depending on the fraction of the waste component to be separated from the main flow. It is also important to mention that, this waste flow is not further directed to the other process intervals; however it can be used to assign a cost value to the produced waste or define a constraint (e.g. constraint on greenhouse gas emissions).

Finally, the third type of separation defined in the generic process interval model is the phase separation, which corresponds simply to the task carried out by the sedimentation

tank. Phase separation is formulated by equation 3.9, where the parameter $split_{i,kk}$, determines the fraction of each component to be diverted into two different streams. Similar to the parameter defining waste separation, the *split* parameter takes different values for different components in different process intervals. Usually, the soluble components and the component defining the total flow rate are given the same split factors whereas particulate components are separated depending on their non-settleable fraction. In this way, the concentration of the soluble components does not change after the separation (as in the case of secondary sedimentation) while particulates accumulate in the underflow.

Definition of sink limitations

In order to ensure a WWTP network selection satisfying the effluent limits defined by the user, sink limitation constraints should be formulated as shown in equation 3.14. To this purpose a parameter is defined - $Lim_{i,kk}$, which stores the limit values for component *i* valid for the sink process interval *kk*. The limit definition, however, is made in two different ways for two different problem types. For the deterministic solution of the problem, the sink limitations are formulated as constraints; therefore, a network (combination of process intervals), which cannot satisfy the limitations, is eliminated by the optimizer. However, when the problem is solved under uncertainty, the constraints are relaxed such that if the effluent limit is violated by a selected network then a penalty should be paid. The penalty is in this case added in the objective function and thus it is minimized together with all the other cost items. The motivation behind defining sink limitations in two different ways can be explained as: (1) the deterministic solution, which can go further through the design stages as the best selected network option, should satisfy the regulated effluent limitations; in other words, a WWTP cannot be designed to pay an effluent penalty for its entire lifetime and (2) it is important to observe how the selected network under deterministic conditions will behave under uncertainty, especially in certain scenarios in which it cannot satisfy the effluent limitations (i.e. how much is the gap between the defined limit and the actual effluent concentration and the regarding effluent penalty that the plant is liable for).

Definition of economic models and objective function

The economic models which constitute the objective function are shown above in section 3.3.2 by equations 3.15 to 3.20. In the formulations of U_{cost}, S_{cost}, P_{cost} and *CAPEX* (i.e. the cost models correspond to utility cost, cost related to sink intervals, product cost and capital cost, respectively) the parameters $P1_k$, $P2_i$ and $P3_{kk}$ are the unit cost parameters

and associated data needed to be collected from the open literature, expert knowledge and/or equipment/service suppliers.

$P1_k$ is used in the capital cost equation and represents the cost of a particular treatment unit (e.g. aerated reactor, sedimentation tank, anaerobic reactor) per unit volume (i.e. unit cost/L^3 units). It is stored in the database in a matrix format with the index *k*, thus having different values for different process intervals. Another parameter used in the capital cost equation is V_k which stands for the volume of the treatment units in L^3. Consequently, the *CAPEX* equation (equation 3.19) calculates the total capital cost of the selected network.

$P2_i$ corresponds to the unit cost for the utilities (i.e. unit cost/amount of utility added) and is used to calculate the total utility cost of the selected network. The parameter can be given in different units depending on the type of the utility. If the utility is oxygen then its unit becomes unit cost/M of oxygen; on the other hand, the utility addition corresponding to electricity used is defined by cost of unit electricity use (i.e. unit cost/kWh).

Lastly, $P3_{kk}$ is the cost parameter associated with any cost item related to individual process intervals, which can be a treatment unit, source or sink process interval. For instance, any taxation related to sinks and sources can be added by this parameter. Moreover, any extra operation cost related to treatment units (e.g. carriers, membrane etc.) are also added into the database by using this parameter.

Definition of uncertain parameters and their domain

When the uncertain domain is sampled by using the LHS method, a number of values (i.e. the determined number of future scenarios) for the parameter are obtained. These values are also stored in the database as matrices. Consequently, for the uncertain parameters, two different matrices are present in the database with two different parameter names: the deterministic values and a set of values representing the future realizations.

In order to define the future scenarios, another index definition is made, which is index *sc,* and it refers to the scenario index. Therefore, the new parameter defined to represent the uncertain domain has an additional index in its representation. For instance, the parameter $\phi_{i,kk}$, which represents the influent wastewater composition, is highly uncertain so it is one of the primary parameters that is considered while performing uncertainty analysis. The new parameter defined to represent the uncertain space is named $\phi^{unc}_{i,kk,sc}$ and represented as shown in Table 4.12. Similarly, all the other uncertain parameters are defined in the database with the addition of the index *sc* and the corresponding values for future scenario definitions are inserted into the matrices.

Table 4.12 Definition of the uncertain domain of wastewater characterization

$\phi_{i,kk,sc}^{unc}$		**sc1**	**sc2**	**sc3**	**…**
i_1	**I-1**	$\phi_{i1,I-1,sc1}^{unc}$	$\phi_{i,I-1,sc2}^{unc}$	…	
i_2	**I-1**	$\phi_{i2,I-1,sc1}^{unc}$	…	…	
i_1	**I-2**	…	…	…	
…	**…**				

An illustrative example

After describing the treatment unit design models and generation of the generic process interval model parameters; in this part of the chapter, an illustrative example is presented. To this end, a pre-denitrification type of treatment unit is selected. However, the design methodology is exemplified in details in the case studies chapter (specifically under the section 5.1.3); therefore, here the design outputs are converted into the generic process model parameters and presented below.

The system is selected as a pre-denitrification type AS treatment unit with an SRT of 10 days and HRT of 9.6 hours – represented as BNR10. The unit was designed according to Design Model no.1 (presented in section 4.1.1.2) and the corresponding mass flows of the components are converted into the flow definitions of the generic process interval model (illustrated in Figure 3.4) as shown below in Table 4.13. All the steps given below from 1-8 are automated in an MS Excel based structure and once the data from unit design model is inserted into the table (as given in red), the remaining data are calculated automatically. The formation of Table 4.13 and generation of model parameters are detailed below in steps 1-8.

Table 4.13 Mass flow of components inside the BNR10 process interval (the numbers in red are the inserted numbers from data collection step, the numbers in black are the calculated numbers)

Component	Unit	F	F_{in}	R	F_{mix}	F_{reac1}	F_{reac}	F_{sep}	F_{w}	F_{rec2}	F_{out1}	F_{out2}	F_{out3}
Q	m^3/d	72000	144000		144000	144000	144000	141120	141120	72000	69120	0	2880
S_I	kg/d	1690.56	3381.438		3381.438	3381.12	3381.12	3313.498	3313.498	1690.878	1622.62	0	67.6224
S_S	kg/d	7765.2	7765.2		7765.2	0	0	0	0	0	0	0	0
S_O	kg/d	0	144.0271	20207	20351.03	288	288	282.24	282.24	144.0271	138.2129	0	5.76
S_{NO}	kg/d	0	763.3435		763.3435	4959.36	1526.4	1495.872	1495.872	763.3435	732.5285	0	30.528
S_{ND}	kg/d	0	0		0	0	0	0	0	0	0	0	0
S_{NH}	kg/d	2365.2	2413.449		2413.449	96.48	96.48	94.5504	94.5504	48.24907	46.30133	0	1.9296
X_I	kg/d	6711.84	167431.9		167431.9	167760	167760	164404.8	164404.8	164076	328.8096	0	3355.2
X_S	kg/d	18118.8	9998.788		9998.788	960.48	960.48	941.2704	941.2704	939.3879	1.882541	0	19.2096
X_{BH}	kg/d	0	132669.2		132669.2	135648	135648	132935	132935	132669.2	265.8701	0	2712.96
X_{BA}	kg/d	0	19435.61		19435.61	19872	19872	19474.56	19474.56	19435.61	38.94912	0	397.44
X_P	kg/d	0	15914.67		15914.67	16272	16272	15946.56	15946.56	15914.67	31.89312	0	325.44
X_{ND}	kg/d	705.6	30506.16		30506.16	30830.4	30830.4	30213.79	30213.79	30153.36	60.42758	0	616.608

1. The components of the optimization problem defined for this specific unit are given in the first column of Table 4.13. These components can also be used to define the other units in the superstructure. If additional components are used for different types of units (e.g. electricity for a UV disinfection unit, ozone for an ozone disinfection unit, methanol for Sharon unit etc.), they can also be added in the components list. The only utility used in this unit is oxygen – S_O and it is specified in the utility list.
2. The stream composition under the flow F is inserted into the table as the pre-defined influent wastewater characterization given in the *Problem Definition* step of the framework. This composition is also given to the optimizer as the wastewater characterization stored in $\phi_{i,kk}$ matrix.
3. F_{in} is calculated by summing up the influent flow F and the recycle flow F_{rec2}.
4. F_{mix} is the flow after mixing the influent flow F_{in} with the utility flow R, which is inserted as the calculated oxygen demand of the unit. At this step the definitions of parameter $\mu_{i,ii,kk}$ - the amount of utility to be added and $\alpha_{i,kk}$ - the fraction of the utility added that is mixed with the main stream, are done. As mentioned above, the only utility considered in this unit is oxygen; it is required in the unit for cell decay and nitrification. The mass flow of oxygen given in Table 4.13 under the column R is the sum of oxygen amount required for two mechanisms; however, the unit design specifies the oxygen requirements for different mechanisms separately and the value of parameter $\mu_{i,ii,kk}$ is calculated based on those values. Accordingly, 12460 kg/d oxygen is required for nitrification and the corresponding $\mu_{i,ii,kk}$ value is calculated based on influent S_{NH} mass flow; and 7747 kg/d is necessary for cell decay and the corresponding $\mu_{i,ii,kk}$ value is calculated based on influent S_S mass flow as shown below. It is required that all the added oxygen is mixed with the main stream therefore the parameter $\alpha_{So,BNR10}$ is taken as 1.

$$\mu_{So,Snh,BNR10} = \frac{12460}{F^{in}_{Snh,BNR10}} \quad 4.96$$

$$\mu_{So,Ss,BNR10} = \frac{7747}{F^{in}_{Ss,BNR10}} \quad 4.97$$

5. The reactions defined in this unit consist of several mechanisms: organics removal, nitrification and denitrification. Here the reaction is defined as to proceed as two consecutive reaction blocks; therefore, an extra flow F_{reac1} is defined. Within the first reaction block, in the first reaction the S_S and X_S are removed and the corresponding particulate organic components are produced. Their concentration is maintained in the system with the recycle flow. In a second reaction in the first reaction block, S_{NH} is nitrified and as a result S_{NO} is produced. In the second reaction block, S_{NO} is removed with a given efficiency, which is also determined from the unit design. Consequently, the flow F_{reac} is also inserted into

the table as the steady state concentrations of the components in the reactor. The calculated $\gamma_{i,kk,rr}$ and $\theta_{react,kk,rr}$ values for two reaction blocks and a total of 4 reactions are given in Table 4.14.

Table 4.14 Reaction definition for BNR10 unit

	Gamma1 for reaction block 1			**Gamma2 for reaction block 2**
	Reactant			**Reactant**
Component	**S_S**	**S_{NH}**	**X_S**	**S_{NO}**
S_I	0			
S_S	-1			
S_O	-2.58371			
S_{NO}		1.810994		-1
S_{ND}		0		
S_{NH}		-1		
X_I	0.042251			
X_S			-1	
X_{BH}	0.383613			
X_{BA}	0.056198			
X_P	0.046017			
X_{ND}		0.13994		
Theta	100%	96%	91%	84%

6. F_{reac} is separated into two streams of the same quality to obtain the sludge wastage flow. The unit design gives the sludge wastage flow rate (as shown in red in the F_{out3} column). Therefore, the corresponding mass flow rates of the components are calculated according to the parameters SP^1_{BNR10}, SP^2_{BNR10} which are calculated as 0.02 and 1, respectively.
7. In this unit, there is no waste flow defined so F_w is identical to F_{sep} and the value of parameter $W_{i,BNR10}$ for all the components are 0.
8. The recycle flow rate is also defined in the design of the treatment unit therefore sludge recycle flow rate is inserted into the table as shown in red in the F_{rec2} column. Then, the effluent water stream flow rate (i.e. F_{out1} stream) is calculated as the difference between F_w and F_{rec2} knowing that there is no secondary outlet (i.e. F_{out2} stream) in this unit because the sludge wastage is done from the tertiary outlet. Then, the next step is the calculation of the $split_{i,kk}$ parameter. This parameter is the ratio between the F_w and F_{out1} streams. It takes different values for different components. However, within the context of this unit, it takes two different values for (1) soluble components and flow rate, and (2) particulate components. The first value is calculated as the ratio of the flow rates (i.e. 69120

/ 141120), and the second value is taken as the fraction of non-settleable particulates in the settler and assumed to be 0.002. Finally the value of parameter SP^{3}_{BNR10} is taken as 1 as there is no defined tertiary outlet and all the settler underflow is directed to the sludge recycle stream.

5 CASE STUDIES

In the fifth chapter, the synthesis, design and retrofitting framework is applied on two case studies constituting examples for a design and a retrofitting study, respectively. In the case studies, the use of the developed methodology and database is highlighted. In the first case study, the wastewater composition given by the Benchmark Simulation Model no.2 is taken and a design study is performed; the second case study deals with two full-scale WWTPs from the Copenhagen region and seeks for retrofitting options by defining novel technologies in the design space. The case studies are presented in a structured way, by following the steps of the proposed framework.

5.1 Benchmark wastewater treatment plant

The Benchmark wastewater treatment plant (B-WWTP) case study has been built as a simple yet representative case study in order to illustrate the application of the proposed methodology. In the context of the case study, the wastewater characterization is taken from Benchmark Simulation Model no.2 (BSM2) (Gernaey et al., 2014). The BSM2 is selected for the case study since this plant layout is generally known in the wastewater treatment modelling community. The formulated optimization problem is solved both under deterministic conditions and uncertainty. Several scenarios are defined and solved and the results are analyzed below in this chapter.

5.1.1 B-WWTP Problem definition

The problem is defined as treatment of domestic wastewater comprising mainly COD, nitrogen and solids as pollutants. The wastewater composition is shown in Table 5.1. Accordingly, the influent total COD is *460.67 g COD/m^3* and total nitrogen is *45.64 g N/m^3*. The objective is to design the WWTP network against the lowest operational cost (aeration cost, sludge disposal cost, pumping and mixing cost as well as biogas price) and capital cost possible; while satisfying the effluent limitations for organic material and nitrogen in the water stream to be discharged into the environment. This problem is defined as a design problem with a given wastewater characterization.

Table 5.1 Influent wastewater characterization, average composition (Gernaey et al., 2014)

Component	Value	Unit
S_I	27.23	g COD/m^3
S_S	58.18	g COD/m^3
X_I	92.49	g COD/m^3
X_S	363.94	g COD/m^3
$X_{B,H}$	50.68	g COD/m^3
$X_{B,A}$	0	g COD/m^3
X_P	0	g COD/m^3
S_O	0	g -COD/m^3
S_{NO}	0	g N/m^3
S_{NH}	23.86	g N/m^3
S_{ND}	5.65	g N/m^3
X_{ND}	16.13	g N/m^3
S_{ALK}	7	mole /m^3
Q	20,648	m^3/d

5.1.2 B-WWTP Superstructure definition

The superstructure developed for this problem is shown in Figure 5.1 together with the explanation about each process interval (i.e. treatment technology in the superstructure) in Table 5.2.

The superstructure consists of a domestic wastewater source interval in the source column and sinks for effluent water, sludge and biogas in the last column. Treatment technologies are located in between the source and the sinks, and include primary treatment, secondary treatment, tertiary treatment, disinfection and sludge treatment as the tasks.

For the primary treatment, the only technology put into the superstructure is the primary clarifier (PC). For the secondary treatment, three different biological treatment units are present: (1) Modified Ludzack Ettinger (MLE) system characterized by its low SRT, two different zones depending on the presence of oxygen: an aerated zone for nitrification and an anoxic zone for denitrification; as well as the internal recirculation flow for nitrate recycle; (2) Oxidation ditch, which has a relatively higher SRT and similar to the MLE technology includes different zones for nitrification and denitrification; however, in this case, since the reactor is designed in the carrousel shape, no separate internal recirculation is needed. Finally (3) the Upflow anaerobic sludge blanket (UASB) technology works under anaerobic conditions and produces biogas as a result of degradation of organics. While the first two technologies are proven to be effective in terms of organic matter and nitrogen removal, the UASB type of reactors only perform organic matter destruction. For this reason, a tertiary treatment is added into the superstructure with the aim of performing nitrogen removal. The two different technologies put here are: Sharon, which is responsible for nitritation – denitritation and a Sharon reactor coupled with an Anammox reactor to perform partial nitritation and anaerobic ammonia oxidation, respectively. Disinfection technologies comprise different means of treatment with respect to the disinfection agent or method applied: UV, O_3 and chlorine. The sludge treatment line consists of sludge stabilization options namely anaerobic digestion and aerobic digestion, which are receiving the sludge from a Thickener.

For each task, there is an additional process interval defined as the By-pass interval (except for the sludge thickener). Therefore, if the task is not needed for the specific problem defined, it can be by-passed through this process interval.

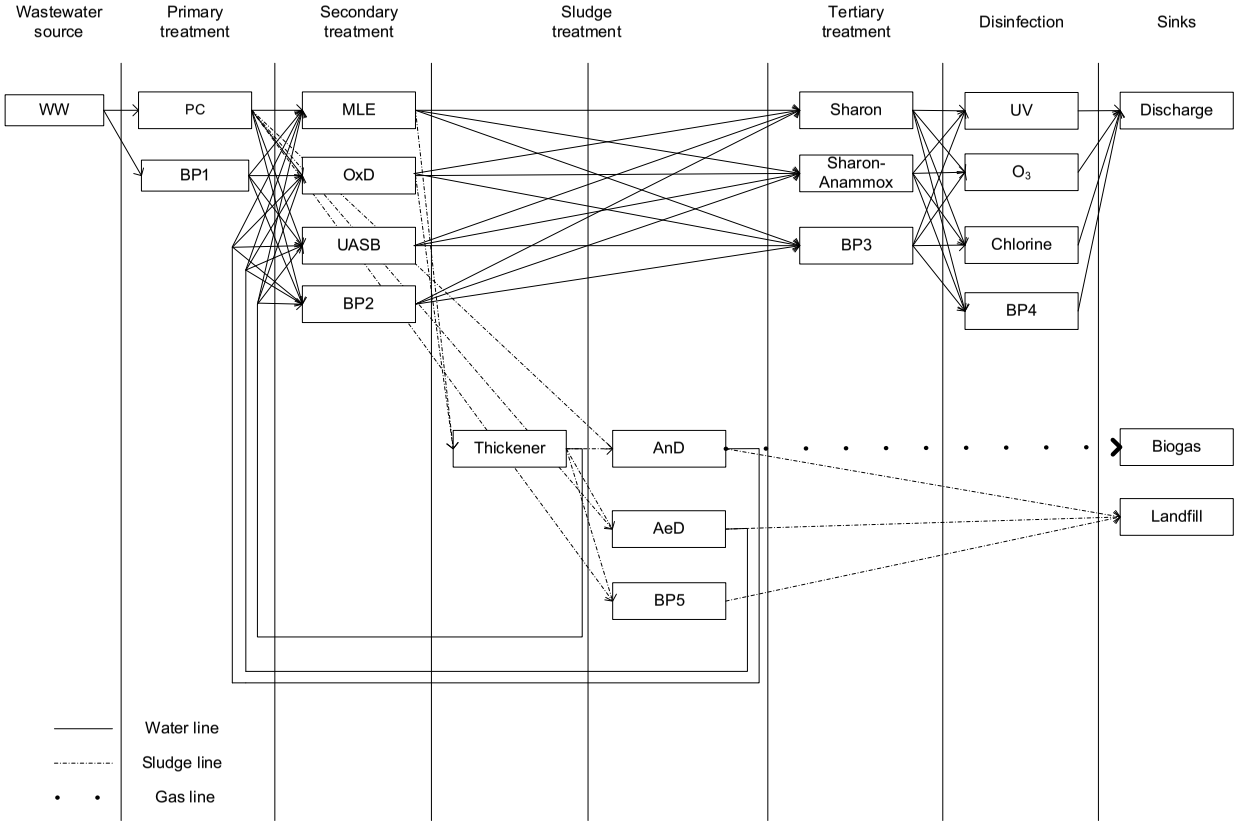


Figure 5.1 Superstructure developed for B-WWTP case study

Table 5.2 Process interval definitions for the B-WWTP superstructure

Name	Definition
WW	Wastewater source
PC	Primary clarifier
MLE	Short-SRT biological nutrient removal system (Modified Ludzack Ettinger)
OxD	Long-SRT biological nutrient removal system (Oxidation Ditch)
UASB	Upflow anaerobic sludge blanket
Thickener	Sludge thickener
AnD	Anaerobic sludge digester
AeD	Aerobic sludge digester
Sharon	Nitritation – Denitrification system
Sharon-Anammox	Partial nitritation – Anammox system
UV	Disinfection by using UV
O_3	Disinfection by using O_3
Chlorine	Disinfection by using chlorine
Discharge	Sink interval for water effluent
Biogas	Sink interval for biogas
Landfill	Sink interval for sludge disposal
BP 1 – 5	By-pass intervals

5.1.3 B-WWTP Data collection & Generic process interval model generation and validation

5.1.3.1 B-WWTP Data collection and design of individual treatment technologies

The development of the database for the represented superstructure was done by following the steps of the systematic data collection and design procedure given in Figure 3.3.

Design of Primary Treatment Alternatives

Primary treatment is carried out in a primary settler which separates a part of the solids from the wastewater stream and directs them to sludge treatment alternatives. The settler design was done so that the *split* values for particulate and soluble components in the wastewater stream were set. Consequently, 99.3% of the soluble and 50% of the particulate components by mass leave the primary sedimentation tank with the water effluent stream while the rest is sent to underflow (Gernaey et al., 2014). The sizing of the settler was done by applying equations 4.73 and 4.75 iteratively. The values for *SOR* and t_d are given by Tchobanoglous (2003) as a range. The resulting volume of the primary sedimentation tank is then calculated to be $1{,}537\ m^3$.

Design of Secondary Treatment Alternatives

The wastewater characterization of BSM2 (i.e. the composition given in Table 5.1) represents a raw wastewater source; in other words, it constitutes a high amount of solids. For this purpose, in order to design the secondary treatment units, the pre-settled wastewater characterization of Benchmark Simulation Model no.1 (BSM1) is used. The BSM1 average dry weather wastewater composition comprises approximately 50% less total suspended solids (TSS) as compared to the raw wastewater composition of BSM2, and is given in Table 5.3 (Copp, 2002). The pollutants are represented by ASM1 components (Henze et al., 2000). The effluent limits given in the Urban Wastewater Treatment Directive (91/271/EEC) are taken as a reference for the sink intervals.

Table 5.3 Pre-settled wastewater characterization taken from BSM1 (Copp, 2002)

Component	Value	Unit
S_I	30.0	g COD/m^3
S_S	69.5	g COD/m^3
X_I	51.2	g COD/m^3
X_S	202.32	g COD/m^3
$X_{B,H}$	28.17	g COD/m^3
$X_{B,A}$	0	g COD/m^3
X_P	0	g COD/m^3
S_O	0	g -COD/m^3
S_{NO}	0	g N/m^3
S_{NH}	31.56	g N/m^3
S_{ND}	6.95	g N/m^3
X_{ND}	10.59	g N/m^3
S_{ALK}	7	mole /m^3
Q	18,446	m^3/d

The treatment plant has been designed for operating at 15°C. System specific design data has been collected from several sources (Tchobanoglous, 2003 and WEF, 2010) together with the temperature dependent biokinetic constants and stoichiometry information (Copp, 2002).

The secondary settler is incorporated into the secondary treatment process intervals (MLE and OxD) as the phase separation (see Figure 3.4). It is designed by defining a thickening factor representing the non-settleable fraction of the particulate components and a flow separation fraction. Accordingly, 48% of the soluble components and 0.2% of the particulates by mass leave with the water stream (Copp, 2002), while the rest is assumed to settle in the sludge zone. In order to satisfy that the concentrations of the soluble components do not change after phase separation the same separation factor is used for the soluble components and the component representing the total flow rate. Moreover, the volume of the sedimentation basin is calculated by assuming specific *SOR* and *SLR* values as well as a certain depth of the tank from a range given for circular clarifiers (WEF, 2010).

The main outcomes of the design procedure for secondary treatment alternatives are summarized in Table 5.4, whereas the details of the design procedure are given in Appendix 3.

Table 5.4 Process information for process intervals under the secondary treatment task

Properties	**Process Interval**		
Corresponding technology	Modified Ludzack-Ettinger (MLE)	Oxidation ditch (OxD)	Upflow Anaerobic Sludge Blanket (UASB)
Temperature (°C)	15	15	15
SRT (days)	14	28	120
HRT (hours)	12	24	14
Reactor volume (m^3)	9,223	18,446	12,956
Settler volume (m^3)	3,774	3,411	-
Anoxic/Aerobic volume ratio	0.6	0.6	-
MLSS (g/m^3)	3,410	3,032	18,590
Sludge wastage flow (% influent flow)	3.5	3.5	-
Sludge recycle flow (% influent flow)	100	100	-
COD removal efficiency (%)	88.4	87.78	68.5
Total N removal efficiency (%)	77.2	78.48	-

Design of tertiary treatment alternatives

The tertiary treatment alternatives are placed in the superstructure for removing the nitrogen from the wastewater stream. For this purpose two technologies were selected: Sharon and a two-stage Sharon/Anammox reactor. Below, the principle design parameters calculated by following the models presented in section 4.1.3 are given.

- For the Sharon system, the SRT is equal to its HRT and selected as *1 d* (Hellinga et al., 1998). The volume of the reactor is then calculated as *18,446 m^3*. For the two-stage Sharon/Anammox system, the sizing of Sharon reactor is maintained and an Anammox reactor is designed with the nitrogen removal rate of *10 kg $N/m^3.d$ (*van der Star et al., 2007). While calculating the nitrogen load into the tertiary treatment process intervals, the influent nitrogen is assumed not to be changing in the secondary treatment task; so that tertiary treatment can handle the maximum amount of nitrogen that is potentially entering the system. With regard to that assumption, the volume of the anammox reactor is calculated as *90 m^3*.
- The stoichiometry of the system is taken from equations 4.64, 4.65 for Sharon and 4.70 and 4.71 for 2-stage Sharon/Anammox reactors. Moreover, the removal efficiencies are taken as 86% and 60% (Hellinga et al., 1998) for the nitritation and denitritation mechanisms occurring in the Sharon reactor, whereas partial

nitritation and anammox are assumed to proceed with 50% and 80% efficiencies, respectively (van Dongen et al., 2001).

Design of sludge stabilization alternatives

- The anaerobic and aerobic sludge digesters are designed by following steps of the design models given in section 4.1.2.
- The influent sludge composition is defined based on the sludge wastage composition of a sample secondary treatment unit (i.e. sludge wastage composition by fixing the SRT of the AS type of unit) with and without the contribution of primary sludge. The design steps are repeated in order to observe the effect of influent characterization on the outputs by using a different influent composition.
- For the anaerobic digestion, the following observations have been made: (1) the change in the concentrations of S_I, S_S, S_O, S_{NO}, S_{ND}, X_I and X_{ND} are either very low or there is no change at all (some of these components are not present in the influent sludge stream); (2) the increase in the concentrations of S_{NH} and X_P are proportional to the decrease in the heterotrophic biomass concentration – X_{BH}; and, (3) the increase in the methane gas production is proportional partly to biomass degradation and partly to particulate biodegradable COD (i.e. X_S) reduction. Thus, the design has been made generic by defining three reactions based on three components- X_{BH}, X_{BA} and X_S where they are removed with 100% efficiency; and all the other components (S_{NH}, X_P and methane gas) are produced accordingly. Below, according to a particular influent composition definition shown in Table 5.5, the definition of design outputs are given in Table 5.6.
- For the design of aerobic digestion, the observations were similar. Only this time, instead of methane production, oxygen consumption is observed to be proportional to the destruction of biomass and particulate biodegradable COD. For the same influent composition defined in Table 5.5, the output of the aerobic digester design can be seen in Table 5.7.

Table 5.5 Sample influent characterization into the anaerobic digester

Parameter	Value	Unit
S_I	27	g COD/m^3
S_S	44	g COD/m^3
X_I	14,326	g COD/m^3
X_S	21,210	g COD/m^3
$X_{B,H}$	8,931	g COD/m^3
$X_{B,A}$	1,131	g COD/m^3
X_P	5,184	g COD/m^3
S_O	-	g -COD/m^3
S_{NO}	1.8	g N/m^3
S_{NH}	22	g N/m^3
S_{ND}	0	g N/m^3
X_{ND}	1,778	g N/m^3
Q	190	m^3/d

Table 5.6 Summary of design parameters in anaerobic digestion for the influent composition given in Table 3.5

Parameter	Value	Unit	Related equation / Reference
HRT	15	hours	Tchobanoglous, 2003
r_h	1.86	g COD/L.d	2.72
S_{bp}	2.69	g COD/L	2.73
Z_{AD}	1.95	g COD/L	2.74
S_{up}	19.51	g COD/L	2.75
S_m	24.69	g COD/L	2.76
X_S	4.26	g COD/L	2.77
X_p	14.32	g COD/L	2.78
S_{NH}	1.45	g N/L	2.81
X_{ND}	0.98	g N/L	2.82

Table 5.7 Summary of design parameters in aerobic digestion for the influent composition given in Table 3.5

Parameter	Value	Unit	Related equation / Reference
HRT	15	hours	Tchobanoglous, 2003
X_a	6.79	g COD/L	2.86
X_e	4.89	g COD/L	2.87
X_i	14.32	g COD/L	2.88
S_{NO}	1.39	g N/L	2.89
X_{ND}	0.89	g N/L	2.90
MO	3,720	kg/d	2.91
MO_n	1,217	kg/d	2.92

- The thickener unit is added into the superstructure as a separate process interval. The dewatering is incorporated into the sludge digestion units as phase separation (see Figure 3.4). The separation factors for the thickening unit are calculated as 0.02 and 0.94 for particulates and soluble components, respectively. In other words, 2% of the particulates and 94% of the soluble components by mass, leave with the water stream while the rest are concentrated into the underflow. These values are set to 1% and 95% for the particulate and soluble components, respectively in the dewatering unit.

Design of disinfection alternatives

All the disinfection units are assumed to remove the pathogens in the wastewater stream with 100% efficiency. At this point, the utility (chemical and/or electricity) addition requirements are defined based on information from the open literature.

- The electricity consumption of the UV system is defined as *45 kWh /m^3* of wastewater to be disinfected. This value is given for low pressure – high intensity systems (URS Corporation, 2004).
- The typical chlorine dosage for effective disinfection is given as *10-25 mg/L* (Tchobanoglous, 2003).
- Finally, the typical ozone dose for disinfection is reported as *10-15 mg ozone/L* of *wastewater treated* (Takahara et al., 2006).

Collection of operational and capital cost data

The objective function represents the TAC and it is formulated to be minimized. OPEX corresponds to the operational cost and is composed of aeration, electricity consumption, chemical addition, pumping, mixing and landfill cost as well as biogas price. CAPEX on the other hand, represents the capital cost. All the cost data are collected from information available in the open literature and summarized in Table 5.8.

Table 5.8 Cost information for operational and capital cost items

Cost item	Unit	Value/Range	Description/Assumption
Electricity consumption of oxygen transfer [1]	kg O_2/kwh	1.9 – 3.2	Coarse bubble diffusor
Sodium hypochlorite cost[2]	euro/kg	0.12	-
Energy requirement for ozone[3]	kwh/kg O_3	21 – 35.2	Sum of ozone generation (air feed), ozone contacting and all other uses (on the average)
Electricity cost[4]	euro/kwh	0.0978	In Denmark for industry
Landfill cost[5]	euro/t	107	In Denmark, on the average
Biogas price[6]	eurocent/m^3 methane	40.3	In Denmark (assumptions: 1 mole of methane is 24 L and 1 mole of methane accounts for 64 g of COD)
Capital cost – UASB[7]	US$/$m^3$	425	Based on the price level of 2006, for 100,000 PE
Capital cost – Aeration tank[7]	US$/$m^3$	175	Based on the price level of 2006, for 100,000 PE
Capital cost – Secondary settler[7]	US$/$m^3$	290	Based on the price level of 2006, for 100,000 PE
Capital cost – Primary settler[7]	US$/$m^3$	375	Based on the price level of 2006, for 100,000 PE
Capital cost – Sludge thickener[7]	US$/$m^3$	400	Based on the price level of 2006, for 100,000 PE
Capital cost – Anaerobic digester[7]	US$/$m^3$	350	Based on the price level of 2006, for 100,000 PE

[1] Siemens (2009)

[2] AWWA Michigan Section (2006)

[3] Tchobanoglous (2003)

[4] URL1 (2013)

[5] URL2 (2013)

[6] Hahn et.al (2010)

[7] van Haandel and van der Lubbe (2012)

5.1.3.2 B-WWTP Generic process interval model generation

After the data has been collected for individual treatment technologies, it has been converted into the generic process interval model parameters (as explained in section 4.2). The components, utilities and reactants of the formulated model are shown in Table 5.9. The formulated superstructure (i.e. process intervals and the interconnections) is illustrated in Appendix 3.

Table 5.9 Components, utilities and reactants for the B-WWTP case study

Components		Utilities	Reactants
Q	S_{NO}	S_O	S_S
S_I	S_{NH}	Ozone	S_{NH}
S_S	S_{ND}	Cl_2	$X_{B,H}$
X_I	X_{ND}	Electricity	$X_{B,A}$
X_S	CH_4		X_S
$X_{B,H}$	N_2		
$X_{B,A}$	Ozone		
X_P	Cl_2		
S_O	Electricity		
S_{ALK}			

The parameters are stored in matrixes in an MS Excel based structure prior to be sent to GAMS by using GDX utilities. All the parameters used for the B-WWTP case study are summarized in Appendix 4. Since, the process interval model, which is formulated in GAMS, is generic, the database is the main element which defines the specific design/retrofit problem. Therefore, the maintenance of the database (i.e. updating necessary data with respect to a change in the source etc.) will be ensured by the user by selecting and using the updated model parameters in the model generation step. Moreover, if there are constraints and conditions that are known about the treatment technologies, their combinations etc. from prior expert knowledge, it can also be included into the process interval model at this step.

For instance, in this particular case study, since it is known from expert knowledge that selection of a high SRT activated sludge technology (in this case oxidation ditch) together with the anaerobic digestion is not meaningful, this combination is eliminated from the search space by simply inserting a constraint in the problem formulation as shown in equation 5.1.

$$y(OxD) + y(AnD) \leq 1 \qquad 5.1$$

5.1.4 B-WWTP MILP formulation and deterministic solution

The MILP problem is formulated as previously shown in equations 3.27 – 3.30. The objective of the optimization problem is to select among the treatment alternatives so that the resulting treatment process flow diagram has the minimum TAC and at the same time satisfies the effluent limits given in the Urban Wastewater Treatment Directive (91/271/EEC). The formulated optimization problem is solved by using GAMS and specifically the solver CPLEX. The details of the deterministic solution are analyzed and discussed in this section for three scenarios corresponding to different objective function formulations:

- Scenario 1: The objective function covers only OPEX and the effluent limit for nitrogen is set to 15 mg N/L.
- Scenario 2: The objective function covers TAC with the effluent nitrogen limit set to 15 mg N/L.
- Scenario 3: The objective function covers TAC; however, this time the effluent nitrogen limit is set to 10 mg N/L.

The optimal process selection and value of the objective function after solution of the optimization problem are given in Table 5.10 for three different scenarios and the selected process flow diagram is illustrated in Figure 5.2. Under the conditions of the first scenario, tertiary treatment and disinfection tasks are by-passed (this is mainly because the secondary treatment is effective enough to meet the effluent nitrogen limit and there is no pathogen defined in the influent wastewater composition); the water stream is sent to the water sink interval after being treated by the primary clarifier and the low SRT MLE system whereas the sludge is stabilized in the anaerobic digester and sent to the sink interval. When the capital cost is also added into the formulation of the objective function (i.e. scenario 2), the network selection does not change; however an expected increase in the objective function is observed due to capital cost.

In the third scenario, the optimizer once again selects the MLE technology coupled with primary clarifier to treat the wastewater, and an anaerobic digester for sludge stabilization purposes.

Although the anaerobic treatment alternative of the UASB coupled with the nitrogen rich wastewater treatment alternatives of the tertiary treatment task can satisfy the effluent total nitrogen limit, the UASB alone cannot generate an effluent stream complying with the COD effluent limit criteria when operated at such low temperatures. Experimental work also showed the decrease in the efficiency of the UASB reactor with a decreasing temperature (Lew et al., 2004). Although anaerobic treatment of domestic wastewater has been successfully demonstrated in full scale all over the world, the conclusion here, however, is that in order to comply with the regulations, the system should either be operated at higher temperatures or it should be integrated with effluent polishing steps which are not included in the current superstructure (i.e. facultative ponds, sand filtration, constructed wetlands, trickling filters, physico-chemical treatment and activated sludge

treatment) (Henze et al., 2008). Therefore, this treatment alternative has not been selected by the optimizer for any of the scenarios as expected from the above-mentioned process engineering expertise.
The cost summary and the performance evaluation for the scenarios are presented in Table 5.11. MLE is favored both for its low operational cost (low utility requirement and high sludge production resulting in high biogas production) and relatively low capital cost.

Table 5.10 Summary of results for different scenarios

Scenario	Objective function	Total N limit (mg/L)	Selected Process Flow Diagram	Value of objective function (unit cost)
1	OPEX	15	WW-PC-MLE-BP3-BP4-Thickener-AnD-Discharge-Sludge-Biogas	219.051
2	TAC	15	WW-PC-MLE-BP3-BP4-Thickener-AnD-Discharge-Sludge-Biogas	912.080
3	TAC	10	WW-PC-MLE-BP3-BP4-Thickener-AnD-Discharge-Sludge-Biogas	912.080

Table 5.11 Cost summary and performance evaluation for the different scenarios

	Unit	Scenario 1	Scenario 2	Scenario 3
Objective function	-	OPEX & Total N limit of 15 mg/L	TAC & Total N limit of 15 mg/L	TAC & Total N limit of 10 mg/L
Aeration cost	unit cost	229.187	229.187	229.187
Landfill cost	unit cost	614.191	614.191	614.191
Biogas price	unit cost	695.058	695.058	695.058
Electricity cost	unit cost	-	-	-
Pumping cost	unit cost	43.687	43.687	43.687
Mixing cost	unit cost	27.044	27.044	27.044
Capital cost	unit cost	-	693.029	693.029
Objective function value	unit cost	219.051	912.080	912.080
Effluent COD	g COD/m^3	39.16	39.16	39.16
Effluent Total N	g N/m^3	9.82	9.82	9.82

The optimizer also gives the flow of components through the selected process flow diagram. The stream table of the components for the solution of Scenario 1 is shown in Table 5.12, where the flows are given as the flows after reaction – F_{reac} – in each process interval. By using this information, the selected process flow diagram is evaluated in terms of its performance, which is presented also in Table 5.11. It can be seen that both COD and total nitrogen concentrations are below the limits set by the regulations. This analysis shows that the selected process flow diagram is capable of decreasing the concentrations of the key pollutants below the effluent discharge limits while using minimum amount of utilities.

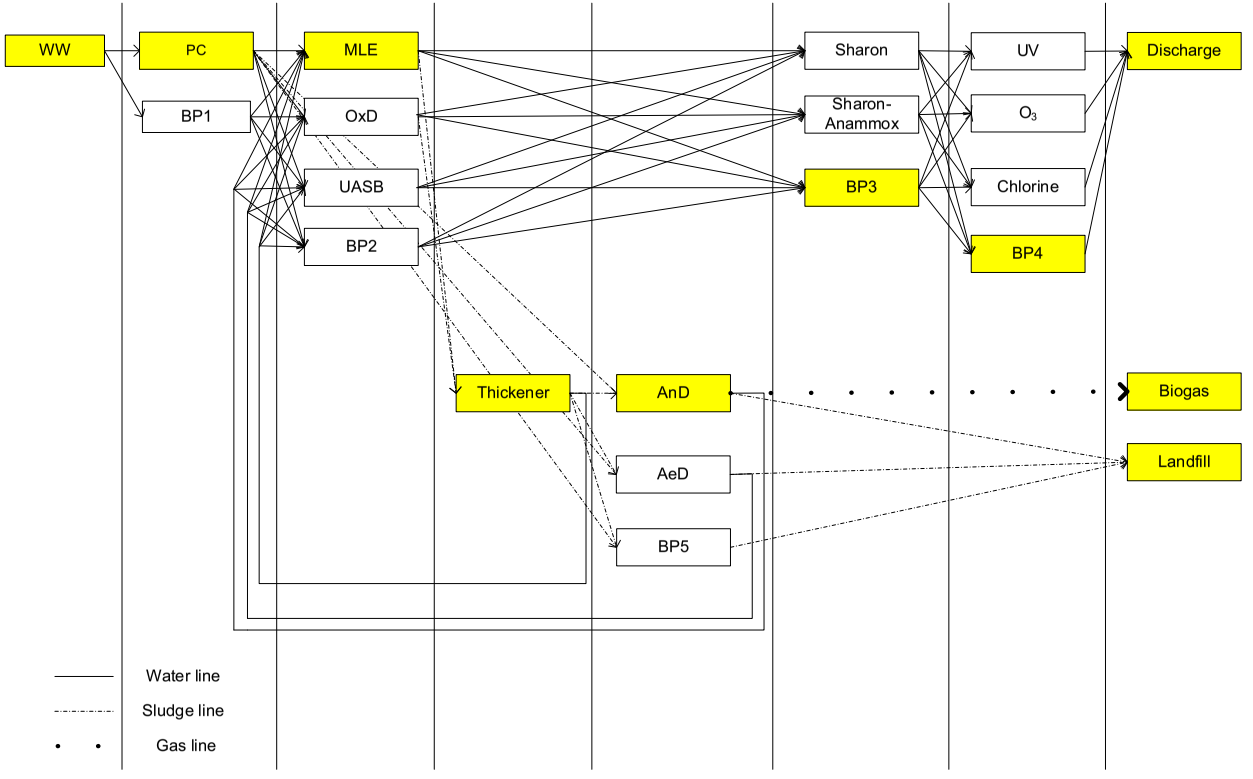


Figure 5.2 Process flow diagram and the interconnections

Table 5.12 Scenario 1 stream table

	Unit	WW	PC	MLE	BP3	BP4	Thickener	AnD	Discharge	Landfill
Q	m^3/d	20,648	20,648	42,633	20,553	20,553	763	190	20,553	95
S_I	kg/d	562	562	1,160.382	559.420	559.420	20.771	5.159	559.420	2.580
S_S	kg/d	1,201	1,201	-	-	-	-	8.407	-	4.203
S_O	kg/d	-	-	85,266	41,106	41,106	1,526	0	41,106	0
S_{NO}	kg/d	-	-	341.204	164.494	164.494	6.108	0.360	164.494	0.180
S_{ND}	kg/d	117	117	-	-	-	-	-	-	-
S_{NH}	kg/d	492	492	22.055	10.633	10.633	0.395	126.268	10.633	63.134
X_I	kg/d	1,909	1.909	52,521.861	105.044	105.044	1,811.664	2,743.809	105.044	2,724.602
X_S	kg/d	7,514	7,514	116.229	0.232	0.232	4.009	752.192	0.232	746.927
X_{BH}	kg/d	1,046	1,046	34,557.848	69.116	69.116	1,192.022	-	69.116	-
X_{BA}	kg/d	-	-	6,344.526	12.689	12.689	218.845	-	12.689	-
X_P	kg/d	-	-	29,234.094	58.468	58.468	1,008.387	1,031.705	58.468	1,024.483
X_{ND}	kg/d	333	333	5,167.206	10.334	10.334	178.235	342.536	10.334	340.138
CH_4	kg/d							4,599.228		

The model and solution statistics of the problem are given in Table 5.13. Accordingly, the solution time required for the problem containing *44,445* equations is *0.172* seconds.

Table 5.13 Model and solution statistics

Number of variables	42,319
Number of binary variables	20
Number of equations	44,445
Objective function	1
Execution time (s)	0.172
Solver	CPLEX

Validation of the deterministic solution

In order to validate the performance of the selected network (PC-MLE-AnD), the Matlab/Simulink model for BSM2 was used (Jeppsson, 2011). The SRT and HRT of the units and the influent wastewater composition are maintained to be the same in both cases and the performance results are summarized in Table 5.14. Accordingly, it is observed that the optimization mass-input output model which is based on steady state unit models performs better in terms of COD, NO_X-N nitrogen and total nitrogen components; on the other hand the more rigorous MATLAB/Simulink model removes the NH_4-N nitrogen with a higher efficiency. All in all, when the effluent limitations are considered for all the components, all the values are seen to be below the limits and therefore the errors are considered to be within acceptable limits.

Table 5.14 Validation of the deterministic solution

		Effluent concentrations	
Component	**Unit**	**GAMS (this study)**	**MATLAB/Simulink model**
COD	g COD/m^3	39.16	48.81
NH_4-N nitrogen	g N/m^3	0.52	0.18
NO_X-N nitrogen	g N/m^3	8.00	10.19
Total nitrogen	g N/m^3	9.82	12.36

5.1.5 B-WWTP Uncertainty analysis

5.1.5.1 Uncertainty characterization

Uncertainty in the B-WWTP case study is characterized with respect to cost related parameters (oxygen transfer efficiency, electricity and landfill prices), effluent total nitrogen limits and influent wastewater characterization. The parameters that are considered uncertain and their probability distribution together with mean, minimum and maximum values are given in Table 5.15. The alpha, beta and fouling factor parameters are used in the equation 5.2 (Tchobanoglous, 2003), in which the correction factor is calculated to convert the standard oxygen transfer rate in tap water (SOTR) to the actual oxygen transfer rate (AOTR) by taking into account the effects of salinity-surface tension, temperature, elevation etc. This affects the electricity consumption needed to supply the oxygen demand to the WWTP. The standard aeration efficiency value is given as a range as shown in Table 5.8. The uncertain domain is defined accordingly. The electricity price is taken as the end-user energy price for industrial consumers in Denmark and a variation of 20% is assumed over the average price given. Landfill cost, given for Denmark by the Confederation of European waste-to-energy Plants as a range, is used while defining the uncertain domain. The effluent total nitrogen limitation is assumed to change between *15* and *10 mg N/L*. Moreover, the possible change in the COD fractionations is taken into account together with the change in influent ammonium nitrogen concentration. Four different COD fractions (S_I, S_S, X_I and X_{BH}) were sampled and the resulting X_S concentration was calculated assuming the total COD in the influent wastewater is constant.

$$AOTR = SOTR\left(\frac{\beta * C_{s,T,H} - C_L}{C_{s,20}}\right)(1.024^{T-20})(\alpha)(F) \qquad 5.2$$

Table 5.15 Uncertain parameters and their domain definition

Data	Probability distribution	Mean	Min	Max	Unit
Alpha (α)	Uniform	0.75	0.30	1.20	dimensionless
Beta (β)	Uniform	0.965	0.95	0.98	dimensionless
Fouling factor (F)	Uniform	0.775	0.65	0.9	dimensionless
Standard aeration efficiency (SAE)	Uniform	2.55	1.9	3.2	kg O_2/kwh
Price of electricity	Uniform	0.0977	0.08	0.12	Euro/kwh
Landfill cost	Uniform	127	75	179	Euro/ton of sludge
Limit – Total N	Uniform	12.5	10	15	g N/m^3
Soluble inert organic matter (S_I)	Uniform	30	27	33	g COD/m^3
Readily biodegradable substrate (S_S)	Uniform	63.18	56.86	69.5	g COD/ m^3
Particulate inert organic matter (X_I)	Uniform	51.2	46.08	56.32	g COD/ m^3
Active heterotrophic biomass ($X_{B,H}$)	Uniform	28.17	25.35	30.99	g COD/ m^3
$NH_4^+ + NH_3$ nitrogen (S_{NH})	Uniform	31.56	28.4	34.72	g N/ m^3

Once the uncertain parameters are selected and their uncertain domain is defined, the domain is sampled through Monte Carlo sampling by using LHS as the sampling technique, as previously explained in section 3.5. In the B-WWTP case study, the uncertain domain is sampled to create 50 future scenarios with respect to realization of 12 uncertain parameters given in Table 5.15. It is assumed that among the uncertain parameters there is no correlation existing. Figure 5.3 illustrates the future scenarios created.

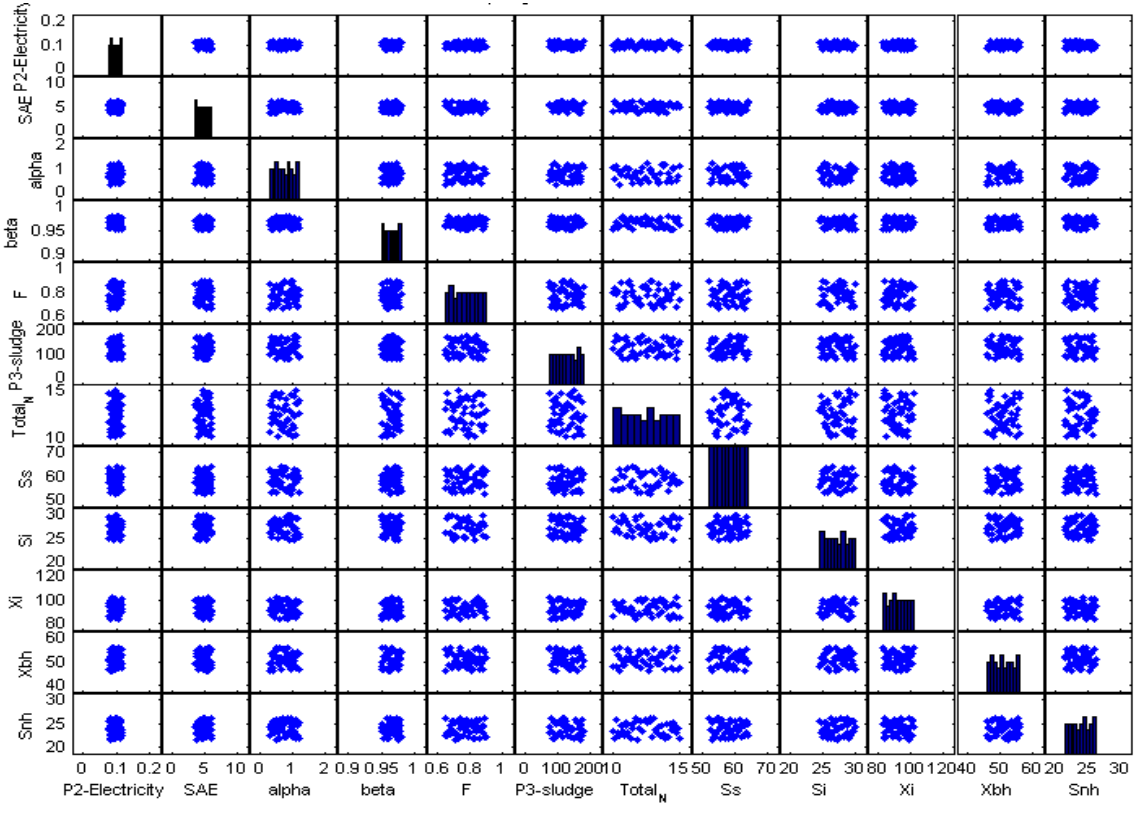


Figure 5.3 Sampling results

5.1.5.2 Uncertainty mapping and analysis

In the second step, the optimization problem was solved for 50 scenarios created in the preceding sampling step. The analysis of the optimization results indicated that two different WWTP networks were identified as optimal with different frequencies as shown in Table 5.16. The majority of the future solutions with respect to future realizations of uncertain parameters resulted in the selection of the same WWTP network as the deterministic solution. Although the probability is very low, in *16%* of the future scenarios the UASB is selected to treat the organic content of the wastewater together with the 2-stage Sharon-Anammox reactor for further nitrogen removal. This network does not comply with the effluent COD limit as explained before under section 5.1.4. However, in the realization of those scenarios, paying the effluent penalty for COD limit violation is found to be more feasible than choosing any other technology – from the limited search space – by the optimizer.

Table 5.16 Uncertainty mapping results

Network	Probability of realization	Selected Intervals
1	84 %	WW-BP1-MLE-BP3-BP4-Thickener-AnD-Discharge-Sludge-Biogas
2	16 %	WW-BP1-UASB-Shar-An-BP4-BP5-Discharge-Sludge-Biogas

The cumulative distribution of the objective function is illustrated in Figure 5.4 where the x-axis shows the objective function value, which represents operational and capital cost, and the y-axis represents the probability that the value of the objective function will be lower than the stated value on the x-axis. This indicates that there is a significant uncertainty on the treatment cost due to the cost related parameters selected to be uncertain; and the objective function value ranges from *693* to *1,606* unit cost. Compared with the deterministic solution case given in Table 5.10, it can be seen that *78%* of the scenarios result in a higher objective function value, and in *16%* of the scenarios a different network configuration is selected. Although the output from uncertainty analysis very much depends on the defined domain of input uncertainties (section 3.5), this comparative analysis already indicates the significance of considering uncertainty analysis for better informed decision making, at least compared to single-point analysis (the case of the deterministic solution).

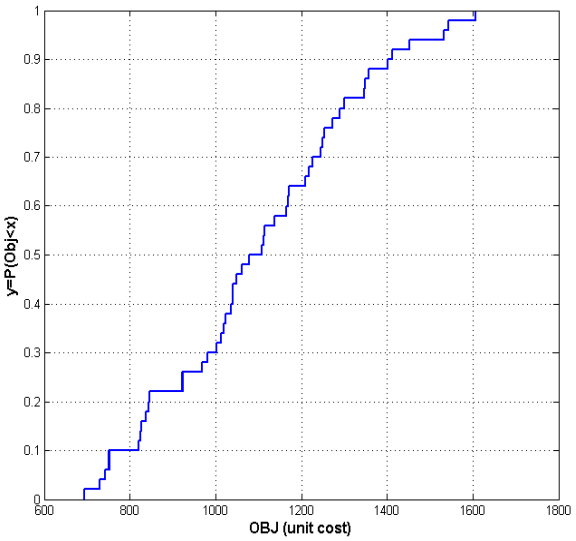


Figure 5.4 Cumulative distribution of the objective function

5.1.5.3 Decision making under uncertainty

In the last step of the uncertainty analysis, the optimization problem is formulated as a stochastic programming problem and solved using the SAA technique as previously explained in section 3.5. The selected network and the cost breakdown for the solution under uncertainty are given in Table 5.17.

Table 5.17 Summary of SAA results

Network	WW-PC-MLE-BP3-BP4-Thickener-AnD-Discharge-Sludge-Biogas
Aeration cost	461.773
Landfill cost	615.289
Biogas price	699.496
Electricity cost	-
Pumping cost	43.687
Mixing cost	27.044
Effluent penalty	-
Capital cost	693.029
OBJ	1,141.326

In order to summarize the results of uncertainty analysis the indicators explained previously in section 3.5 are calculated and analyzed. The EVPI is calculated as *39.833* (4.36% of the deterministic value of TAC). VSS, on the other hand, is *0* because the network selection did not change under uncertain conditions (i.e. deterministic network selection is the same as network selection under uncertainty). Lastly, UP is found to be *229.246.*

The calculated EVPI value is very low as compared to the objective function value of the deterministic solution which indicates that the optimizer did not identify a better solution in the design search space (i.e. the treatment alternatives defined in the superstructure). Hence this means that the current network selection is mature to go further through the project development stages. The VSS value is found to be *0*; since both stochastic and deterministic formulation ended up in the same network solution, the performance is the same and therefore the difference is *0*. The UP on the other hand, is relatively high, *25%* of the deterministic objective function value itself, which indicates that the uncertainties inherent in the operation of the plant, namely wastewater composition and load and changes in the prices of cost items will likely increase the operation cost of the project by that much within the project lifetime. Therefore, by considering all the indicators, and especially the UP indicator, the user can conclude that the uncertainty in the model parameters affects the performance of the selected WWTP network significantly and the uncertainty should be reduced in order to achieve a more optimal design decision. If uncertainties affecting the system cannot be decreased, e.g. by improving the available wastewater characterization through a long term measurement campaign, then one can consider designing a flexible network which is a solution that is addressed elsewhere (Quaglia et al., 2013).

5.1.6 General conclusions on B-WWTP case study

The B-WWTP case study has been formulated to constitute a simple but representative, illustrative example for the application of a synthesis, design and retrofitting framework for the design of municipal wastewater treatment plants.

Although the definition of the problem was limited to only three pollutants (i.e. organics, nitrogen and solids), 19 components were defined, which constitute the pollutants, utilities as well as end products of the defined reactions. The superstructure developed for this case study encompasses 5 different tasks responsible for different means of wastewater and sludge treatment. With the 12 treatment alternatives defined in the design space, around 190 alternative treatment networks are created and compared within the optimization algorithm. It was also shown that the definition of the design space is flexible and expert-driven in the sense that the tasks, alternative technologies and the interconnection between them are defined by the user with previous experiences and/or a detailed market search.

Use of the design models for individual treatment units (detailed in section 4.1) was demonstrated by collecting real operational data from the literature by following the steps of the data collection and design procedure (Figure 3.3). Through the formulation of a MILP problem, the process synthesis problem for the specified wastewater composition was solved and some key conclusions are given below:

- As a result of the deterministic solution of the formulated optimization problem, the optimizer favored the low SRT pre-denitrification activated sludge type of treatment unit – *MLE* in combination with the primary clarifier and anaerobic

sludge stabilization unit. This network is characterized by its low volume requirement, high biogas production and effective treatment in terms of organics and nitrogen.

- The anaerobic treatment unit together with nitrogen removal satisfied by tertiary treatment is effective for nitrogen removal; however, without operating it in higher temperatures or integrating with effluent polishing steps, it cannot comply with effluent COD requirements.
- Uncertainty in wastewater composition and several input parameters of early stage design, such as; cost parameters and effluent limits are known to have great influence on design outputs (i.e. selected network, operational cost etc.) through the project lifetime. This is demonstrated by performing the uncertainty analysis. Accordingly, considerable variations in the network performance and objective function value were observed within the defined uncertain domain.

It is believed that, the novel approach of superstructure optimization for early stage design studies was used in the case study to promote the effective formulation and management of the complexity of the wastewater treatment process synthesis problem.

5.2 Retrofitting of full scale WWTPs

The second case study (Retrofitting case study) has been formulated as a retrofitting problem focusing on the challenges that many, if not the majority, of the wastewater treatment plants in EU and North America are facing due to tightened legal effluent discharge limits which put considerable demand on increasing nitrogen removal performance. To this end, two Danish WWTPs were used in the context of this case study and the tool was applied to represent the design space for retrofitting alternatives for novel technologies (side stream treatment processes as well as main stream) and identify the optimal solution for various scenarios. The solutions were further analyzed considering various sources of uncertainties including influent quantity and quality as well as expected utility costs and effluent limit variations in the project investment horizon. In this section, the details of the case study are presented by following the steps of the superstructure based optimization methodology.

5.2.1 Retrofitting case study – Problem definition

In the context of the retrofitting case study, two Danish WWTPs were analyzed: Lynetten WWTP and Avedøre WWTP. Lynetten WWTP is located east of Copenhagen, Denmark. It has a capacity to serve approximately 750,000 PE by treating around 60 million m^3 of wastewater annually. Avedøre WWTP, on the other hand, is located west of Copenhagen, Denmark and receives wastewater from 10 suburban municipalities with a population of approximately 265,000 people. Annually, around 25-30 million m^3 of wastewater is treated in the plant. Both of the treatment plants utilize physical, biological and chemical means of treatment to process the incoming wastewater; whereas the produced sludge is incinerated in fluidized bed incineration plants. The location of the plants are illustrated in Figure 5.5. Both Lynetten WWTP and Avedøre WWTP have similar existing plant facilities (i.e. treatment network), which is demonstrated in Figure 5.6.

(a)

(b)

Figure 5.5 Location of (a) Avedøre WWTP (b) Lynetten WWTP

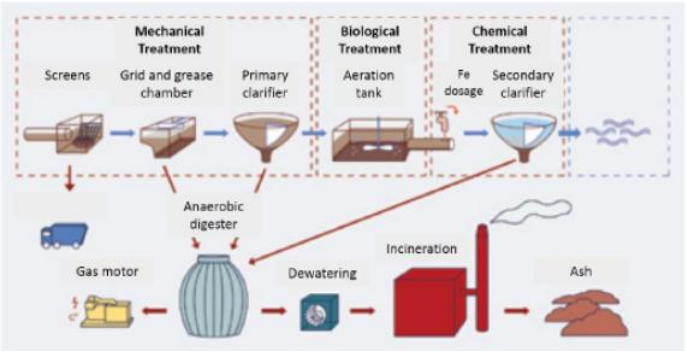


Figure 5.6 Layout for Avedøre and Lynetten WWTPs

The WWTPs receive organics, nutrients and solids with the influent wastewater. The yearly average pollutant loads for the year 2012, in terms of concentration units, are shown in Table 5.18. The table also summarizes the average effluent water composition of the same year (Note: For Lynetten WWTP there is no information available for the fractionation of influent total nitrogen).

Table 5.18 Avedøre WWTP influent and effluent composition (2012 yearly average)

		Avedøre WWTP		Lynetten WWTP	
	Unit	**Influent**	**Effluent**	**Influent**	**Effluent**
Flow rate	m^3/d	72,037	67,113	162,465	162,465
COD	g/m^3	476	23	657	56
BOD	g/m^3	180	2	306	9
NH_4-N	g/m^3	33	1.2		
NOx-N	g/m^3	-	3		
Total-N	g/m^3	43	4.8	51	8.9
Total-P	g/m^3	6.5	0.6	8.1	1.7

For practical purposes, the influent wastewater composition was characterized in terms of ASM1 components (Henze et al., 2000). The conversion procedure and influent characterization after conversion are illustrated below in Table 5.19. The influent wastewater was assumed not to contain any biomass (X_{BH}, X_{BA}), no particulates from biomass decay (X_P), nitrate / nitrite nitrogen (S_{NO}), soluble organic nitrogen (S_{ND}) and oxygen (S_O).

Accordingly, all the effluent COD was assumed to be in the form of soluble inert materials - S_I (Eq. 5.19.1). The ratio of BOD to biodegradable COD was taken as 0.595 and used in the conversion procedure (Fall et al., 2012). The effluent BOD concentration (i.e. 2 and 9 g/m^3 for Avedøre and Lynetten WWTPs, respectively; which correspond to approximately 3.4 g/m^3 and 15 g/m^3 of biodegradable COD) was assumed to be negligible

and therefore was not included in the COD calculation. COD was assumed to be composed of biodegradable COD and soluble and particulate inert COD; therefore equation 5.19.3 was used to calculate the concentration of particulate inert COD – X_I. Biodegradable COD includes soluble and particulate fractions – S_S and X_S respectively. It was assumed that it contains 30% soluble and 70% particulate biodegradable COD. According to our assumption, total nitrogen is composed of ammonium nitrogen - S_{NH} and particulate biodegradable organic nitrogen - X_{ND} (equations 5.19.5 - 5.19.8). Since the fractionation information for total nitrogen in Avedøre WWTP is known, equations 5.19.5 and 5.19.7 were used to calculate the ammonium nitrogen and particulate organic nitrogen concentrations for this WWTP. On the other hand, for Lynetten WWTP the two fractions were determined by equations 5.19.6 and 5.19.8. It should be noted that the influent fractionation procedure provided a base case on which a comprehensive uncertainty analysis was further performed to robustify the solutions as part of the systematic framework in step 5.

Table 5.19 Avedøre WWTP influent characterization in terms of ASM1 components (2012 yearly average)

Component	Unit	Value		Description	Eqn.
		Avedøre	Lynetten		
S_I	g/m^3	23.48	56.52	$S_I = COD_{out}$	5.19.1
S_S	g/m^3	107.85	153.25	$S_S = COD_{biodegradable} * 0.3$	5.19.2
X_I	g/m^3	93.22	89.98	$X_I = COD - S_I - COD_{biodegradable}$	5.19.3
X_S	g/m^3	251.65	357.59	$X_S = COD_{biodegradable} * 0.7$	5.19.4
X_{BH}	g/m^3	0	0		
X_{BA}	g/m^3	0	0		
X_P	g/m^3	0	0		
S_O	g/m^3	0	0		
S_{NO}	g/m^3	0	0		
S_{NH}	g/m^3	32.85	45.6	$S_{NH} = NH_4\_N$	5.19.5
				$S_{NH} = Total - N - X_{ND}$	5.19.6
S_{ND}	g/m^3	0	0		
X_{ND}	g/m^3	9.8	5.4	$X_{ND} = Tot\_N - NH_4\_N$	5.19.7
				$X_{ND} = X_I * i_{xp}$	5.19.8

The retrofitting problem was defined so that the feasibility of extending/modifying the existing treatment line will be analysed in two ways:

(1) Addition of a new task responsible for nitrogen removal and several alternative technologies will be considered in that respect in the sludge reject water treatment line,

(2) Evaluating alternative novel treatment technologies in the main wastewater treatment line.

The objective function was defined such that it covers the operational and capital cost (only for the new treatment units) – i.e. total annualized cost (TAC) – which has to be minimized. The operational cost covers utility cost (i.e. aeration, electricity consumption, chemical addition etc.), sludge production via landfill price, biogas price, mixing and pumping.

5.2.2 Retrofitting case study – Superstructure definition

The design space formulation for the retrofitting case study is done by formulating a superstructure. In this specific case study, the individual treatment technologies are selected so that the design space consists of novel approaches and emerging technological developments. The superstructure developed for this retrofitting problem is illustrated in Figure 5.7; Table 5.20 summarizes and describes the treatment units selected in the design space within the context of this problem.

The process intervals (i.e. individual treatment units) shown in grey are the existing treatment units in the Avedøre and Lynetten WWTPs. The wastewater source was defined in the source column – *WW*, as previously summarized in Table 5.19. The wastewater first goes through primary treatment and some fraction of the particulates are directed to sludge treatment line in the primary clarifier – *PC* unit. Afterwards, the primary effluent is sent to biological treatment for removal of organics, nitrogen and phosphorus. This unit was represented as activated sludge – *AS* unit in the superstructure. The sludge treatment line is composed of a sludge thickener, anaerobic digestion unit and a dewatering unit (i.e. *Thick*, *AD* and *Dewat* in the superstructure). The sink intervals for water and sludge effluents were represented as *Water* and *Sludge*, respectively.

In this specific retrofitting problem, the alternative technologies were located under three different treatment tasks: *Primary Treatment*, *Secondary Treatment* and *Reject Water Treatment.* The primary treatment task is basically for treating/separating the particulate organics in the influent wastewater. Together with the primary clarifier of the base case, a high-rate oxic reactor – *A-stage* and an Upflow Anaerobic Sludge Blanket reactor – *UASB* were placed here as alternative treatment units. The secondary treatment task is responsible for removal of the remaining organics together with nitrogen and phosphorus. Several different biological nutrient removal (BNR) type of systems with different SRTs (i.e. *BNR10*, *BNR14* and *BNR28*), a low-rate oxic system in a pre-denitrification structure – *B-stage*, an Anaerobic Ammonium Oxidation reactor operating in low temperatures (i.e. main stream wastewater temperature) – *Anammox*, an activated sludge type of reactor with granular sludge – *Granular AS* and a membrane bioreactor – *MBR* were selected among the secondary treatment technologies and placed in the superstructure. The sludge treatment line is composed of a thickener, an anaerobic digester and a dewatering unit, which already exist in the base case design of the treatment plant. Finally, within the context of the sludge reject water treatment task, several different treatment units were

included in the database and shown in the superstructure. These units are responsible for treating the nitrogen rich water stream resulting from thickener and dewatering units. Finally, three by-pass units are added under three tasks having treatment alternatives; this allows the optimizer to by-pass the task when it is not needed.

After defining the treatment tasks and alternative treatment processes, the superstructure definition was finalized by identifying the interconnections between the process intervals. The *PC* unit is connected to all the secondary treatment alternatives while *A-stage* technology is connected to the *B-stage* and *Anammox* alternatives of the secondary treatment and *UASB* directs their effluent only to the *Anammox* unit. The secondary treatment effluent water stream is sent to the sink interval for effluent water. The sludge generated in primary treatment and secondary treatment units is directed to the sludge thickener prior to be sent to anaerobic digester. After being dewatered, the waste sludge is directed to the sludge sink interval. The reject water stream originating from thickener and dewatering units of the sludge treatment line is recirculated back to the influent wastewater stream after passing through the reject water treatment task.

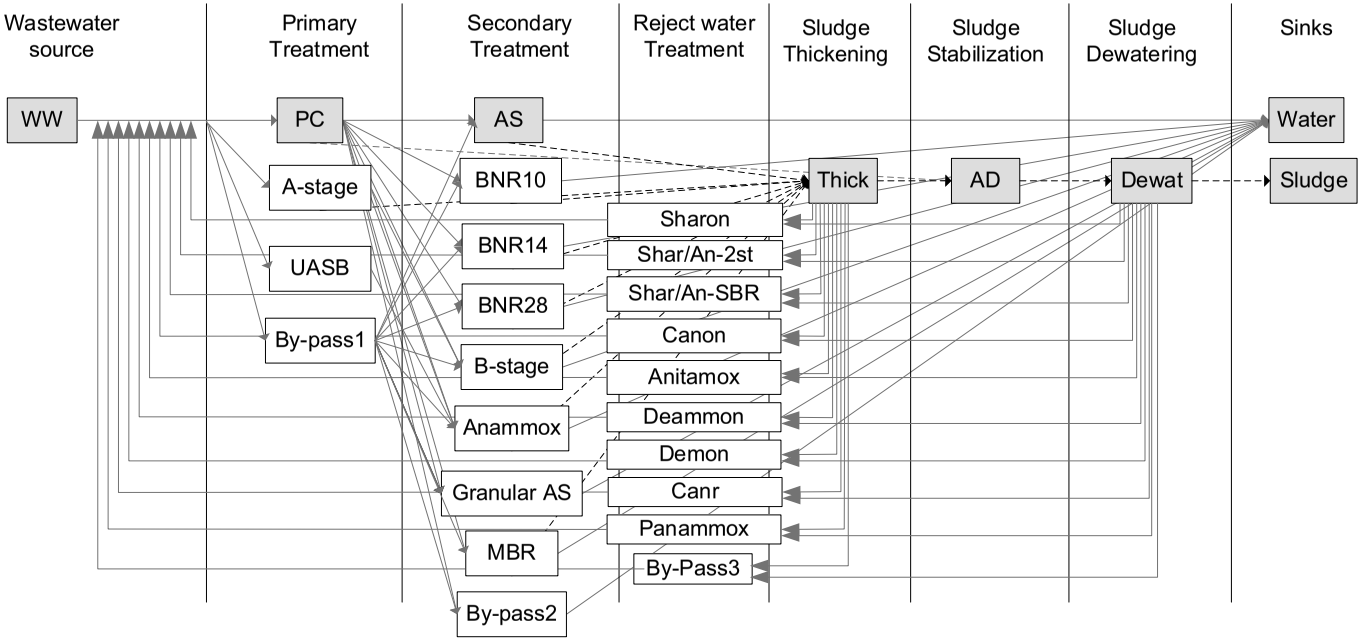


Figure 5.7 Superstructure developed for the Retrofitting case study representing the design space considering novel primary, secondary and reject water treatment technologies

Table 5.20 Treatment technologies represented in the superstructure

Unit	Description	Unit	Description
WW	Wastewater source	Sharon	Single reactor system for high activity ammonium removal over nitrite
PC	Base case primary clarifier	Shar/An-2st	2 stage Sharon and Anammox reactors
A-stage	High-rate oxic reactor	Shar/An-SBR	1 stage (SBR) Sharon and Anammox reactor
UASB	Upflow anaerobic sludge blanket	Canon	Completely autotrophic nitrogen removal over nitrite
AS	Base case activated sludge type of reactor	Anitamox	Partial nitritation/Anammox in a moving bed biofilm reactor
BNR10	Biological nutrient removal, SRT=10 d	Deammon	Deammonification in a biofilm type of reactor
BNR14	Biological nutrient removal, SRT=14 d	Demon	Deammonification in a SBR type of reactor
BNR28	Biological nutrient removal, SRT=28 d	Canr	Complete autotrophic nitrogen removal in an SBR type of reactor
B-stage	Low-rate oxic reactor	Panammox	Two-step partal nitritation/anammox process
Anammox	Main stream anaerobic ammonium oxidation reactor	Thick	Base case sludge thickener
Granular AS	Granular activated sludge reactor	AD	Base case anaerobic digester
MBR	Membrane Bioreactor	Dewat	Base case dewatering unit
		Water	Water effluent
		Sludge	Sludge effluent
		By-pass	By-pass intervals

5.2.3 Retrofitting case study – Data collection & Generic process interval model generation and validation

5.2.3.1 Retrofitting case study – Data collection and design of individual treatment technologies

Treatment technologies in the superstructure, including the base case treatment units, were designed by following the steps of the systematic data collection and design procedure previously described in section 3.3.1. In this section, the design specifications of separate treatment units are given in three different groups:

- Base case treatment units
- Main wastewater treatment line alternatives
- Sludge reject water stream treatment technologies.

Design of base case treatment units

The base case units were designed based on the design data obtained from the treatment plants according to the design models previously described in section 4.1. Separation in primary clarifier – *PC* was defined so that 99% of the total flow and 52% of the particulates by mass leave with primary effluent while the rest is directed to the anaerobic digester – *AD*. These numbers were selected so that the resulting concentrations comply with the influent and effluent stream compositions of *PC* taken from the WWTP.

The secondary treatment unit, which is referred to as *AS* in the superstructure, is a biological nutrient removal unit (i.e. responsible for removal of organics, nitrogen and phosphorus). The configuration of this technology is referred to as Bio-denipho in the literature and nutrient removal is performed with intermittent or phased operations (Bundgaard et al., 1989). The SRT of the system was taken as 35 days while the HRT was fixed to 20 hours for Avedøre and 22 hours for Lynetten *AS* unit. The system therefore operates with 90% COD, 95% NH_4-N, 82% total-N and 93% total-P removal. The biological treatment effluent was directed to a secondary settler unit which separates the particulates with 99.8% efficiency.

The concentrated sludge stream from the secondary treatment is sent to thickener, where it is further concentrated with an efficiency of 95%. The primary sludge (i.e. the underflow of *PC* unit) together with the concentrated sludge stream from the thickener unit are sent to the anaerobic digester. *AD* unit operates with a retention time of 30 days at 35°C and converts the biodegradable COD into methane gas with an efficiency of 37%. The dewatering unit, which receives the sludge from the anaerobic digester separates the liquid and solid fractions with a 95% efficiency. The water stream resulting from sludge treatment (i.e. the water effluent from thickener and dewatering unit), which is characterized by its high ammonium nitrogen concentration, is recycled back to the influent of the wastewater treatment line to be further treated in the main wastewater

treatment units. The base case design is summarized in Table 5.21 in terms of the compositions of the influent, effluent–both sludge and water- and sludge reject water streams.

Table 5.21 Base case design summary (a) for Avedøre WWTP and (b) for Lynetten WWTP

(a)

Parameter	Unit	Influent	Effluent		Sludge reject water
			Water	Sludge	
Flow rate	m^3/d	72,037	71,950	46.2	2,489
COD	g COD/m^3	476	36.3	$3.1*10^5$	302
BOD	g COD/m^3	180	-	$2*10^4$	3.8
NH_4-N	g N/m^3	33	1.78	328	116
NO_X-N	g N/m^3	-	4.95	-	3.2
Total-N	g N/m^3	43	8.1	$1.1*10^4$	136
Total-P	g P/m^3	6.5	0.45	114	40
CH_4	g COD/m^3	-	-	$9.2*10^3$	-

(b)

Parameter	Unit	Influent	Effluent		Sludge reject water
			Water	Sludge	
Flow rate	m^3/d	162,465	156,700	286	5474
COD	g COD/m^3	657	60	$1.2*10^5$	353
BOD	g COD/m^3	306	2	$1.5*10^4$	8.3
NH_4-N	g N/m^3	46	1.13	276	131
NO_X-N	g N/m^3	-	6.22	-	3.3
Total-N	g N/m^3	51	8.83	$1.1*10^4$	165
Total-P	g P/m^3	8.1	0.81	105	50
CH_4	g COD/m^3	-	-	$8.7*10^3$	-

Design of main wastewater line treatment units

As stated earlier, the main wastewater line treatment alternatives are placed under primary and secondary treatment tasks. In this section, their design specifications and performance data are summarized. In Table 5.22, the design data for conventional activated sludge (AS) type of treatment technologies are shown. These technologies were designed following the steps of a systematic data collection procedure as well.

The *A-stage* technology is a high rate oxic reactor receiving high organic loads (i.e. the raw wastewater) and oxidizing the incoming COD by 60% efficiency (Versprille et al.,

1984). The reactor is coupled with a sedimentation tank; therefore, the settleable organics are separated and sent to the sludge treatment line. Since the SRT of the system is very low (i.e. 0.5 days), nitrifiers do not grow in the medium thus nitrification does not occur in the reactor.

The *B-stage* technology is a pre-denitrification type of conventional activated sludge configuration operating with 13 days of SRT. The reactor has two different compartments; one being aerated, where nitrification and COD oxidation occur and the other being anoxic where the recirculated nitrate is denitrified by the incoming organics. It is coupled with a sedimentation basin which separates the liquid and solid fractions and sends the settleable solids to the sludge treatment line. The reaction proceeds by 78% efficiency in terms of COD removal and 67% efficiency in terms of total nitrogen removal. Phosphorus, on the other hand, is precipitated chemically by the addition of $FeCl_3$ and this removal mechanism operates with 90% efficiency.

The biological nutrient removal (BNR) type of technologies have similar mechanisms in terms of organics and nitrogen removal; however they operate with different SRTs resulting in different performance in terms of removal efficiencies. For phosphorus removal, the high SRT BNR system (i.e. *BNR28*) incorporates an anaerobic reactor different than other conventional AS type of technologies, which is operated with 0.5 hours of retention time. It is assumed that approximately 60% of the incoming phosphorus is removed by biological means while the remaining is precipitated chemically by the addition of $FeCl_3$ to achieve a 90% overall removal efficiency.

Table 5.22 Design data for AS type of treatment technologies

Unit	Mechanism	SRT (d)	HRT (h)	Reactor type	Performance
A-stage	COD oxidation	0.5	2	Aerated reactor + sedimentation basin	60 % biodegradable COD removal
B-stage	COD oxidation Nitrification Denitrification Chemical P removal	13	4 (aerobic) 3 (anoxic)	Pre denitrification type of reactor + sedimentation basin	78 % COD 67 % total N 90 % total P removal
BNR10	COD oxidation Nitrification Denitrification Chemical P removal	10	7.2 (aerobic) 2.4 (anoxic)	Pre denitrification type of reactor + sedimentation basin	88 % COD 84 % total N 90 % total P removal
BNR14	COD oxidation Nitrification Denitrification Chemical P removal	14	9 (aerobic) 3 (anoxic)	Pre denitrification type of reactor + sedimentation basin	87 % COD 85 % total N 90 % total P removal
BNR28	COD oxidation Nitrification Denitrification Biological and chemical P removal	28	15 (aerobic) 5 (anoxic) 0.5 (anaerobic)	Pre denitrification type of reactor + sedimentation basin	87 % COD 86 % total N 90 % total P removal

For the *UASB* technology, the SRT is selected as 120 days at 20°C while the HRT is taken as 14 hours (WEF, 2010). The total COD reduction is assumed to be fixed and taken as 68% at this temperature (WEF, 2010). There is no nitrogen removal in the system. Sludge is produced with a yield of 0.15 g COD sludge/g COD applied (WEF, 2010) whereas the decay coefficient is taken as 0.03 1/d (Tchobanoglous, 2003). Methane production is calculated with respect to the removed COD with the relation given by Tchobanoglous (2003), which is 0.38 m^3 methane/kg COD removed. The concentration of soluble inert COD fraction does not change during the reaction. The effluent COD was assumed to be in the form of soluble inert COD - S_I, particulate inert COD - X_I and slowly biodegradable COD – X_S. The readily biodegradable COD - S_S was assumed to be completely oxidized in the system. Since the reactor is operated with granular sludge formulation, there is no

sludge wastage; the only particulates leaving the system (determined from SRT) are leaving with the water effluent and very low in concentration. The sizing of the reactor is done based on the selected HRT together with upflow velocity and gas collection height that are taken from reported values (Tchobanoglous, 2003).

The *Anammox* technology, placed under secondary treatment task, operates partly with partial nitritation/anammox and partly with denitrification mechanisms at low temperatures. When operated in optimal conditions, it can reduce the concentration of NH_4-N to 4 g/m^3 and NO_X-N to 4 g/m^3 as well. NO_2/NO_X ratio is given as 0.7. Moreover, COD reduction via denitrification is reported to be 78% (Regmi et al., 2014). In order to satisfy the given operating conditions by Regmi et al. (2014), the following assumptions were made:

- The partial nitritation proceeds with 65% efficiency (i.e. 65% of the NH_4-N is converted to NO_X-N while the rest is remained as NH_4-N). The corresponding oxygen requirement is calculated from stoichiometry.
- NH_4-N is used by anammox microorganisms, remaining a residue of 4 g N/m^3. The corresponding NO_X-N, which is determined from stoichiometry, is also consumed by anammox.
- The amount of NO_X-N, after subtracting the amount used by anammox and the assumed effluent (i.e. 4 g/m^3), is used in denitrification.
- The remaining COD after denitrification is removed by aerobic heterotrophic activity and the corresponding oxygen requirement is calculated from biomass yield (i.e. growth and decay of microorganisms).
- Heterotrophic SRT is assumed to be 10 days and accordingly the sludge production is calculated.
- The sizing of the reactor is done based on the total nitrogen loading rate, which is taken as 0.25 – 0.3 kg N/m^3.d (Wett et al., 2013; Lotti et al., 2014).
- The phosphorus is assumed to be removed by chemical precipitation with the addition of iron chloride, which proceeds with 90% efficiency.

The *Granular AS* technology is placed under secondary treatment task. The sizing of the reactor is based on the data received from a full scale application in Groningen, The Netherlands, as given below:

- Dry matter concentration in the system is reported as 8.5 g/L.
- Total sludge loading rate is 0.09 kg COD.

An optimal operation results in BOD<1 mg/L, total nitrogen<7 mg/L, NH_4-N<1 mg/L and o-phosphate<0.5 mg P/L. The efficiency of the treatment unit is calculated based on the given effluent concentrations. It follows the nitrification/denitrification mechanism for nitrogen removal. Given the achievable NO_X-N effluent concentration, the COD requirement for denitrification is determined and the rest of the organic removal occurs

via oxidation until it reaches the pre-determined organic effluent concentration. The oxygen demand for nitrification and organic oxidation are calculated from stoichiometry. Finally, the SRT of the system is assumed to be 30 days and the corresponding wastage flow rate is calculated accordingly.
The last treatment alternative that has been considered in this retrofitting problem is the *MBR* unit. It is designed as a submerged type of *MBR* with hollow fibre or plate membrane modules, which are reported as most commonly used type of reactor and membrane designs in municipal wastewater treatment by Melin et al. (2006). The design data is also collected from the same study and summarized below:

- Membrane flux is given in the range of 15-30 $L/m^2.h$ and taken as the average value 22.5 $L/m^2.h$. This information is used to determine the size of the membrane area.
- SRT of the system is selected as 25 days while the HRT is taken as 5 hours.
- Reactor performance is reported to be 89-98% for COD, 80-90% for NH_3-N and 36-80% for total-N removal. Moreover, when it is operated with complete nitrification/denitrification, which is the selected mechanism in this study, it effectively achieves total-N concentrations below 10 mg/L in the effluent stream.
- Biomass concentration in the system is in the range 12,000-15,000 mg/L.
- Total energy consumption is given as 0.2 – 0.4 kWh/m^3. The breakdown of this consumption is reported to be 80-90% for membrane aeration and the remaining 10-20% is consumed for pumping for permeate extraction.
- The phosphorus removal is assumed to be conducted chemically by the addition of $FeCl_3$ with 90% efficiency.

Design of sludge reject water stream treatment units

In the sludge reject water treatment task definition, the main purpose is removal of nitrogen from this highly contaminated stream so that the total nitrogen load into the main stream treatment unit is lowered while decreasing the operational cost of this unit (mainly in terms of aeration requirements and extra carbon dosage). In the context of this retrofitting study, two different treatment mechanisms and nine different technology alternatives are considered under the related task. Sharon reactor operates with nitritation/denitritation mechanism; whereas, all the other treatment units treat nitrogen by partial nitritation/anammox mechanism. The stoichiometry for the two mechanisms are given below in equations 5.3-5.4 and 5.5-5.6, respectively.

- Stoichiometry for nitritation/denitritation (Hellinga et al., 1998)

$$NH_4{}^+ + 1.5\ O_2 \rightarrow NO_2{}^- + H_2O + 2H^+ \quad 5.3$$

$$NO_2^- + 0.5CH_3OH + 0.5CO_2 \rightarrow 0.5N_2 + HCO_3^- + 0.5H_2O \quad 5.4$$

- Stoichiometry for partial nitritation/anammox (van Dongen et al., 2001)

$$NH_4^+ + HCO_3^- + 0.75O_2 \rightarrow 0.5NH_4^+ + 0.5NO_2^- + CO_2 + 1.5H_2O \quad 5.5$$

$$NH_4^+ + NO_2^- \rightarrow N_2 + 2H_2O \quad 5.6$$

Table 5.23 summarizes the design specifications for the treatment alternatives of sludge reject water treatment task. The *Sharon* unit operates with nitritation / denitritation and it is the only unit in Avedøre retrofitting problem design space using this mechanism. The other alternative units operate with partial nitritation / anammox mechanism either in single reactor or separate reactors for partial nitritation and anammox. The sizing of the units are done based on the given HRT for *Sharon* and reported volumetric nitrogen loading / removal rate values for the other units. In order to determine the performance of the systems in terms of their nitrogen (total nitrogen or NH_4 nitrogen) removal efficiencies, the removal efficiencies at optimal operating conditions reported by the stated studies in Table 5.23 are used.

Table 5.23 Design data for sludge reject water treatment alternatives

	# of reactors	Reactor type	Volumetric N removal rate (kg N /m^3 d)	Volumetric N loading rate (kg N /m^3 d)	Efficiency	Comments	References
Sharon	1	CSTR			86% for 1st reaction 60% for second reaction	1 d HRT for Sharon reactor	Hellinga (1998)
Shar/An-2st	2	CSTR-granular sludge	10		50% in Sharon 80% in anammox		vanDongen(2001) Van der Star(2007)
Shar/An-SBR	1	SBR	0.55		90% overall N conversion to N_2		Joss(2009)
Canon	1	Granular sludge		1.5	95% for ammonium 81% for total N		Abma(2010)
Anitamox	1	MBBR	0.8		85% for ammonium		Lemaire(2011)
Deammon	1	MBBR	0.3-0.4	0.42-0.5	70% for total N		Rosenwinkel(2005)
Demon	1	SBR		0.61	90% for ammonium		Wett(2010)
Canr	1	SBR		0.75	89% for total N		Vangsgaard(2013)
Panammox	2	SBR-granular sludge		1.8 – PN 0.46 - Anammox	89% for ammonium 86% for total N		Personal contact- Jesus Colprim

Collection of operational and capital cost data

As stated earlier, the objective function of the optimization problem comprises the operational – *OPEX* and capital cost – *CAPEX* of the treatment plant. In this retrofitting problem, the capital cost was calculated with the calculated volume of the units; whereas operational cost consists of aeration cost, electricity cost, cost of the chemicals, sludge production cost calculated via landfill taxes and the gains from biogas production. All the cost data are collected from information available in open literature and summarized in Table 5.24.

Table 5.24 Cost information for operational and capital cost items

Cost item	Unit	Value/Range	Description/Assumption
Electricity consumption of oxygen transfer [1]	kg O_2/kwh	3 – 5	Range given by different equipment suppliers
Methanol cost[2]	euro/kg	0.35	-
Ferric chloride cost[1]	euro/kg	0.13	Spildevandcenter Avedøre
Electricity cost[3]	euro/kwh	0.0978	In Denmark for industry
Landfill cost[4]	euro/t	107	In Denmark, on the average
Biogas price[5]	eurocent/m^3 methane	40.3	In Denmark (assumptions: 1 mole of methane is 24 L and 1 mole of methane accounts for 64 g of COD)
Capital cost – UASB[6]	US$/$m^3$	425	Based on the price level of 2006, for 100,000 PE
Capital cost – Aeration tank[6]	US$/$m^3$	175	Based on the price level of 2006, for 100,000 PE
Capital cost – Secondary settler[6]	US$/$m^3$	290	Based on the price level of 2006, for 100,000 PE
Capital cost – Primary settler[6]	US$/$m^3$	375	Based on the price level of 2006, for 100,000 PE
Capital cost – Sludge thickener[6]	US$/$m^3$	400	Based on the price level of 2006, for 100,000 PE
Capital cost – Anaerobic digester[6]	US$/$m^3$	350	Based on the price level of 2006, for 100,000 PE

[1] Spildevandcenter Avedøre (2014)

[2] URL3 (2015)

[3] URL1 (2013)

[4] URL2 (2013)

[5] Hahn et.al (2010)

[6] van Haandel and van der Lubbe (2012)

5.2.3.2 Retrofitting case study – Generic process interval model generation

The information about the superstructure generated and the design of the treatment technologies, which are placed in the superstructure, is converted into a generic mass input-output type simple model as given previously in section 4.2 (mathematical model was described in section 3.3.2). The optimization problem has a number of parameters defined, and the values of these parameters are calculated based on the individual treatment unit designs employed, stored in matrices in an MS Excel based structure and finally sent to the optimizer for being used in the solution of the optimization problem. The components, utilities and the reactants of the formulated optimization model are summarized in Table 5.25; while the superstructure formulation with the defined interconnections together with values of all the parameter values used in the Retrofitting case study are given in Appendix 3.

Table 5.25 Components, utilities and reactants for Retrofitting case study

Components		Utilities	Reactants
Q	CH_4	S_O	S_S
S_I	N_2	Electricity	S_{NH}
S_S	Ozone	Methanol	S_{NO}
X_I	Cl_2	$FeCl_2$	$X_{B,H}$
X_S	Electricity		$X_{B,A}$
$X_{B,H}$	Methanol		X_S
$X_{B,A}$	X_{AOB}		X_I
X_P	X_{NOB}		P
S_O	X_{AnAOB}		
S_{ALK}	X_{Den}		
S_{NO}	P		
S_{NH}	$FeCl_2$		
S_{ND}	$FePO_4$		
X_{ND}			

5.2.4 Retrofitting case study – MILP formulation and deterministic solution

The superstructure optimization problem was formulated as a Mixed Integer Linear Programming (MILP) problem as previously shown in equations 3.27 – 3.30.
The deterministic solution of the optimization problem results in the optimal network, fate of pollutants/components throughout the selected treatment network and the value of the objective function together with the cost breakdown into the components of the objective function (i.e. utility cost, product cost, capital cost etc.).
The retrofitting case study has been conducted by considering two different scenarios:

- Scenario 1: process selection for sludge reject water treatment
- Scenario 2: full-scale retrofitting study covering treatment alternatives for main wastewater treatment line and sludge reject water line as well.

Scenario 1 – Process selection for sludge reject water treatment

In the first scenario, in addition to the base case treatment layout, an additional task has been defined in the superstructure to treat the nitrogen rich water stream resulting from sludge treatment. The optimization results (represented as the selected alternative) together with the base case cost breakdown and a ranking of all the other alternatives with respect to objective function values are given in Table 5.26 and the selected network is illustrated in Figure 5.8. For both treatment plants, the selected alternative and ranking of all the other alternatives were the same. The biogas price, pumping cost and mixing cost are 1914, 491 and 240 unit cost for Avedøre WWTP and 6136, 1108 and 540 unit cost for Lynetten WWTP, respectively. They are not included in the cost breakdown since they do not change with the different reject water treatment alternative selections. It is important to mention that although the objective function value increased with the increased plant size from Avedøre WWTP to Lynetten WWTP (i.e. increased aeration cost, pumping and mixing requirements together with higher amount of sludge produced); the gains from biogas production are higher in Lynetten WWTP case with the higher organic load entering the plant with higher biodegradable fraction.
It is seen that the base case treatment units perform very well in terms of nitrogen removal i.e. the effluent NO_X-N and NH_4-N concentrations are very low; however, it should also be noted that the base case design has been made with respect to the yearly average influent characterization and performance of the units. The effects of reject water treatment technologies are known to be more significant when the treatment plant operates with effluent total nitrogen concentrations greater than 10 g N/m^3.
The *Canon* technology is a one stage partial nitritation/anammox unit working with granular sludge formulation. Its required volume, which has been calculated with respect to the reported volumetric nitrogen loading/removal rate, is very small and utility consumption is very low. Although the base case scenario has no associated capital cost

with it, the overall cost to the plant becomes lower and *Canon* is favored by the optimizer. Moreover, approximately 6% of an improvement in the performance is observed in terms of total nitrogen removal.

The *Sharon* technology, which is ranked as the last alternative (i.e. the most costly alternative) by the optimizer, requires extra utility cost due to methanol addition for denitritation and pH control; therefore, it is not feasible for full scale applications especially after the discovery of anammox microorganisms and its successful full scale applications.

2-stage applications (i.e. *Panammox* and *Shar/An-2*) are known to have advantages during operation (e.g. better control of nitritation and anammox) (Vlaeminck et al., 2012); however, mostly because of the capital cost requirements, they are not favored by the optimizer and also not much favored for full scale applications recently (Vlaeminck et al., 2012; Lackner et al., 2014).

For the commercial and experimental applications of one stage partial nitritation/anammox processes (i.e. *Canon*, *Anitamox*, *Canr*, *Shar/An-SBR*, *Demon* and *Deammon*), the difference in terms of cost and removal efficiency does not seem significant. This simply means that in terms of technical and economic performance criteria most of these side-stream technologies analyzed are similar. Hence the decision maker needs to consider other criteria when making a decision about which technology to select. This analysis is actually in agreement with the discussion of van Loosdrecht and Salem (2006). These additional criteria may include but not be limited to flexibility, ease of operation, risk for failure, site specific conditions, experience of the plant staff etc. (van Loosdrecht and Salem, 2006).

Table 5.26 Summary of results for deterministic solution of scenario 1 (all the cost parameters are given in 'unit cost' and the concentrations of nitrogen components are reported in 'g/m^3') (a) Avedøre WWTP (b) Lynetten WWTP

(a)

	Process interval	**Utility cost**	**Landfill cost**	**Capital cost**	**OBJ**	**Eff S_{NO}**	**Eff S_{NH}**
Base case	By-pass3	891	1763	-	1471	4.79	1.01
Selected alternative	Canon	883	1762	8.08	1470	4.54	0.95
2	Anitamox	884	1762	12.89	1477	4.58	0.96
3	Canr	882	1762	16.17	1478	4.53	0.95
4	Shar/An-SBR	883	1762	19.85	1482	4.54	0.95
5	Demon	883	1762	19.87	1483	4.56	0.95
6	Deammon	884	1762	24.25	1488	4.58	0.96
7	Panammox	882	1762	33.09	1495	4.54	0.95
8	Shar/An-2st	883	1762	36.72	1500	4.56	0.95
9	Sharon	926	1762	35.74	1542	4.61	0.96

(b)

	Process interval	**Utility cost**	**Landfill cost**	**Capital cost**	**OBJ**	**Eff S_{NO}**	**Eff S_{NH}**
Base case	By-pass3	2579	4816	-	2907	5.75	1.21
Selected alternative	Canon	2553	4814	18.2	2899	5.40	1.13
2	Anitamox	2558	4814	28.9	2915	5.46	1.13
3	Canr	2553	4814	36.4	2917	5.40	1.13
4	Shar/An-SBR	2552	4814	44.7	2925	5.40	1.13
5	Demon	2555	4814	44.7	2928	5.43	1.14
6	Deammon	2558	4814	54.6	2940	5.46	1.14
7	Panammox	2553	4814	74.4	2955	5.40	1.13
8	Shar/An-2st	2555	4814	82.6	2966	5.43	1.14
9	Sharon	2689	4814	80.4	3097	5.49	1.14

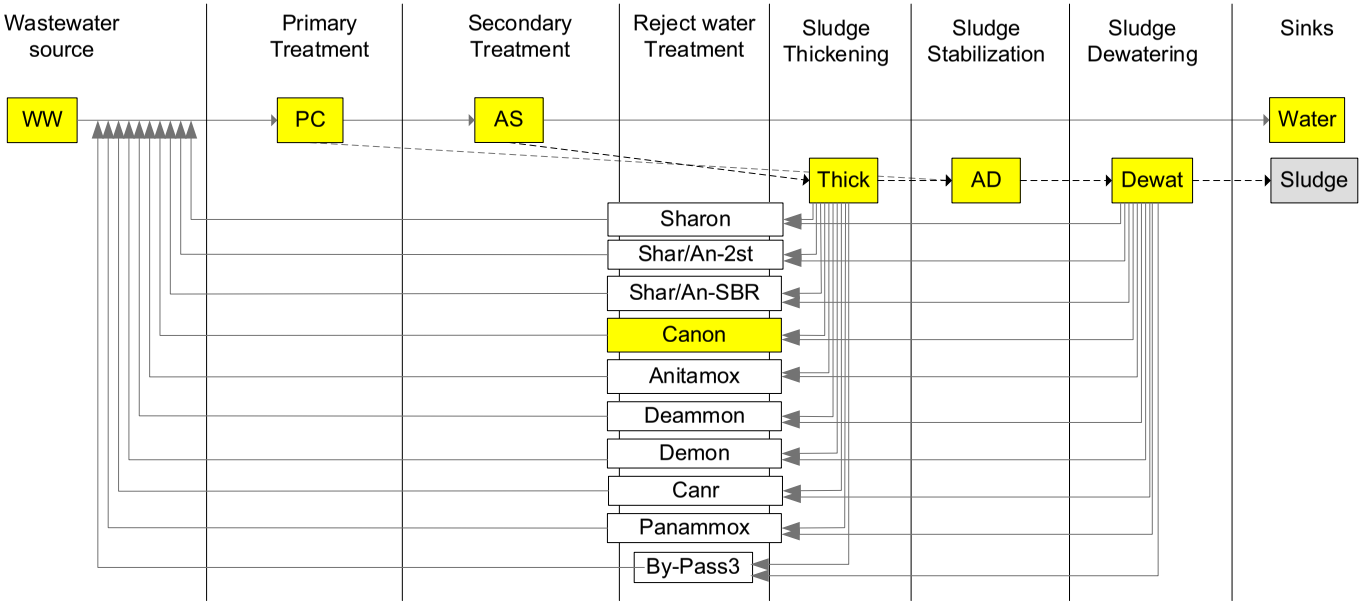


Figure 5.8 Process flow diagram and the interconnections for the selected alternative for scenario 1

Scenario 2 – Full-scale retrofitting study

The second scenario considers a full-scale retrofitting study. In other words, in this scenario, the alternative treatment technologies are placed in the superstructure not only under the sludge reject water treatment task, but also under the primary and secondary treatment tasks as illustrated previously in Figure 5.7.

Table 5.27 summarizes the cost breakdown information for the selected alternative together with the simulation results for other secondary treatment alternative units. Figure 5.9 illustrates the selected network. Since all the treatment units are designed in their optimality, their performances in terms of removal efficiencies of key contaminants are satisfactory and very similar to each other. Therefore, the main comparison is done here based on the cost breakdown information. Among the reject water treatment alternatives, the *Canon* technology was selected unless the task is by-passed. Since the performance and cost related differences among one stage partial nitritation/anammox technologies are very minor as stated previously under the discussion of Scenario 1, the selection of the *Canon* technology reflects the selection of the one stage partial nitritation/anammox mechanism as other alternatives can also do well.

The optimizer favors the *A-stage – Anammox* and *Canon* units for primary, secondary and sludge reject water treatment tasks, respectively. In other words, this network is selected as the best network in the predefined design space with regard to its reported cost and performance criteria. This network is characterized by its low utility consumption, which mainly results from the lower oxygen consumption of anammox technology as compared to the conventional nitrification/denitrification route. Another important factor is that only a fraction of COD is oxidized in the *A-stage* unit while the rest is directed to the sludge line to be digested in the *AD* unit; this also explains the high biogas production. The capital cost associated with the selected network is relatively low as compared to most of the networks shown in the summary table.

The *Granular AS* technology is coupled with the *PC* of the base-case and the *Canon* unit of the sludge reject water treatment task and ranked as the second best network favored by the optimizer with respect to the objective function value. The stoichiometric oxygen requirement of *Granular AS* technology (i.e. oxidation of organic material and nitrification/denitrification route for nitrogen removal) and the required chemical dosage for phosphorus removal are similar to the conventional biological nutrient removal system; therefore, the utility cost – consisting of aeration and chemical requirement – is similar to the conventional BNR units. However, the main advantage of this technology is that, there is no sludge return flow and internal recirculation flow; as well as no mixing provided; therefore, the pumping and mixing costs associated with this network are significantly lower. Moreover, it is a compact technology requiring less space as can also be observed from the low capital cost.

The low SRT BNR units (*BNR10* and *BNR14*) selected together with the *PC* and *Canon* units, as well as the combination of *A-stage* and *B-stage* technologies incorporate

chemical phosphorus treatment, which can be observed with the high utility cost reported for those units; on the contrary, the high SRT *BNR28* system has an anaerobic compartment for biological phosphorus removal, which increases its capital cost but decreases the utility consumption (i.e. less chemical addition for chemical precipitation of phosphorus). Increasing SRT results in less biogas production because less organics – mainly the inert fractions – are diverted to the sludge treatment line. When the *A-stage* technology is selected in the network, the biogas production increases as compared to the other BNR units because of the diversion of more organics to the *AD* unit in this technology. The pumping cost for those four networks are similar to each other; however, mixing cost increases with the increased SRT, in other words with the increasing volume. The *MBR* technology is selected together with *PC* and *Canon* units. The *MBR* is known to have high energy consumption and the utility cost in the cost breakdown evaluation reflects this, and includes the energy consumption of the unit together with aeration requirements. On the contrary, the associated capital cost, pumping and mixing cost are seen to be low. The *MBR* technology is designed as a compact technology because it operates with high biomass concentrations and it does also not incorporate a settler, which decreases the system volume (i.e. reactor + settler) significantly. Since the membrane cost is not incorporated into the capital cost calculation in this study (due to difficulty in obtaining data), the capital cost for the *MBR* unit is very low as compared to other units. However in practice, the capital costs associated with MBR are expected to be rather high (Tchobanoglous, 2003).

When the results for two different wastewater compositions are compared (i.e. Avedøre WWTP vs. Lynetten WWTP), the ranking does not change significantly and the above-discussed points seem to hold for both cases. However, one very important conclusion is that; since the organics concentration in the Lynetten WWTP influent is higher as compared to Avedøre WWTP, the biogas production increases. When comparing the selected network cost breakdown for the two cases, the value of the objective function decreases although the size of the treatment plant increases almost three fold from Avedøre to Lynetten resulting in the increase in utility cost, landfill cost, capital cost as well as pumping and mixing cost; this is mainly due to the increasing biogas production.

Table 5.27 Summary of results for deterministic solution of scenario 2 (all the cost parameters are given in 'unit cost') (a) Avedøre WWTP (b) Lynetten WWTP

(a)

	Network	Utility cost	Landfill cost	Biogas price	Pumping cost	Mixing cost	Capital cost (*)	OBJ
Base case	PC AS By-Pass3	891	1763	1914	491	240	-	1471
Selected alternative	A-stage Anammox Canon	761	871	2354	188	58	1630	1154
2	PC GranularAS Canon	1128	1145	1830	191	-	745	1380
3	PC BNR10 Canon	965	1387	2355	500	127	2243	2868
4	A-stage B-stage Canon	949	1165	2584	484	156	2736	2906
5	PC BNR14 Canon	992	1383	2185	496	148	2614	3450
6	PC MBR Canon	3083	1060	1832	188	53	940	3492
7	PC BNR28 Canon	827	1377	1929	491	219	3849	4834

(b)

	Network	Utility cost	Landfill cost	Biogas price	Pumping cost	Mixing cost	Capital cost (*)	OBJ
Base case	PC AS By-Pass3	2706	4719	6137	1109	540	-	2937
Selected alternative	A-stage Anammox Canon	2459	1928	7562	424	130	3668	1047
2	PC GranularAS Canon	3526	2918	5870	433	-	1675	2682
3	A-stage B-stage Canon	3023	2772	8298	1093	350	6157	5098
4	PC BNR10 Canon	2918	3164	6705	1129	287	5046	5838
5	PC BNR14 Canon	3007	3114	6356	1120	335	5882	7102
6	PC MBR Canon	7885	2690	5874	424	120	2115	7360
7	PC BNR28 Canon	2571	4517	6192	1109	493	8661	11159

* The capital cost is calculated based on the volume of the units, no other equipment or supporting materials (i.e. membrane, carriers, filters etc.) are included.

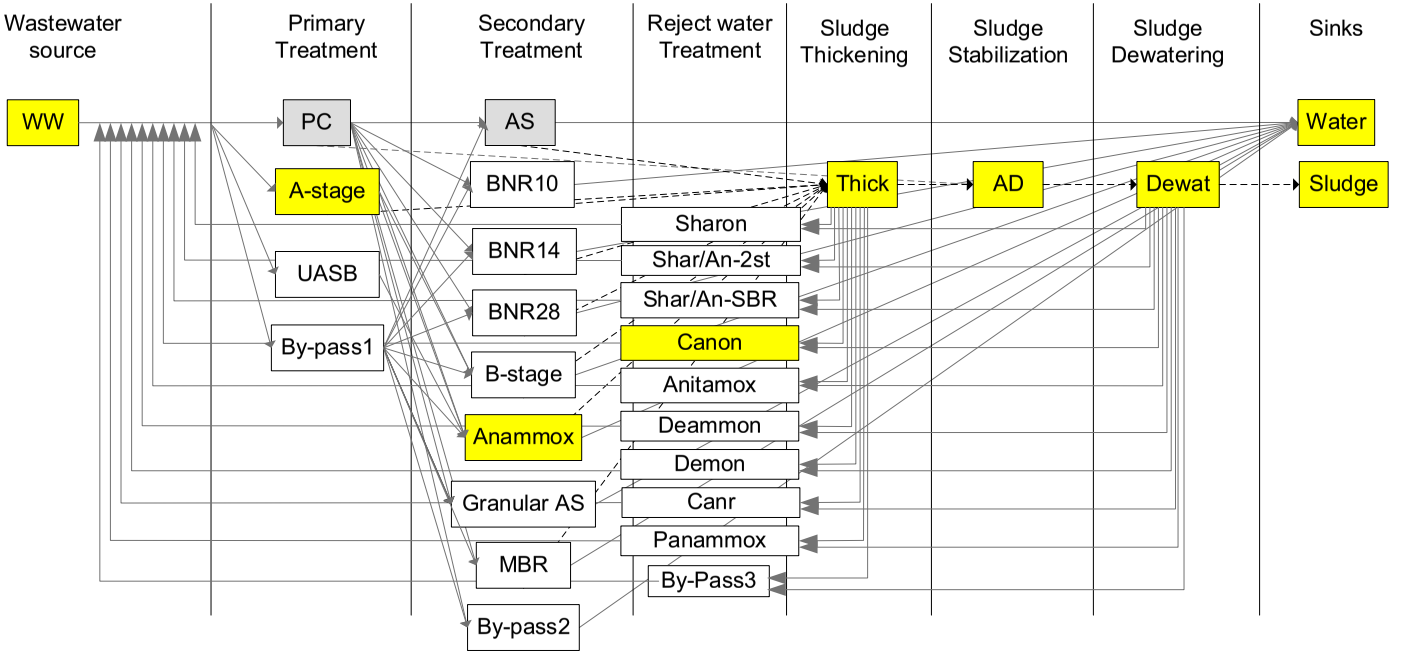


Figure 5.9 Process flow diagram and the interconnections for the selected alternative for scenario 2

The model and solution statistics for the deterministic solution for the two scenarios are summarized in Table 5.28.

Table 5.28 Model and solution statistics

	Scenario 1	**Scenario 2**
Number of variables	36,963	144,944
Number of binary variables	16	34
Number of equations	39,119	150,531
Objective function	1	1
Execution time (s)	0.141	0.624
Solver	CPLEX	CPLEX

5.2.5 Retrofitting case study – Uncertainty analysis

The uncertainty analysis was done by considering two different scenarios for the full-scale superstructure shown in Figure 5.7, taking into account:

- The effect of influent composition,
- The effect of cost and effluent limitation uncertainty.

5.2.5.1 Uncertainty characterization

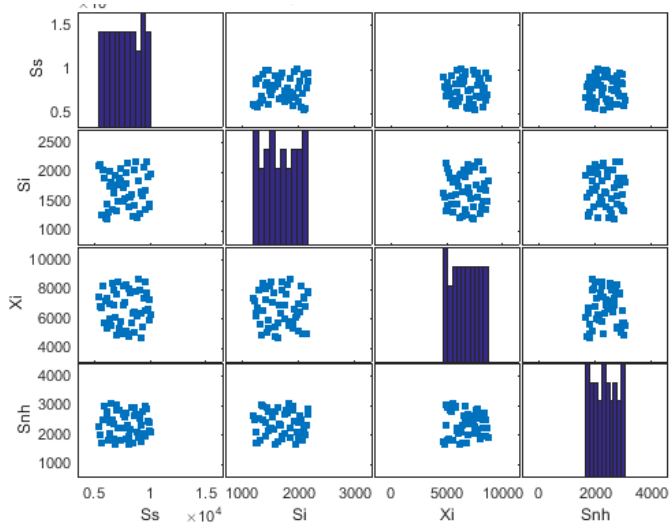
In the first step of the uncertainty analysis, the uncertain parameters are selected and their uncertain domain is identified. In order to characterize the uncertainty range, a uniform distribution is assigned to the uncertain parameters. The minimum, maximum and mean values of the parameters are recorded in the database.

In the Retrofitting case study, two main inputs to the problem were considered uncertain: the influent composition and cost related data together with effluent limits. In the first scenario, the influent COD fractionation and NH_4-N concentration were considered uncertain. Accordingly, a 30% variation around the deterministic value was assumed in the S_S, S_I and X_I fractions of COD and the resulting X_S concentration was calculated assuming that the total influent COD concentration is constant. Similarly, a 30% variation around the deterministic value was assumed in the influent S_{NH} concentration. In a second scenario the cost related parameters (oxygen transfer efficiency and electricity price) together with effluent total nitrogen limitation were selected as uncertain parameters. Table 5.29 summarizes the uncertainty characterization step.

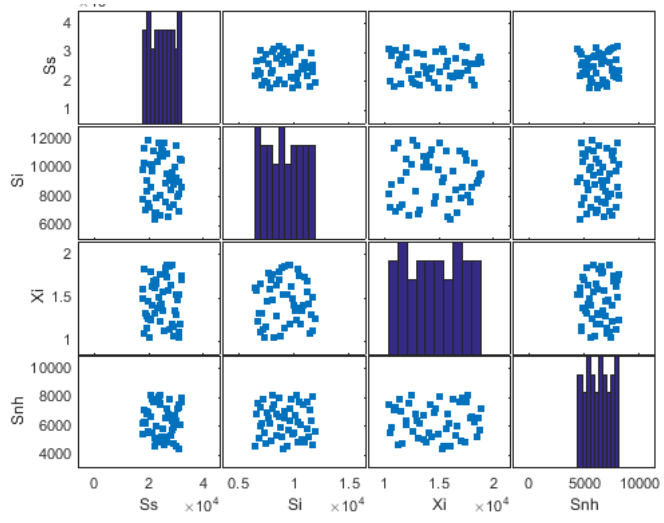
Table 5.29 Summary of uncertainty characterization

Sc.	Parameter	Unit	Mean		Minimum		Maximum	
			Avedøre	Lynetten	Avedøre	Lynetten	Avedøre	Lynetten
1	S_S	g /m^3	107.85	153.25	75.50	107.58	140.21	199.8
	S_I	g /m^3	23.48	56.52	16.44	39.68	30.52	73.69
	X_I	g /m^3	93.22	89.98	65.25	63.17	121.19	117.31
	S_{NH}	g /m^3	32.85	45.6	23.00	31.9	42.71	59.28
2	Electricity price	Euro/ kWh	0.098		0.08		0.12	
	O_2 transfer efficiency	kg O_2/kWh	4.85		4.12		5.58	
	Total N limit	g N/m^3	12.5		10		15	

The uncertainty domain was then sampled through Monte Carlo sampling. By means of sampling the uncertain domain, 50 future scenarios were generated assuming different realizations of the uncertain parameters. The sampling technique used at this step is Latin Hypercube Sampling (LHS) with its effective coverage of the uncertain domain. Figure 5.10 illustrates the future scenarios created.



(a)



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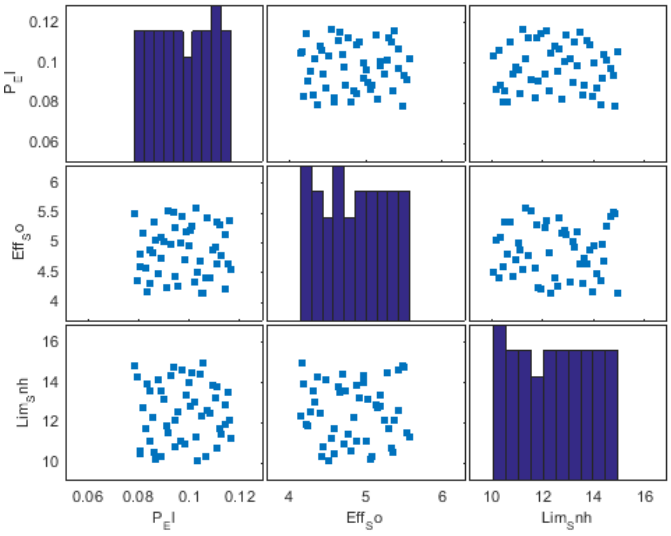


(c)

Figure 5.10 Sampling results (a) scenario 1 for Avedøre WWTP (b) scenario 1 for Lynetten WWTP and (c) scenario 2

5.2.5.2 Uncertainty mapping and analysis

In this step, the deterministic optimization problem was solved for the realization of 50 different future cases for two different scenarios. The results are illustrated in Table 5.30 and the cumulative distribution of the objective function, where the x-axis shows the objective function value, which represents operational and capital cost, and the y-axis represents the probability that the value of the objective function will be lower than the stated value on the x-axis, is shown in Figure 5.11.

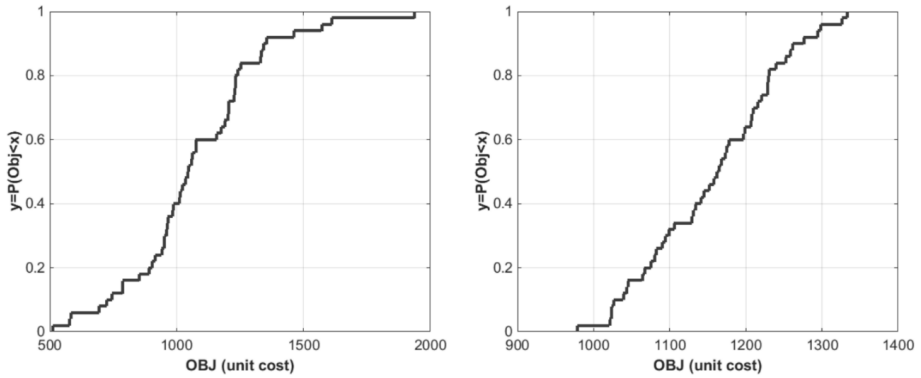
It is indicated by the results of scenario 1 that the uncertainty on influent composition had a significant effect on the network selection as well as on the value of the objective function. 60% of the future realizations resulted in the selection of the same network of the deterministic solution for Avedøre WWTP; on the other hand, for the Lynetten WWTP case, two network selections have almost the same probability of realization within the uncertain future domain. Different network selections seem also to be possible despite their relatively low possibility of occurrence. When the distribution of the value of the objective function is considered, it ranges from 513 to 1938 unit cost for Avedøre WWTP. In other words, 40% of the future realizations have higher TAC as compared to the deterministic problem solution. For Lynetten WWTP, the objective function value ranges from -1858 to 2736 unit cost. A negative objective function value does not necessarily mean that the treatment plant will operate with a profit; it shows that the

biogas production, in some future conditions, might dominate all the other operational cost elements considered. In the Lynetten WWTP case, 28% of the future scenarios have higher TAC as compared to the deterministic case.

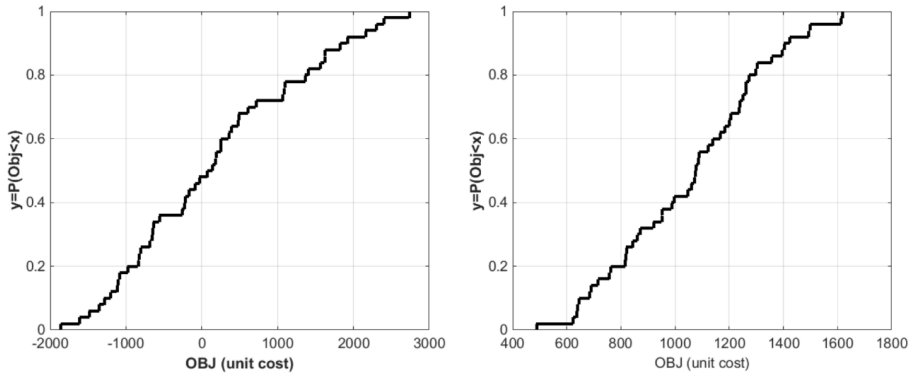
When the results of scenario 2 are analyzed, which takes into account cost related uncertainty as well as possible changes in effluent nitrogen limitation, the network selection seem to be more stable. For all of the future realizations, the deterministic network selection has not changed. Similarly, the variation in the objective function value is not as significant as for scenario 1; it changes from 978 to 1333 unit cost for Avedøre WWTP and 488 to 1619 for Lynetten WWTP, which indicates that 56% of the future realizations have higher TAC than the deterministic problem solution for both Avedøre and Lynetten WWTP cases.

Table 5.30 Summary of uncertainty mapping results

	Scenario	**Network**	**Probability of realization**	**Selected intervals**
Avedøre	1	1	60%	A-stage – Anammox - Canon
		2	20%	PC – Granular AS – By-Pass3
		3	8%	PC – AS – Canon
		4	8%	PC – AS – By-pass3
		5	2%	PC – Granular AS – Canon
		6	2%	A-stage – Anammox – By-pass3
Lynetten	1	1	48%	PC – Anammox – By-Pass3
		2	46%	A-stage – Anammox - Canon
		3	4%	PC – Granular AS – Canon
		4	2%	PC – AS – Canon
Avedøre	2	1	100%	A-stage – Anammox - Canon
Lynetten	2	1	100%	A-stage – Anammox - Canon



(a)



(b)

Figure 5.11 Cumulative distribution of the objective function for scenario 1 (left) and scenario 2 (right) for (a) Avedøre WWTP and (b) Lynetten WWTP

5.2.5.3 Decision making under uncertainty

The final step of the uncertainty analysis is where the optimization problem is formulated as a stochastic programming problem and solved by using the sample average approximation (SAA) technique (Birge and Louveaux, 1997). The results of this step are summarized in Table 5.31. Both scenarios resulted in the same network selection as the deterministic solution. Although different future realizations result in a significant variation especially for the objective function value as previously shown in Figure 5.11, when the results of 50 future scenarios are averaged by solving with the SAA technique, the effect of uncertainty seem to be insignificant. It is important to note that, the uncertainty characterization (i.e. selection of uncertain parameters and definition of the uncertain domain) play an important role in the generation of the results and is highly subjective and depends on the user's priorities. Several indicators are defined in order to summarize the results of uncertainty: Expected value of the perfect information (EVPI),

value of stochastic solution (VSS) and uncertainty price (UP) (Birge and Louveaux, 1997).

In scenario 1, the uncertainty had a positive effect on the solution for both Avedøre and Lynetten WWTPs; in other words, the SAA solution resulted in a lower objective function value as compared to the deterministic solution. When the cost breakdown is analyzed, this mainly results from the increase in the biogas production as a result of the variation in the COD fractionation. The EVPI is very low as compared to the objective function – 6% of the deterministic objective function value – in Avedøre WWTP. This shows that the current design is robust and can go further through the project development stages. However, for Lynetten WWTP, the high EVPI – 64% of the deterministic objective function value – represents that the selected network is not robust enough for the wastewater characterization of Lynetten WWTP and should further be improved or eventually replaced by another network to ensure a more robust selection. The negative UP for both cases results from the increase in the biogas price.

When the results of scenario 2 are analyzed, it can be concluded that the cost and effluent limitation related uncertainty, with its defined domain, do not have significant effect on the problem solution in terms of both network selection and cost breakdown for both WWTPs.

Since the network selection is the same for deterministic solution and solution under uncertainty, the possible gain from solving the stochastic optimization problem which is indicated by VSS is calculated as 0 for both scenarios.

Table 5.31 Summary of SAA results

		Scenario 1	Scenario 2	Deterministic solution
Avedøre	**Network**	A-stage-Anammox-Canon	A-stage-Anammox-Canon	A-stage-Anammox-Canon
	Utility cost	764	765	761
	Landfill cost	877	871	871
	Capital cost	1630	1630	1630
	Biogas price	2376	2354	2354
	Mixing cost	58	58	58
	Pumping cost	188	188	188
	OBJ	1141	1157	1154
	EVPI	69	0	-
	VSS	0	0	-
	UP	-13	3	-
Lynetten	**Network**	A-stage-Anammox-Canon	A-stage-Anammox-Canon	A-stage-Anammox-Canon
	Utility cost	2479	2471	2459
	Landfill cost	1937	1928	1928
	Capital cost	3668	3668	3668
	Biogas price	7792	7562	7562
	Mixing cost	130	130	130
	Pumping cost	424	424	424
	OBJ	846	1059	1047
	EVPI	674	0	-
	VSS	0	0	-
	UP	-201	12	-

5.2.6 General conclusions on Retrofitting case study

In this second case study, two real WWTPs of different scale from the Copenhagen region in Denmark have been selected as examples and the developed methodology was applied for retrofitting purposes. The wastewater characterization was obtained from the WWTP operators and yearly averaged values have been used constituting organics, nutrients (i.e. nitrogen and phosphorus) and solids. While the amount of wastewater to be treated is approximately tripled from Avedøre WWTP to Lynetten WWTP (i.e. 265,000 PE to 750,000 PE); a significant increase in concentrations of key pollutants was also observed. To this end, a design space covering novel treatment technologies was defined and the superstructure was formulated accordingly. The problem formulation was done so that the design space covers not only alternative technologies and network definitions for the already existing primary and secondary treatment tasks, but also introduces a new task responsible for sludge reject water treatment and several alternative technologies responsible for it. Overall, the superstructure includes 18 new technologies resulting in approximately 240 different possible network designs. The optimization problem was formulated as a MILP problem and solved for different scenario definitions under both deterministic conditions and uncertainty. The main conclusions of the study can be summarized as:

- A comprehensive design space was developed and formulated as a superstructure in a compact way. The design space includes many latest innovative concepts and technologies for both side-stream and main-stream wastewater treatment.
- By solving the problem under uncertainty, the effect of the variations in influent wastewater composition, cost and effluent limitation parameters on problem outputs are investigated.
- The application of a high rate oxic reactor (A-stage) coupled with anammox technology in the main wastewater treatment line is ranked as the best *design concept* by the optimizer with its low utility consumption, high biogas production and relatively low area requirement.
- Among the sludge reject water treatment alternatives, the commercial one stage partial nitritation-anammox technologies considered in the design space seem to be superior with respect to economic criteria as compared to two stage partial nitritation-anammox as well as nitritation/denitritation concepts.
- The increasing organic content (especially the biodegradable particulate organic fraction) resulted in a higher biogas production. Although the size of the plant is bigger in Lynetten WWTP as compared to Avedøre WWTP, resulting in higher capital cost and operational requirements (such as aeration, mixing, pumping etc.), the increase in the biogas production decreased the TAC considerably.

6 CONCLUSIONS AND PERSPECTIVES

The final chapter is the *Conclusions and perspectives* section where the summary of the outcomes of the PhD project together with the achievements are given. Moreover, some comments on the possible future improvements of the methodology and its applications in the wastewater engineering field are presented.

6.1 Summary of outcomes and achievements

In this study, a superstructure based optimization methodology has been developed to support optimal treatment process selection which is a critical and challenging step in the early stage of wastewater treatment plant design and retrofitting studies. A novel framework to help effective formulation and management of the complexity of the optimization problem is developed. The underlying theory and mathematical concepts, the required methods for its solution and analysis and its practical implementation as a tool is presented, using design and retrofitting case studies.

The main outcomes of the project are listed below:

- Within this project, a framework for synthesis, design and retrofit of WWTPs has been developed primarily to support the early stage decision making studies. The framework is composed of several steps and brings together different engineering practices. The first two steps of the framework, where the problem is analyzed and defined, as well as the design space is generated and presented in a superstructure form, require significant expert input. Different unit models for steady state design of treatment technologies were put together within a systematic data collection and design procedure, constituting the next step of the proposed framework; prior to the generation of the generic process interval model and formulation of the optimization problem. The uncertainties are also considered in the framework, where the optimization problem is solved to find the optimal network that can further go through the subsequent steps of detailed design, and is also solved within the uncertain domain to find out the effects of the expert / user defined uncertain parameters on the proposed solution.
- In this study, the design space is represented as a superstructure. The novel superstructure approach enables not only to cover numerous treatment alternatives but also to be flexible in the sense that any task, any treatment alternative and any connection can be included or excluded in the search space. Eventually, the search space covers a high number of WWTP network alternatives including well-known as well as innovative combinations of treatment units.
- A generic process interval is defined and described using a mass input-output model. This formulation of a generic model to define any unit or process in a treatment plant is important in order to handle the complexity of the MINLP problem formulation and solution for network design. The generic process interval encompasses several phenomena so that it can represent a complete reaction unit (e.g. a BNR unit composed of a series of reactors / compartments together with a settler and recycle flows in between as illustrated in Figure 6.1) as well as a single separation unit or a by-pass unit where the influent and effluent flow compositions are exactly the same. By inserting the parameters of the model into the database, which define the individual phenomena in the process interval – e.g. the amount of utility added, the performance in terms of COD, N, P removal,

the fraction of flow to be diverted for the internal recycle etc. – the treatment unit designs are converted into an algorithm for the optimization problem. Moreover, the mathematical formulation of the optimization problem and the database are separated from each other, which is very important because (1) the mathematical formulation is generic and can be used for any search / design space (i.e. superstructure) generated; and, (2) the maintenance of the database, which is required in order to keep the data updated and valid, is very straightforward.

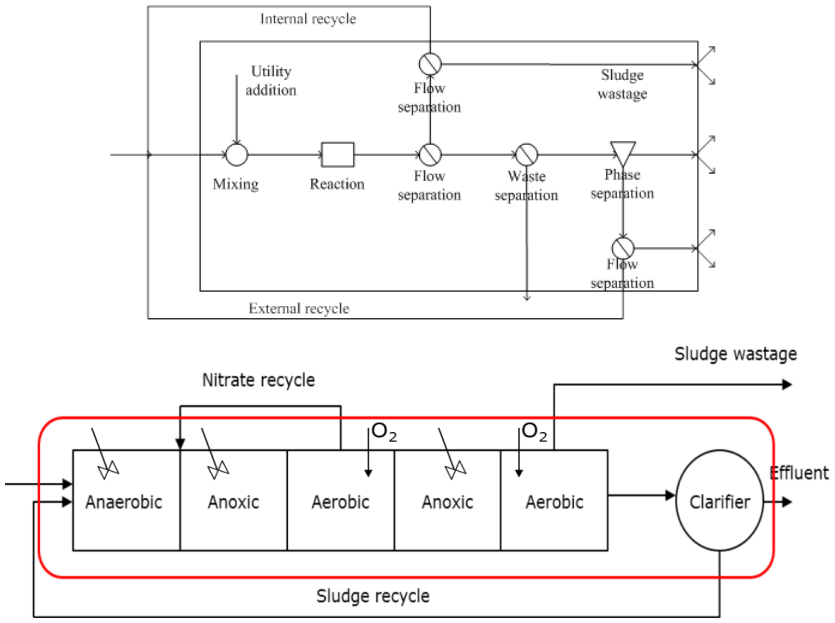


Figure 6.1 Illustration of the generic process interval

- One of the main features of the methodology used is the utilization of simple design models to collect data related to each technological alternatives (i.e. the treatment units are designed at their optimality, at steady state by fixing the design parameters and environmental conditions rather than optimizing them). This approach facilitates the definition of large search / design spaces and enables the solution not only for one deterministic scenario but also a number of future scenarios, e.g. generated through LHS sampling. The index definition of the mathematical formulation (component index, reaction index etc.) allows for investigating the fate of numerous pollutants / components in the treatment network, defining many different utilities and by-products as well as covering many single reactions and reactions in series in the search space.

- In order to highlight the applicability of the proposed methodology, two case studies of design and retrofitting origin were formulated and presented by following the steps of the synthesis, design and retrofitting framework.
    - The first case study, which is defined as a design problem, is dealing with a very well-known wastewater composition in the wastewater engineering community: the composition defined in the BSM2. In this case study, a rather limited superstructure was defined covering several tasks responsible for wastewater and sludge treatment. The treatment alternatives were designed to remove organics, nitrogen and solids from the incoming wastewater stream. To this end, two pre-denitrification type of technologies in different process configurations and an anaerobic treatment unit were included in the design space. Moreover, the anaerobic unit was coupled with innovative nitrogen treatment units in the mainline. Two sludge stabilization units – anaerobic digester and aerobic digester – were included in the sludge treatment line. Consequently, a network characterized by low capital cost, low utility consumption and low sludge production as well as high biogas revenue was selected as the best network design by the optimizer within the defined design space with respect to the defined constraints.
    - The second case study deals with two full-scale treatment plants located in the Copenhagen region in Denmark. These plants receive a wastewater mainly characterized by its organics, nutrients and solids content. This case study was designed as a retrofitting case study covering many novel technologies in the main wastewater treatment line as well as for the sludge reject water stream for nitrogen removal. As the optimization results suggest, the application of the combination of a high-rate oxic reactor and the novel anammox technology is promising with low energy requirements as well as high biogas potential. On the other hand, the one stage PN/anammox applications seem to be effective both in performance and economic terms; however, the commercial applications of a dozen of other side-stream nitrogen removing technologies do not differ significantly when the cost and performance are concerned; therefore, the main selection is based on local conditions such as ease of operation, preference and experience of staff, etc..

Finally, it is believed that the novel superstructure based optimization approach for facilitating early stage design and retrofitting decisions is seen as a big step towards filling the gap between optimization-based design methods and wastewater engineering. The proposed framework and the resulting tool are promising in the sense that they are expected to support the process design experts and engineers in their continuous efforts to identify and design novel, optimal and efficient WWPTs for a given wastewater treatment problem.

6.2 Future perspectives

In this presented work, we addressed the early stage decision making for WWTP design and retrofitting studies, which has become a formidable challenge with the increasing number of treatment technologies as well as various driving factors such as the need for nutrient recovery, energy efficiency, water and sludge reuse. However, the content and therefore impact of the proposed framework can be increased and some further development ideas are presented below.

- In the wastewater engineering field, it is known that there are numerous treatment alternatives utilizing different means of treatment for the removal of various types of pollutants. Therefore, one of the most important suggestions for future work is enlarging the database to cover many more treatment technologies including for example Enhanced Biological Phosphorus Removal (EBPR) technologies, Biological Aerated Filters (BAF) etc.
- As the treatment technologies are numerous in the market, the novel approaches and considerations are as well. Recently considerable attention was paid to climate change and specifically the release of greenhouse gases (GHG) together with the recognition of WWTPs as significant contributors to the GHG emissions. As a result there are currently many studies focusing on mitigating the release of especially N_2O from WWTPs. Moreover, diminishing of important resources like phosphorus, potassium and fossil fuels and their derivatives combined with the fact that wastewater is a significant 'resource' containing many useful elements and materials brings the importance of resource recovery in WWTPs increasingly in focus. Furthermore, with more strict regulations put on several compounds, their fate in WWTPs gained importance. Examples of such compounds are: micropollutants and heavy metals. Thus, their introduction into the component list and inclusion of their removal mechanisms into unit models would be an important improvement. Models for this type of components have for example been formulated and integrated in the WWTP simulation benchmark platform by Snip et al. (2014). Therefore, the scope of the design / retrofitting problem can be extended to cover such approaches to the end where the wastewater treatment facility become more of a resource recovery facility rather than being only a treatment facility.
- In the current framework, the step 2, where the superstructure is generated is done manually by incorporating expert knowledge and previous experiences. However, this step can also be done through mathematical programming by for instance combining the superstructure optimization based tool with the knowledge-based decision support systems developed successfully by Comas et al. (2003).
- Currently, the sink definitions for treated water and sludge are implemented such that they only cover discharge into surface waters and disposal into landfills, respectively. However, the environments where the effluents of WWTPs are discharged to are considered as an integrated part of the treatment plant and play

a very important role in the early stage design decisions. For instance, when the sludge is intended to be used in agriculture, many more pollutants come into the picture such as metals, trace organics etc. and they need to be removed to some extent prior to the agricultural use. Therefore, definition of different sink alternatives with different constraints would be a good idea when extending the scope of the tool.

- In the design methodology used within this study, the design parameters are fixed by collecting data for optimal operation of the treatment units from the open literature. In a future expansion, the design methodology can include the optimization of these parameters rather than fixing them.
- A final remark can be the extension of the scope to cover the sewer systems as well. In the current state of the tool, the wastewater characterization is done at the point it enters the treatment plant. However, sewer systems are considered as important elements of the wastewater management with many reactions occurring and significant costs are allocated to the sewer system. The addition of sewer facilities might also contribute to the discussion on the selection of centralized or decentralized treatment facilities, and provide valuable ideas from an optimization point of view.

A APPENDICES

A.1 Appendix 1 – Nomenclature

Abbreviations

A2O	Anaerobic-anoxic-oxic biological nutrient removal technology
AD	Anaerobic digester
ADM1	Anaerobic Digestion Model no.1
AeD	Aerobic digester
Anammox	Anaerobic ammonium oxidation
AnD	Anaerobic digester
AOB	Ammonium oxidizing bacteria
AOTR	Actual oxygen transfer rate
AS	Activated sludge
ASM1	Activated Sludge Model no.1
ASM2(d)	Activated Sludge Model no.2(d)
ASM3	Activated Sludge Model no.3
BAT	Best available techniques
BNR	Biological nutrient removal
BOD	Biochemical oxygen demand
BP	By-pass
BSM1	Benchmark Simulation Model no.1
BSM2	Benchmark Simulation Model no.2
B-WWTP	Benchmark wastewater treatment plant
C	Carbon
Canon	Completely autotrophic nitrogen removal over nitrite
Canr	Completely autotrophic nitrogen removal
CAPEX	Capital cost
COD	Chemical oxygen demand
CSTR	Continuous stirred tank reactor
DO	Dissolved oxygen
EBPR	Enhanced biological phosphorus removal
ESCAPE	European Symposium on Computer Aided Process Engineering
EU	European Union
EVPI	Expected value of perfect information

GDX	GAMS data exchange
GHG	Greenhouse gases
HRT	Hydraulic retention time
IWA	International Water Association
LHS	Latin hypercube sampling
MBBR	Moving bed biofilm reactor
MBR	Membrane bioreactor
MI(N)LP	Mixed Integer (non)Linear Programming
MLE	Modified Ludzack Ettinger
MLSS	Mixed liquor suspended solids
N	Nitrogen
NLP	Nonlinear Programming
NOB	Nitrite oxidizing bacteria
NS	Number of samples
O_3	Ozone
OBJ	Objective function
OPEX	Operational cost
OxD	Oxidation ditch
P	Phosphorus
PC	Primary clarifier
PE	Population equivalence
PN	Partial nitritation
PN/A	Partial nitritation/Anammox
SBR	Sequencing batch reactor
SHARON	Single reactor High activity Ammonia Removal over Nitrite
SLR	Solids loading rate
SOR	Surface overflow rate
SOTR	Standard oxygen transfer rate
SRT	Sludge retention time
SAA	Sample average approximation
TAC	Total annualized cost
TKN	Total kjeldahl nitrogen
TSS	Total suspended solids
UASB	Upflow anaerobic sludge blanket
UCT	University of Cape Town biological nutrient removal technology
UP	Uncertainty price
UV	Ultraviolet
VSS	Value of stochastic solution

WFD	Water Framework Directive
WW	Wastewater
WWTP	Wastewater treatment plant

Indexes

ae	Aerobic
an	Anoxic
i,ii	Component index
in	Influent
k,kk	Process interval index
out	Effluent
react	Reactant index
rr	Reaction index
sc	Uncertainty index
T	Total

Greek letters

α	Amount of utility mixed with the main flow
γ	Stoichiometry matrix
η	Removal efficiency
θ	Conversion efficiency of the key reactant
Θ	Uncertain data
μ	Mass of utility added per mass flow of corresponding component
ν	Stoichiometric coefficient in ASM1 matrix
ρ	Process rate expression in ASM1 matrix
φ	Matrix storing wastewater characterization

Symbols

F	Influent flow to the process interval from another process interval
b	Decay coefficient in AeD model
b_A	Decay rate coefficient of autotrophic microorganisms
b_{AD}	Decay coefficient in AD model
b_H	Decay rate coefficient of heterotrophic microorganisms

CN	Sum of NH4-N nitrified and assimilated into the biomass
COD_b	Biodegradable COD
DO_{sp}	Dissolved oxygen set point
DP	Denitrification potential
E_Θ	Expected value of the objective function
f	Ratio of endogenous residue solids to active solids in AeD model
F_1, F_2, F_3	Outlet streams directed to the other process intervals
F_{in}	Sum of influent flows to the process interval
F_{mix}	Flow after mixing
f_n	Nitrogen content of the active solids in AeD model
f_{ns}	Non-settleable fraction of particulate material
F_{out1},F_{out2},F_{out3}	Primary, secondary and tertiary outlet streams
f_P	Fraction of biomass ends up as inert particulate matter
F_{reac}	Flow after reaction
F_{rec2}	External recycle flow
F_{rec3}	Internal recycle flow
F_{sep}	Flow after internal separation
f_{thick}	Thickening factor
f_{thin}	Thinning factor
F_w	Flow after waste separation
f_{xi}	Non-biodegradable fraction of the biomass
h	Height
i_{XB}	Mass of nitrogen per mass of cellular COD
i_{XP}	Mass of nitrogen per mass of inert particulate COD
K_2	Denitrification rate
k_a	Ammonification rate
k_h	Maximum specific hydrolysis rate
K_m, K_s	Kinetic parameters in AD model
K_{NH}	Kinetic parameter regarding nitrification
K_{NO}	Kinetic parameter regarding denitrification
K_{OA}	Half saturation coefficient for dissolved oxygen (autotrophs)
K_{OH}	Half saturation coefficient for dissolved oxygen (heterotrophs)
K_S	Kinetic parameter for growth of heterotrophic microorganisms
K_X	Half saturation coefficient for hydrolysis of slowly biodeg. substrate
Lim	Effluent limit
MO	Oxygen requirement for oxidation of carb. material in AeD model
MO_n	Oxygen requirement for nitrification in AeD model
NS	Nitrogen content of the biomass
P_1, P_2, P_3	Unit cost for components or process intervals

P_{cost}	Product cost
p_{thick}	Percentage of suspended solids in the underflow
Q	Flow rate
q	Volumetric loading/removal rate
R	Utility flow
r	Reaction in ASM1 matrix
R	Retention time in AD model and in AeD model
r_h	Hydrolysis rate in AD model
RO	Oxygen requirement
S	Superstructure information
S_{ALK}	Alkalinity
S_{bp}	Particulate biodegradable COD
S_{bsf}	Readily biodegradable soluble COD
S_{cost}	Cost related to the sink intervals
S_I	Soluble inert organic matter
S_m	Methane production
S_{ND}	Soluble biodegradable organic nitrogen
S_{NH}	$NH_4^+ + NH_3$ nitrogen
S_{NO}	Nitrate and nitrite nitrogen
S_O	Oxygen
SP_1, SP_2, SP_3	Flow separation fractions
split	Phase separation fraction
S_S	Readily biodegradable substrate
Sup	Unbiodegradable particulate COD
Sus	Unbiodegradable soluble COD
t	Project lifetime
U_{cost}	Utility cost
V	Volume
W	Waste separation fraction
X_a	Active solids in AeD model
$X_{B,A}$	Active autotrophic biomass
$X_{B,H}$	Active heterotrophic biomass
X_e	Endogenous residuals in AeD model
X_I	Particulate inert organic matter
Xi	Inert solids in AeD model
x_{LO}, x_{UP}	Lower and upper boundaries defined for variable x
X_{ND}	Particulate biodegradable organic nitrogen
X_P	Particulate products arising from biomass decay
X_S	Slowly biodegradable substrate

y	Binary variable assigned to process intervals
Y_A	Autotrophic yield
Y_{AD}	Yield coefficient in AD model
Y_{AnAOB}	Yield coefficient for anammox bacteria
Y_{AOB}	Yield coefficient for ammonium oxidizers
Y_{denit}	Yield coefficient for denitrifiers
Y_H	Heterotrophic yield
Z_{AD}	Acidogen biomass concentration
η_g	Denitrification correction factor
η_h	Hydrolysis rate correction factor
μ_A	Growth rate of autotrophic microorganisms
μ_H	Growth rate of heterotrophic microorganisms

A.2 Appendix 2 – Data collection and design of individual treatment technologies

A.2.1 Matlab® scripts for treatment unit designs

Below in this section, the automated Matlab® script together with the script containing influent wastewater characterization and biokinetic constants are given.

Matlab® script containing data for influent characterization and biokinetic constants

```
% Design tempetarure: 15 degree C

%% Influent characterization

Si_i=23.48;          % g/m3
Ss_i=107.85;
Xi_i=46.61;
Xs_i=125.82;
Xbh_i=0;
Xba_i=0;
Xp_i=0;
So_i=0;
Sno_i=0;
Snh_i=32.85;
Snd_i=0;
Xnd_i=9.8/2;
Salk_i=7;            % mol HCO3/m3
Q=72000;             % m3/d

influent=[Si_in Ss_in So_in Sno_in Snd_in Snh_in Salk_in Xi_in
Xs_in Xbh_in Xba_in Xp_in Xnd_in  Q_in]';

%% Effluent requirements in g/m3
COD_eff=10;
N_eff=15;
Snh_eff=4;

%% Parameters (15 degree C) values from BSM2 and ASM3

fxi=0.2;             % g COD Xi / g COD Xbm
inbm=0.07;           % gn/gcod. asm3 values.
inxp=0.06;           % gn/gcod
inxs=0.04;           % Xnd/Xs
inss=0.03;           % Snd/Ss
inxi=0.02;           % N/Xi
insi=0.01;           % N/Si
Ya=0.24;             % g cell COD formed / g N oxidized
Yh=0.67;             % g cell COD formed / g COD oxidized
```

```
muh=4;                % 1/d
Ks=10;                % g COD/m3
Koh=0.2;              % g O2/m3
Kno=0.5;              % g NO3-N/m3
bh=0.3;               % 1/day
nug=0.8;              % dimensionless
nuh=0.8;              % dimensionless
kh=3;                 % g slowly biodeg COD / g cell COD * day
Kx=0.1;               % g slowly biodeg COD / g cell COD
mua=0.5;              % 1/day
Knh=1;                % g NH3-N/m3
ba=0.05;              % 1/day
Koa=0.4;              % g O2/m3
ka=0.05;              % m3 * COD/g day
DOsp=2;               % DO set point (mg/L)
fp=0.08;              % g COD Xp / g COD Xbm
```

Matlab® script for BNR design

```
%% Assumptions used in the model
% All COD removal occurs in the anoxic zone by using nitrate as
an electron
% acceptor

%% load the data file
data_avedore;

%% Define system specific design data

SRT=14;                       %total SRT in days
HRTae=(9/24);                 %aerobic HRT in days
HRTan=(3/24);                 %anoxic HRT in days
HRT=HRTae+HRTan;              %total HRT
volumeratio=HRTan/HRT;        %anoxic volume / total volume
SRTae=SRT*(1-volumeratio);    %aerobic sludge retention time in
days
SRTan=SRT*volumeratio;        %anoxic SRT in days
Vae=Q*HRTae;                  %aerobic volume (m3)
Van=Q*HRTan;                  %anoxic volume (m3)
Vtot=Vae+Van;                 %total volume (m3)

fns_part=0.002;               %fraction of non-settleable solids
in the settler

%% Influent
%ASM --> Lumped parameters (e.g.COD, N)
%COD
Sbsfi=Ss_i;                                  %readily biodegrada-
ble soluble (influent)
```

```
Sbpi=Xs_i+Sbsfi-DOsp;                          %particulate biode-
gradable (influent) corrected for oxygen in the recycle sludge
Supi=Xi_i+Xp_i+fxi*(Xbh_i+Xba_i);              %particulate unbio-
degradable (influent)
Susi=Si_i;                                     %soluble unbiode-
gradable (influent)

COD_in=Sbpi;                                   %total soluble COD
in
TNi1=inxs*Xs_i+inss*Ss_i+(Xbh_i+Xba_i)*inbm;%nitrogen content of
biodegradable COD
TNi2=inxi*Xi_i+inxp*Xp_i;                      %nitrogen content of
unbiodegradable COD

N_in=TNi1+TNi2+Snh_i+Sno_i+Snd_i;              %total nitrogen in
TKN_in=Snh_i+Snd_i+Xnd_i;                      %total biodegradable
nitrogen in



%% Model equations
% Carbon removal in aerobic tank
% effluent COD (independent of the influent amount)
COD_out=(Ks*(1+bh*SRT))/(SRT*(muh*(volumeratio)-bh)-1);

%Nitrogen removal in aerobic tank (nitrification)
Snh_out=(Knh*(ba+(1/SRT)))/(mua*(1-volumeratio)-(ba+(1/SRT)));

%% sludge production
MXbh=(Q*(COD_in-COD_out)*Yh*SRT)/(1+bh*SRT);%het. biomass (g)
MXp_bh=(fp*bh*MXbh*SRT);                       %particulates aris-
ing from decay of het biomass (g)
MXi=Q*Xi_i*SRT;                                %inert particulates

Ns=(inbm*MXbh)/(SRT*Q);                        %NH4 assimilation by
growth g/m3
CN=TKN_in-Snh_out-Ns;                          %nitrogen balance
MXba=(Q*CN*Ya*SRT)/(1+ba*SRT);                 %aut. biomass (g)
MXp_ba=(fp*ba*MXba*SRT);                       %particulates aris-
ing from decay of aut biomass (g)
MXp=MXp_ba+MXp_bh;

MXt=MXbh+MXp+MXi+MXba;                         %total solids pro-
duced (g)
Xt_design=MXt/Vtot;                            %design solids con-
centration in biological tank (g/m3)

Xbh=MXbh/Vtot;                                 %from mass to con-
centration
Xba=MXba/Vtot;
Xi=MXi/Vtot;
Xp=MXp/Vtot;
```

```
%% calculation of wastage flowrate (assuming that it is wasted
from the reactor prior to
%secondary settler
Px=MXt/SRT;
Qw=Px/Xt_design;

%% Oxygen requirement (in Predenit. system all COD is oxidized
using Nitrate)
%oxygen is mainly maintenance /decay!
ROb1=(((1-fxi)*bh*MXbh)*(Vae/Vtot));%oxygen requirement in aero-
bic tank het.cell decay
ROb2=(((1-fxi)*ba*MXba)*(Vae/Vtot));%oxygen requirement in aero-
bic tank aut.cell decay
ROb=ROb1+ROb2;
ROn=4.57*Q*CN;                      %oxygen requirement for ni-
trification
ROt=ROb+ROn;                        %total oxygen requirement in
g/day

%% denitrification potential (DP=DP1+DP2+DP3)
DP1=Ss_i*(1-Yh)/2.86;       % mgN/L
CODb=Xs_i-(COD_out);
K2=0.01;
DP2=K2*CODb*Yh*SRTan/(1+bh*SRT);
DP3=((1-fxi)*bh*MXbh*(Van/Vtot)/2.86)*(1/Q);
DP=DP1+DP2+DP3;
CN2=Snh_i-Snh_out-Ns;
Sno_eff=CN2+Sno_i-DP;


%% Effluent
%COD, N to ASM1
%concentrations after reaction (effluent of the aeration tank)
Si=Si_i;            % g/m3
Ss=0;
Xi=Xi;
Xs=COD_out;
Xbh=Xbh;
Xba=Xba;
Xp=Xp;
So=DOsp;
Sno=Sno_eff;
Snh=Snh_out;
Snd=0;
Xnd=inbm*(Xbh+Xba)+inxs*Xs+inxp*Xp+inxi*Xi;
Salk=Salk_i;        % mol HCO3/m3
Q=Q;                % m3/d
```

A.2.2 Treatment unit models

Table A.1 ASM1 Matrix (Copp, 2002)

Component, i		1	2	3	4	5	6	7	8	9		10	11	12	13	Process rate, ($ML^{-3}T^{-1}$) ρ_j
j	Process	S_I	S_S	X_I	X_S	X_{BH}	X_{BA}	X_P	S_O	S_{NO}		S_{NH}	S_{ND}	X_{ND}	S_{ALK}	
1	Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$			$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\mu_h\left(\frac{S_S}{K_s+S_S}\right)\left(\frac{S_O}{K_{OH}+S_O}\right)X_{BH}$
2	Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2.86Y_H}$		$-i_{XB}$			$\frac{1-Y_H}{14*2.86Y_H}$ $-i_{XB}/14$	$\mu_h\left(\frac{S_S}{K_s+S_S}\right)\left(\frac{K_{OH}}{K_{OH}+S_O}\right)$ $*\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{BH}$
3	Aerobic growth of autotrophs						1		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$		$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\mu_a\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{OA}+S_O}\right)X_{BA}$
4	Decay of heterotrophs				$1-f_p$	-1		f_p						i_{XB} $-f_p i_{XP}$		$b_H X_{BH}$
5	Decay of autotrophs				$1-f_p$		-1	f_p						i_{XB} $-f_p i_{XP}$		$b_A X_{BA}$
6	Ammonification of soluble organic nitrogen											1	-1		$\frac{1}{14}$	$k_a S_{ND} X_{BH}$
7	Hydrolysis of entrapped organics		1		-1											$k_h\frac{X_S/X_{BH}}{K_X+(X_S/X_{BH})}\left[+\eta_h\left(\frac{K_{OH}}{K_{OH}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{BH}$
8	Hydrolysis of entrapped organic nitrogen												1	-1		$\rho_7(X_{ND}/X_S)$
Observed conversion rates ($ML^{-3}T^{-1}$)		$r_i=\sum_j \nu_{ij}\rho_j$														
		soluble inert organic matter (M(COD) L^{-3})	readily biodegradable substrate (M(COD) L^{-3})	particulate inert organic matter (M(COD) L^{-3})	slowly biodegradable substrate (M(COD) L^{-3})	active heterotrophic biomass (M(COD) L^{-3})	active autotrophic biomass (M(COD) L^{-3})	particulate products arising from biomass decay (M(COD)	oxygen (negative COD) (M(-COD) L^{-3})	Nitrate ant nitrite nitrogen (M(N) L^{-3})		$NH_4^+ + NH_3$ nitrogen (M(N) L^{-3})	soluble biodegradable organic nitrogen (M(N) L^{-3})	particulate biodegradable organic nitrogen (M(N) L^{-3})	alkalinity - molar units	

Table A.2 Validation for systematic data collection procedure – continued

(a)

Parameter	ASM1		Design model no.1		Design model no.2	
Corresponding technology	Pre-denitrification activated sludge					
Temperature (°C)	15					
Anoxic / Aerobic volume ratio	0.6					
TKN/COD ratio	0.14					
HRT (hours)	**20**	22.8	**20**	22.8	**20**	22.8
SRT (days)	**28**	35	**28**	35	**28**	35
COD (g COD / m^3)						
Influent	**381.19**	381.19	**381.19**	381.19	**381.19**	381.19
Effluent	**45.06**	44.50	**45.07**	45.92	**41.71**	42.27
Reduction (%)	**88.18**	88.33	**88.17**	87.95	**89.05**	88.91
Nitrogen (g N / m^3)						
Total-N influent	**54.43**	54.43	**54.43**	54.43	**54.43**	54.43
S_{NO} effluent	**10.05**	9.68	**12.16**	11.84	**9.56**	9.03
S_{NH} effluent	**0.14**	0.13	**0.38**	0.34	**0.47**	0.47
Total-N effluent	**11.79**	11.36	**14.15**	13.86	**11.30**	10.81
Reduction (%)	**78.34**	79.12	**73.98**	74.52	**79.23**	80.14
Suspended Solids (g COD / m^3)						
Influent	**211.27**	211.27	**211.27**	211.27	**211.27**	211.27
Effluent	**10.815**	10.41	**11.30**	11.94	**8.85**	9.27
Reduction (%)	**94.88**	95.07	**94.65**	94.34	**95.80**	95.60

(b)

Parameter	ASM1		Design model no.1		Design model no.2	
Corresponding technology	Pre-denitrification activated sludge					
Temperature (°C)	15					
Anoxic / Aerobic volume ratio	0.33					
TKN/COD ratio	0.1					
HRT (hours)	**20**	22.8	**20**	22.8	**20**	22.8
SRT (days)	**28**	35	**28**	35	**28**	35
COD (g COD / m^3)						
Influent	**476.2**	476.2	**476.2**	476.2	**476.2**	476.2
Effluent	**39.87**	39.39	**46.44**	47.99	**42.2**	43.77
Reduction (%)	**91.62**	91.73	**90.25**	89.92	**91.13**	90.81
Nitrogen (g N / m^3)						
Total-N influent	**48.24**	48.24	**48.24**	48.24	**48.24**	48.24
S_{NO} effluent	**5.14**	5.10	**4.78**	4.78	**5.52**	5.57
S_{NH} effluent	**0.15**	0.12	**0.29**	0.26	**0.49**	0.49
Total-N effluent	**6.94**	6.85	**7.43**	7.52	**8.02**	8.16
Reduction (%)	**85.59**	85.81	**84.61**	84.41	**83.36**	83.08
Suspended Solids (g COD / m^3)						
Influent	**258.62**	258.62	**258.62**	258.62	**258.62**	258.62
Effluent	**11.78**	11.43	**17.22**	18.38	**14.49**	15.30
Reduction (%)	**95.44**	95.58	**93.34**	92.89	**94.39**	94.08

A.3 Appendix 3 – Case study Data

A.3.1 B-WWTP Case Study

A.3.1.1 Design of Secondary Treatment Alternatives

Design of pre-denitrification type of activated sludge systems

In the following steps, the design of a pre-denitrification type of activated sludge processes will be given in detail by following the Design model no.1 presented earlier in section 4.1.1.2.

- Two different pre-denitrification systems are considered as treatment alternatives in the B-WWTP case study; namely, Modified Ludzack-Ettinger (MLE) and Oxidation Ditch (OxD).
- The SRT and HRT of the systems are selected from a given range (Tchobanoglous, 2003) as *14 days* and *12 hours* for MLE, and *28 days* and *24 hours* for OxD. The anoxic to aerobic volume ratio is assumed to be *0.6* for both systems.
- The total COD and nitrogen are calculated by using equations 4.3 and 4.4 respectively as *292.36 g COD/m^3* and *49.1 g N/m^3,* where the non-biodegradable fraction of biomass – f_{Xi} is taken as *0.2*.
- By using equations 4.5 and 4.6, the volumes of the different compartments are calculated. Accordingly, V_{ae} and V_{an} for the MLE system are calculated as *5,693 m^3* and *3,530 m^3,* respectively; whereas these values are *11,375 m^3* and *7,071 m^3* for OxD.
- Next, by using the equations 4.7 – 4.24, the concentrations of different components in the reactor, the oxygen consumption and the sludge production are calculated. The results are summarized in Table A.3.

Table A.3 The design results for MLE and OxD technologies

Parameter	Unit	Value		Related equation
		MLE	OxD	
COD_b^{out}	g COD/m^3	3.29	2.8	2.37
S_{NH}^{out}	g N/m^3	0.64	0.39	2.38
X_{BH}	g COD/m^3	961	533	2.39
X_{BA}	g COD/m^3	182	133	2.42
X_P	g COD/m^3	833	932.5	2.43
X_I	g COD/m^3	1,434	1,434	2.44
RO_b	kg O_2/d	1,372	1,515	2.46
RO_n	kg O_2/d	3,883	3,994	2.47
Q_W	m^3/d	658	658	2.48
S_{NO}^{out}	g N/m^3	9.49	7.77	2.53
X_{ND}	g N/m^3	141.42	109.23	2.54

Design of UASB system

- The system is designed at 15°C, accordingly the SRT and HRT of the system are selected as *120 days* and *14 hours*, respectively (WEF, 2010).
- The total volume of the reactor is a combination of liquid volume and gas volume. The calculations are done based on the following equations (A.1 – A.5) and data given by Tchobanoglous (2003). The liquid volume - V_{liq}, was calculated from the known influent flow rate and the selected HRT which resulted in a volume of *10,760 m^3*. The area of the reactor (A) is calculated to be *1,098 m^2* assuming the upflow velocity (v_{up}) to be *0.7 m/h*. The total height (h_t) of the reactor is calculated as *11.8 m* as the summation of liquid height (h_{liq}), which is calculated to be *9.8 m* and gas collection height (h_{gas}), which is assumed to be *2 m*. Consequently, the total volume of the reactor (V_t) is *12,956 m^3*.

$$V_{liq} = Q * HRT \quad \text{A.1}$$

$$A = \frac{Q}{v_{up}} \quad \text{A.2}$$

$$h_{liq} = \frac{V_{liq}}{A} \quad \text{A.3}$$

$$h_t = h_{liq} + h_{gas} \quad \text{A.4}$$

$$V_t = h_t * A \quad \text{A.5}$$

- The following equations (A.6 – A.12) are solved iteratively to calculate the overall COD removal and the sludge produced by the system. The assumptions made here are (1) there is only one effluent stream leaving the tank, no sludge wastage is done and (2) all the soluble COD is degraded except for the inert soluble COD (S_I), and therefore the effluent stream contains only inert soluble COD and particulate COD (where X_{AB} is the anaerobic biomass X_E is the effluent particulate COD).
  The COD removal efficiency (η_{COD}) is taken as 68.5 % from a range (WEF, 2010) resulting in an effluent COD concentration of *120 g COD/m³*. Taking the anaerobic sludge production yield (Y_{an}) and decay coefficient (k_d) as *0.15 g COD sludge/g COD applied* and *0.03 1/d*, respectively; the solids produced are calculated to be X_{AB}*=1,751 g COD/m³,* X_P*=6,305 g COD/m³* and X_I*=10,533 g COD/m³*. The effluent COD consists of the influent inert soluble COD and COD from the solids. In order to keep the SRT in the desired range, X_E is calculated to be *90 g COD/m³* by changing the COD removal efficiency.

$$COD_{eff} = COD_t * (1 - \eta_{COD}) \quad \text{A.6}$$

$$X_{AB} = \frac{1}{V_{liq}} \frac{(Q*(COD_t - COD_{eff})*Y_{an}*SRT)}{(1+k_d*SRT)} \quad \text{A.7}$$

$$X_P = k_d * X_{AB} * SRT \quad \text{A.8}$$

$$X_I = Q * X_I^{in} * SRT \quad \text{A.9}$$

$$X_T = X_{AB} + X_P + X_I \quad \text{A.10}$$

$$X_E = COD_{eff} - S_I^{in} \quad \text{A.11}$$

$$SRT = \frac{X_T * V_{liq}}{Q * X_e} \quad \text{A.12}$$

- Methane production is calculated from COD reduction by using the *0.38 m³ methane / kg COD* as the conversion factor (Tchobanoglous, 2003). Then the methane volume is converted into mass by multiplying it with the density of methane which is *0.66 kg /m³*. Consequently, the amount of methane produced is calculated as *1,208 kg/d.*

- In the UASB system, there is no specific mechanism for nitrogen removal. However, the degradable and non-degradable COD in the effluent stream contain some nitrogen determined by the following composition parameters (Henze et al., 2000): $i_{N,Xs}$*=0.04,* $i_{N,Ss}$*=0.03,* $i_{N,BM}$*=0.07,* $i_{N,Xi}$*=0.02* and $i_{N,Xp}$*=0.06*. According to equations 6.13 and 6.14, the nitrogen originating from degradable COD is calculated to be *0.59 g N/m³* and nitrogen originating from non-degradable COD is calculated to be *2.85 g N/m³* and added to the total nitrogen of the influent stream.

$$N_{deg.COD} = i_{N,Xs}X_S + i_{N,Ss}S_S + i_{N,BM}X_{AB} \quad \text{A.13}$$

$$N_{nondeg.COD} = i_{N,Xi}X_I + i_{N,Xp}X_P \quad \text{A.14}$$

- There is no clarifier used in the UASB system, due to the fact that UASB system operates with granular sludge.

A.3.1.2 Generic process interval model generation

Table A.4 shows the formulation of the superstructure for the B-WWTP case study. As previously explained in section 4.2; the letters P, S and T represent the primary, secondary and tertiary outlet streams, respectively.

In Table A.5, all the parameters of the optimization problem are shown. The description of the parameters can be seen in the mathematical formulation of the optimization problem, which was previously described in section 3.3.2.

Table A.4 Superstructure formulation for the B-WWTP case study

	WW	PC	BP1	MLE	OxD	UASB	BP2	SHARON	SHAR-AN	BP3	UV	Ozone	Chlorine	BP4	Thickener	AnD	AeD	BP5	Discharge	Landfill
WW		P	P																	
PC				P	P	P	P									S	S	S		
BP1				P	P	P	P													
MLE								P	P	P					S					
OxD								P	P	P					S					
UASB								P	P	P										
BP2								P	P	P										
SHARON											P	P	P	P						
SHAR-AN											P	P	P	P						
BP3											P	P	P	P						
UV																			P	
Ozone																			P	
Chlorine																			P	
BP4																			P	
Thickener				S	S	S	S									P	P	P		
AnD				S	S	S	S													P
AeD				S	S	S	S													P
BP5																				P
Discharge																				
Landfill																				

Table A.5 Generic process interval model parameters

Treatment process	Mixing	$\alpha_{i,kk}$	$\mu_{i,ii,kk}$	Key reactant(s) (*react*)	Reaction stoichiometry ($\gamma_{i,kk,rr}$)	Reaction efficiency ($\theta_{react,kk,rr}$)	Sludge wastage (SP^3_{kk})	Waste separation ($W_{i,kk}$)	Sludge recycle (rec_{kk})	Flow separation ($Split_{i,kk}$)
PC	-	-	-	-	-	-	-	-	-	99.3% for solubles and water 50% for particulates
MLE	S_O to S_S ratio	1	4.09	S_S, S_{NH}, X_S	With respect to S_S S_S=-1, S_O=-4.07, X_I=0.77, X_{BH}=0.6, X_{BA}=0.19, X_P=0.87 With respect to S_{NH} S_{NH}=-1, S_{NO}=0.25, X_{ND}=0.03 With respect to X_S: X_S=-1	100% S_S removal 96% S_{NH} removal 97% X_S removal	3.5% of incoming flow	-	100% of incoming flow	48% for solubles and water 0.2 % for particulates
OxD	S_O to S_S ratio	1	4.29	S_S, S_{NH}, X_S	With respect to S_S:S_S=-1, S_O=-4.27, X_I=0.77, X_{BH}=0.15, X_{BA}=0.14, X_P=0.97 With respect to S_{NH}: S_{NH}=-1, S_{NO}=0.20, X_{ND}=-0.03 With respect to X_S: X_S=-1	100% S_S removal 98% S_{NH} removal 97% X_S removal	3.5% of incoming flow	-	100% of incoming flow	48% for solubles and water 0.2 % for particulates
UASB	-	-	-	S_S	S_S=-1, S_{NH}=0.05, X_I=-0.002, X_S=-2.91, X_{BH}=-0.41, X_P=0.36, X_{ND}=-0.15, CH_4=0.94	100% S_S removal	-	1 for CH_4	-	-
SHARON	-S_O to S_{NH} ratio -Methanol to S_{NH} ratio	1 1	3.14 2.85	S_{NH}	S_{NH}=-1, S_{NO}=0.99, S_O=-6.18	50% S_{NH} removal	-	-	-	-
SHARON-Anammox	S_O to S_{NH} ratio	1	1.78	S_{NH}	S_{NH}=1, S_{NO}=0.137, S_O=-2.16, N_2=1.08	80% S_{NH} removal	-	1 for N_2	-	-
UV	Electricity to water ratio	0	15.87	Pathogens	Pathogens=-1	100% pathogen removal	-	-	-	-
Ozone	Ozone to water ratio	0	12.5	Pathogens	Pathogens=-1	100% pathogen removal	-	-	-	-
Chlorine	-Electricity to water ratio -Chlorine to water ratio	- 0 - 1	-2.12 -17.5	Pathogens	Pathogens=-1	100% pathogen removal	-	-	-	-
AnD	-	-	-	X_{BH}, X_{BA}, X_S	With respect to X_{BH}: X_{BH}=-1, S_{NH}=0.07, X_P=0.02, CH_4=0.81 With respect to X_{BA}: X_{BA}=-1, With respect to X_S: X_S=-1,	100% X_{BH} and X_{BA} removal 80% X_S removal	-	1 for CH_4	-	50% for solubles and 0.7% for particulates
AeD	S_O to X_{BH} ratio	1	0.99	X_{BH}, X_{BA}	With respect to X_{BH}: X_{BH}=-1, S_O=-1.35, S_{NO}=0.07, X_P=0.27 With respect to X_{BA}: X_{BA}=-1,	100% X_{BH} and X_{BA} removal	-	-	-	50% for solubles and 0.7% for particulates

A.3.2 Retrofitting case study

A.3.2.1 Generic process interval model generation

Table A.6 shows the formulation of the superstructure for the retrofitting case study. As previously explained in section 4.2; the letters P, S and T represent the primary, secondary and tertiary outlet streams, respectively.

The model parameters are presented below in this section for different phenomena employed in the generic process interval model through Tables A.7 – A.12.

Table A.6 Superstructure formulation for the retrofitting case study

	WW	PC	A-st	UASB	BP1	AS	BNR10	BNR14	BNR28	B-st	MBR	Granular-AS	Anammox	BP2	Thick	AD	Dewat
WW		P	P	P	P												
PC						P	P	P	P	P	P	P	P	P		S	
A-stage										P			P	P	S		
UASB													P	P			
By-pass1						P	P	P	P	P	P	P	P	P			
AS															S		
BNR10															S		
BNR14															S		
BNR28															S		
B-stage															S		
MBR															T		
Gran-AS															T		
Anammox															S		
By-pass2																	
Thick																S	
AD																	P
Dewat																	
Sh/An2st		P	P	P	P												
Sh/AnSBR		P	P	P	P												
Canon		P	P	P	P												
Anitamox		P	P	P	P												
Deammon		P	P	P	P												
Demon		P	P	P	P												
Canr		P	P	P	P												
By-pass3		P	P	P	P												
Water																	
Sludge																	

Table A.6 Superstructure formulation for the retrofitting case study (continued)

	Sh/An 2st	Sh/An SBR	Canon	Anitamox	Deammon	Demon	Canr	BP3	Water	Sludge
WW										
PC										
A-stage										
UASB										
By-pass1										
AS									P	
BNR10									P	
BNR14									P	
BNR28									P	
B-stage									P	
MBR									P	
Gran-AS									P	
Anammox									P	
By-pass2									P	
Thick	P	P	P	P	P	P	P	P		
AD										
Dewat	P	P	P	P	P	P	P	P		S
Shar/An 2st										
Shar/An SBR										
Canon										
Anitamox										
Deammon										
Demon										
Canr										
By-pass3										
Water										
Sludge										

Utility addition and mixing

The parameters $\mu_{i,ii,kk}$ and $\alpha_{i,kk}$ are shown in Table A.7 and A.8 respectively.

Table A.7 Values for parameter $\mu_{i,ii,kk}$ for the retrofitting case study

$\mu_{i,ii,kk}$		Interval								
Utility	**Component**	**A-st**	**AS**	**BNR10**	**BNR14**	**BNR28**	**B-st**	**MBR**	**Granular AS**	**Anammox**
S_O	**S_S**	0.88	1.65	1.49	1.62	1.81	1.26	3.07	3.11	
S_O	**S_{NH}**		5.7	7.74	8.02	8.39	6.31	6.45	6.45	3.34
S_O	**X_S**									0.27
$FeCl_3$	**P**		5.28	5.28	5.28	2.11	5.28	5.28	5.28	5.28

$\mu_{i,ii,kk}$		Interval								
Utility	**Component**	**Shar**	**Shar/An-2st**	**Shar/An-SBR**	**Canon**	**Anitamox**	**Deammon**	**Demon**	**Canr**	**Panammox**
S_O	**S_{NH}**	5.14	2.57	2.57	2.57	2.57	2.57	2.57	2.57	2.57
Methanol	**S_{NH}**	1.14								

Table A.8 Values for parameter $\alpha_{i,kk}$ for the retrofitting case study

$\alpha_{i,kk}$	Interval								
Utility	**A-st**	**AS**	**BNR10**	**BNR14**	**BNR28**	**B-st**	**MBR**	**Granular AS**	**Anammox**
S_O	1	1	1	1	1	1	1	1	1
$FeCl_3$		1	1	1	1	1	1	1	1

$\alpha_{i,kk}$	Interval								
Utility	**Shar**	**Shar/An-2st**	**Shar/An-SBR**	**Canon**	**Anitamox**	**Deammon**	**Demon**	**Canr**	**Panammox**
S_O	1	1	1	1	1	1	1	1	1
Methanol	1								

Table A.9 Gamma values for different intervals where R represents different reactions and gamma1 and gamma2 represent the stoichiometry for two consecutive reactions

		Gamma1				Gamma2
Component	**Interval**	**R1**	**R2**	**R3**	**R4**	**R5**
S_S	AS	-1				
S_O	AS	-2.2				
S_{NO}	AS		1.8			-1
S_{NH}	AS		-1			
X_I	AS	0.54				
X_S	AS			-1		
X_{BH}	AS	0.24				
X_{BA}	AS	0.06				
X_P	AS	0.23				
X_{ND}	AS		0.04			
P	AS				-1	
$FeCl_3$	AS				-5.28	
$FePO_4$	AS				4.88	

		Gamma1		
Component	**Interval**	**R1**	**R2**	**R3**
S_{NH}	AD	0.07		
X_S	AD			-1
X_{BH}	AD	-1		
X_{BA}	AD		-1	
X_P	AD	0.02		
CH_4	AD	0.08		1.07

		Gamma1	
Component	**Interval**	**R1**	**R2**
S_S	A-Stage	-1	
S_O	A-Stage	-1.33	
X_I	A-Stage	1.06	
X_S	A-Stage		-1
X_{BH}	A-Stage	3.37	
X_P	A-Stage	0.04	
X_{ND}	A-Stage	0.16	

		Gamma1		
Component	**Interval**	**R1**	**R2**	**R3**
S_S	UASB		-1	
S_{NH}	UASB	0.04		
X_I	UASB			-1
X_S	UASB	-1		
CH_4	UASB	0.56		

		Gamma1				Gamma2
Component	**Interval**	**R1**	**R2**	**R3**	**R4**	**R5**
S_S	BNR10	-1				
S_O	BNR10	-2.58				
S_{NO}	BNR10		2.17			-1
S_{NH}	BNR10		-1			
X_I	BNR10	0.88				
X_S	BNR10				-1	
X_{BH}	BNR10	1.1				
X_{BA}	BNR10	0.11				
X_P	BNR10	0.67				
X_{ND}	BNR10		0.23			
P	BNR10			-1		
$FeCl_3$	BNR10			-5.28		
$FePO_4$	BNR10			4.88		

		Gamma1				Gamma2
Component	**Interval**	**R1**	**R2**	**R3**	**R4**	**R5**
S_S	BNR14	-1				
S_O	BNR14	-2.71				
S_{NO}	BNR14		2.24			-1
S_{NH}	BNR14		-1			
X_I	BNR14	0.9				
X_S	BNR14				-1	
X_{BH}	BNR14	0.85				
X_{BA}	BNR14	0.1				
X_P	BNR14	0.74				
X_{ND}	BNR14		0.18			
P	BNR14			-1		
$FeCl_3$	BNR14			-5.28		
$FePO_4$	BNR14			4.88		

		Gamma1				Gamma2
Component	**Interval**	**R1**	**R2**	**R3**	**R4**	**R5**
S_S	BNR28	-1				
S_O	BNR28	-2.91				
S_{NO}	BNR28		2.35			-1
S_{NH}	BNR28		-1			
X_I	BNR28	0.93				
X_S	BNR28				-1	
X_{BH}	BNR28	0.48				
X_{BA}	BNR28	0.08				
X_P	BNR28	0.83				
X_{ND}	BNR28		0.11			
P	BNR28			-1		
$FeCl_3$	BNR28			-2.11		
$FePO_4$	BNR28			1.95		

		Gamma1				Gamma2
Component	**Interval**	**R1**	**R2**	**R3**	**R4**	**R5**
S_S	B-stage	-1				
S_O	B-stage	-4.13				
S_{NO}	B-stage		1.64			-1
S_{NH}	B-stage		-1			
X_I	B-stage	0.07				
X_S	B-stage				-1	
X_{BH}	B-stage	0.89				
X_{BA}	B-stage	0.22				
X_P	B-stage	0.79				
X_{ND}	B-stage		0.17			
P	B-stage			-1		
$FeCl_3$	B-stage			-5.28		
$FePO_4$	B-stage			4.88		

		Gamma1		Gamma2	
Component	**Interval**	**R1**	**R2**	**R4**	**R5**
S_S	Anammox				-0.49
S_O	Anammox	-4.29			-0.02
S_{NO}	Anammox	0.98		-2.28	
S_{NH}	Anammox	-1		-1	
X_I	Anammox				
X_S	Anammox				-1
X_{BH}	Anammox				
X_{BA}	Anammox				
X_P	Anammox				
N_2	Anammox			2	
P	Anammox		-1		
$FeCl_3$	Anammox		-5.28		
$FePO_4$	Anammox		4.88		

		Gamma1				Gamma2
Component	**Interval**	**R1**	**R2**	**R3**	**R4**	**R5**
S_S	GranularAS	-1				
S_O	GranularAS	-3.41				
S_{NO}	GranularAS		1.76			-1
S_{NH}	GranularAS		-1			
X_I	GranularAS	0.01				
X_S	GranularAS				-1	
X_{BH}	GranularAS	0.21				
X_{BA}	GranularAS	0.03				
X_P	GranularAS	0.18				
X_{ND}	GranularAS		-0.16			
P	GranularAS			-1		
$FeCl_3$	GranularAS			-5.28		
$FePO_4$	GranularAS			4.88		

		Gamma1				Gamma2
Component	**Interval**	**R1**	**R2**	**R3**	**R4**	**R5**
S_S	MBR	-1				
S_O	MBR	-3.41				
S_{NO}	MBR		1.74			-1
S_{NH}	MBR		-1			
X_I	MBR	0.02				
X_S	MBR				-1	
X_{BH}	MBR	0.25				
X_{BA}	MBR	0.03				
X_P	MBR	0.17				
X_{ND}	MBR		-0.15			
P	MBR			-1		
$FeCl_3$	MBR			-5.28		
$FePO_4$	MBR			4.88		

		Gamma1	Gamma2
Component	**Mechanism**	**R1**	**R2**
S_O	Nitritation/Denitritation	-3.42	
S_{NO}	Nitritation/Denitritation	1	-1
S_{NH}	Nitritation/Denitritation	-1	
Methanol	Nitritation/Denitritation		-1.14
N_2	Nitritation/Denitritation		1
X_{den}	Nitritation/Denitritation		0.55
X_{AOB}	Nitritation/Denitritation	0.15	

		Gamma1	Gamma2
Component	**Mechanism**	**R1**	**R2**
S_O	PN/Anammox	-3.4	
S_{NO}	PN/Anammox	1	-0.986
S_{NH}	PN/Anammox	-1	-1
N_2	PN/Anammox		1.974
X_{AnAOB}	PN/Anammox	0.15	0.157

Table A.10 Reaction efficiencies - $\theta_{react,kk,rr}$ given for different intervals and reactions together with the associated reactant

	Reaction									
	R1		R2		R3		R4		R5	
Interval	**Reactant**	$\theta_{react,kk,rr}$	**Reactant**	$\theta_{react,kk,rr}$	**Reactant**	$\theta_{react,kk,rr}$	**Reactant**	$\theta_{react,kk,rr}$	**Reactant**	$\theta_{react,kk,rr}$
AS	S_S	1	S_{NH}	0.94	X_S	1	P	0.9	S_{NO}	0.85
AD	X_{BH}	1	X_{BA}	1	X_S	0.8				
A-stage	S_S	0.43	X_S	0.43						
UASB	X_S	0.58	S_S	0.58	X_I	1				
BNR10	S_S	1	S_{NH}	0.96	P	0.9	X_S	0.95	S_{NO}	0.84
BNR14	S_S	1	S_{NH}	0.97	P	0.9	X_S	0.96	S_{NO}	0.86
BNR28	S_S	1	S_{NH}	0.98	P	0.9	X_S	0.96	S_{NO}	0.88
B-stage	S_S	1	S_{NH}	0.95	P	0.9	X_S	0.95	S_{NO}	0.7
Anammox	S_{NH}	0.65	P	0.9	S_{NH}	0.65	X_S	0.58		
Granular AS	S_S	1	S_{NH}	0.94	P	0.9	X_S	1	S_{NO}	0.85
MBR	S_S	1	S_{NH}	0.94	P	0.9	X_S	1	S_{NO}	0.85

Table A.10 Reaction efficiencies - $\theta_{react,kk,rr}$ given for different intervals and reactions together with the associated reactant (continued)

		Reaction			
		R1		R2	
Mechanism	**Interval**	**Reactant**	$\boldsymbol{\theta_{react,kk,rr}}$	**Reactant**	$\boldsymbol{\theta_{react,kk,rr}}$
Nitritation/Denitritation	**Shar**	S_{NH}	0.86	S_{NO}	0.60
PN/Anammox	**Shar/An-2st**	S_{NH}	0.5	S_{NH}	0.80
PN/Anammox	**Shar/An-SBR**	S_{NH}	0.5	S_{NH}	0.91
PN/Anammox	**Canon**	S_{NH}	0.5	S_{NH}	0.90
PN/Anammox	**Anitamox**	S_{NH}	0.5	S_{NH}	0.70
PN/Anammox	**Deammon**	S_{NH}	0.5	S_{NH}	0.71
PN/Anammox	**Demon**	S_{NH}	0.5	S_{NH}	0.80
PN/Anammox	**Canr**	S_{NH}	0.5	S_{NH}	0.89
PN/Anammox	**Panammox**	S_{NH}	0.5	S_{NH}	0.89

Flow, waste and phase separation

Table A.11 Definition of phase separation parameter $split_{i,kk}$

$split_{i,kk}$	PC	A-stage	AS	BNR10	BNR14	BNR28	B-stage	MBR	Granular AS	Anammox	Thick	Dewat
Soluble	0.99	0.42	0.49	0.48	0.48	0.49	0.49	0.50	0.50	0.49	0.9	0.95
Particulates	0.52	0.002	0.002	0.003	0.002	0.003	0.002	0.002	0.002	0.002	0.05	0.01

Table A.12 Definition of waste separation parameter $W_{i,kk}$

$W_{i,kk}$	UASB	Anammox	AD	Shar	Shar/An-2st	Shar/An-SBR	Canon	Anitamox	Deammon	Demon	Canr	Panammox
CH_4	1		1									
N_2		1		1	1	1	1	1	1	1	1	1

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