UNIVERSITEIT GENT

Faculty of Bioscience Engineering

Academic year 2016-2017

Opportunities and limitations of connecting Life Cycle Assessment to a dynamic wastewater treatment plant model

Tom Lauriks
Promoters: prof. dr. ir. Ingmar Nopens and prof. dr. ir. Steven De Meester
Tutor: ir. Chaïm De Mulder

Masterproef voorgedragen tot het behalen van de graad van
Master in de bio-ingenieurswetenschappen: Milieutechnologie

Ghent, June 2012

The promoters,	The tutor,	The author,
Prof. dr. ir. Ingmar Nopens Prof. dr. ir. Steven De Meester	ir. Chaïm De Mulder	Tom Lauriks

Acknowledgements

I am very grateful for the support I got while writing my master thesis. The support already started before I selected this topic. My promoters, professor Nopens and professor De Meester, patiently listened to my personal interests during several meetings. Finally, the topic of coupling life cycle assessment to dynamic wastewater treatment plant modelling was created. Since I am very enthusiastic about modelling and protecting the environment, the topic for this master thesis could not have been more suited for me.

The excellent support continued when I started working on this thesis. My tutor, Chaïm De Mulder, has put a lot of effort into correcting my writings and answering my questions. He also played a role in the creative thinking. For instance, he came up with the idea of calculating LCA results in very small time intervals. In addition, his advice was always straight to the point and very valuable. This resulted in the fact that I went through an immense learning process. Finally, Chaïm was very open minded about my own input and perspectives. In could not have imagined better tutoring. Moreover, both professor Nopens and professor De Meester were always there to steer everything in the right direction.

I am also very grateful to Waterschap the Dommel, the Eindhoven wastewater treatment plant governing body. First of all, they fund the research needed to develop the wastewater treatment plant model. This, hence, contributes to the science of wastewater treatment. Furthermore, Tony Flameling was kind enough to answer the questions I had regarding the Eindhoven wastewater treatment plant.

Abstract

Our freshwater resources need to be safeguarded. The most widely used technologies to treat wastewater are wastewater treatment plants (WWTPs) based on biological activated sludge processes. However, they cause considerable environmental impacts themselves. Life cycle assessment (LCA) is a tool to analyse those impacts and can thus assist in the search for optimal or alternative solutions. A WWTP model is furthermore a tool that can speed up scenario analysis and/or alleviate the problem that modifying full-scale installations merely for experimenting is technically difficult and expensive. If these models are coupled to LCA, a thorough environmental analysis of the investigated scenarios can assist in the decision making phase, where it is decided which technologies will assist in building a sustainable future. This seems very interesting indeed and the coupling of modelling and LCA was already performed in a number of articles.

There are, in addition, indications that dynamic WWTP modelling results give a more accurate description of reality than steady state modelling results. Dynamic models were also already coupled to LCA, but - to the best of the author's knowledge - the dynamic aspect of the modelling results was not yet incorporated into the LCA results.

It was therefore the main goal of this thesis to incorporate the dynamic aspect of WWTP modelling results into the LCA results and to analyse if this is actually useful. Another goal was the following: investigate whether or not dynamic LCA can lead to selecting additional scenario(s), that have the potential to improve the environmental performance of the WWTP under study.

The model used in this thesis is a model of the Eindhoven WWTP. It was calibrated and validated with data from 2013. This model was coupled to LCA through Python™ scripts, written in a Jupyter notebook. They are available online for downloading: `https://github.com/TomLauriks/dynamic_WWTP_model_plus_LCA`. The notebook provides both classic LCA and dynamic LCA as output. In addition, different functional units (FUs) can be chosen, for instance 1 m^3 influent, 1 kg chemical oxygen demand (COD) in the influent, 1 kg total nitrogen (TN) in the influent, and a day of WWTP operation. The ReCiPe life cycle impact assessment method was used. The notebook calculates results

for all 18 ReCiPe midpoint and 3 ReCiPe endpoint impact categories.

A first important result of this work is the development of improved visualisation tools for dynamic LCA results. This includes histograms and heatmaps, both helping in pinpointing time instants where environmental performance can be improved substantially, thus providing additional information for decision making.
It was also found that the resulting time series of dynamic LCA cannot be used directly to determine differences between scenarios. However, a classic result and an average dynamic result for one and the same impact category and scenario can deviate substantially. For example, for the FU kg COD in the influent, a difference of 40 % occurred in the impact category fossil depletion. It was therefore concluded that, for scenario comparison, taking the classic LCA approach is advised, while dynamic LCA can increase the amount of information available.
Also with regards to identification of impact peaks, it was shown that dynamic LCA is a very valuable addition to classic LCA. After a better look at the dynamic LCA results, which resulted in identifying the most important impacts to lower, it was decided to further investigate the effects of lowering the total impact in freshwater eutrophication, i.e. lowering phosphorus (P) emissions. A way of decreasing P emissions, for instance, is increasing overall chemical P removal, i.e. aluminium (Al) dosing in the case of the Eindhoven WWTP.
This was tested by simulating different scenarios. The current situation - the reference scenario - was firstly compared to an increased overall Al dosing, and secondly to applying a proposed feed-forward controller. For the former, this resulted in 16.3 % improvement of FE and for the latter 7.5 %. In conclusion, the combination of classic and dynamic LCA assisted in identifying scenarios that could lead to efficient improvements of the current situation.
Finally, an increased total suspended solids (TSS) concentration in the activated sludge tanks (ASTs) was included into the scenario analysis, which resulted in an increased sludge production. This led to an overall environmental performance that was considerably worse than the other scenarios. Results, however, indicate that the cause of this might be the start-up behaviour of the modelled WWTP controllers and that longer simulations are needed to affirm whether or not these results seem logical.

Contents

List of Symbols

$wt\%$ weight percent.

$\bar{x}$ arithmetic mean of the concerning variable.

List of Abbreviations

[g L^{-1}] example of units: [gram $(liter)^{-1}$].

[n M L T] physical properties: [mole mass length time].

AcOH acetic acid.

AD anaerobic digestion.

ALO agricultural land occupation.

ASM1 Activated Sludge Model No. 1.

ASM2 Activated Sludge Model No. 2.

ASM2d Activated Sludge Model No. 2d.

ASM3 Activated Sludge Model No. 3.

AST activated sludge tank.

CC climate change.

CCES climate change ecosystems.

CCHH climate change human health.

COD chemical oxygen demand.

CSO combined sewer overflow.

CSTR continuous stirred-tank reactor.

DALY disability adjusted life years.

DB dichlorobenzene.

DM dynamic modelling.

DO dissolved oxygen.

eq equivalent.

ES ecosystems.

FD fossil depletion.

FE freshwater eutrophication.

FET freshwater ecotoxicity.

FU functional unit.

GHG greenhouse gas.

GWP global warming potential.

HH human health.

HT human toxicity.

IR ionising radiation.

IWA International Water Association.

LCA life cycle assessment.

LCI life cycle inventory.

LCIA life cycle impact assessment.

m^2a m^2·annum.

MD metal depletion.

ME marine eutrophication.

MET marine ecotoxicity.

N nitrogen.

NLT natural land transformation.

NMVOC non methane volatile organic compounds.

OD ozone depletion.

ODE ordinary differential equation.

P phosphorus.

PE person equivalent.

PMF particulate matter formation.

POF photochemical oxidant formation.

PST primary sedimentation tank.

RAS return activated sludge.

RBT rain buffer tank.

RSC resource surplus cost.

SIF sludge incineration facility.

SST secondary secondary sedimentation tank.

STF sludge treatment facility.

TA terrestrial acidification.

TE terrestrial ecotoxicity.

tkm ton.km.

TKN total Kjehldahl nitrogen.

TN total nitrogen.

TP total phosphorus.

TSS total suspended solids.

ULO urban land occupation.

WD water depletion.

WDD Waterboard De Dommel.

WRRF water and resource recovery facility.

WWTP wastewater treatment plant.

List of Figures

List of Tables

CHAPTER 1

Literature study

1.1 Issues regarding wastewater and possible solutions

1.1.1 Freshwater: a resource under pressure

The planet's freshwater resources, if managed sustainably and effectively, can meet the water demand of the world's growing population. However, the widespread water quality degradation across the world is a serious problem, not only threatening human health and the integrity of ecosystems, but also representing a major concern for sustainable management of water resources and sustainable development of countries. In addition, new water quality challenges such as emerging pollutants and safe wastewater reuse also bring great concerns. This all calls for urgent attention. (UNESCO, 2016) Thus, both water quality degradation and safe wastewater reuse are clearly important issues. This stresses the importance of dealing with issues regarding wastewater.

1.1.2 Wastewater treatment plant: a solution with consequences

Aerobic biological treatment is the most widely used approach to manage domestic wastewaters (Semblante et al., 2014). This treatment is based on the fact that a simple aeration permits micro-organisms to grow on biodegradable carbon compounds present in wastewater. The micro-organisms incorporate part of the biodegradable carbon compounds into newly formed biomass and oxidize another part to CO_2 to obtain energy. The suspended particles in the wastewater and the carbon consuming micro-organisms form a sludge, which is know as “activated sludge”. Systems based on this technology, are hence also known as activated sludge systems. In order to purify the water, the sludge has to be separated from it. This can be done by gravitational settlers. (Verstraete and Vlaeminck, 2011; Tchobanoglous et al., 2003)

This simple treatment already dates back to 1914 and leads to the removal of organic compounds from wastewater, which would otherwise lead to excessive dissolved oxygen (DO) depletion in the receiving waters (Tchobanoglous et al., 2003). Fleming Training Center (2016) for instance advises that most activated sludge systems should be designed to remove 85-95% of biodegradable organic matter and the of Eindhoven (which will be the object under study in this thesis) is reported to have removed 97.7% of biodegradable organic matter and 91.8% of all oxidizable - but not necessarily biologically oxidizable - matter in 2013 (Blom, 2013). In addition, colloidal and suspended solids - whether or not organic - are removed. They would otherwise create nuisance and settle - and thus accumulate - in the receiving waters. (Tchobanoglous et al., 2003) The latter would lead to the need for periodic dredging (Nopens, 2017).
Thus, activated sludge systems remove pollution from wastewater. However, since aeration is needed, energy is consumed during this process, which obviously also creates environmental impacts. Furthermore, the generated sludge - i.e. the newly formed biomass - also has to be treated or disposed of, which also bears considerable amounts of environmental impacts (see Section 1.4)

The original activated sludge systems, in addition, evolved during the last decades to become increasingly complex, incorporating biological removal of nitrogen (N) and phosphorus (P) containing compounds (also called nutrients) through nitrification/denitrification and enhanced biological P removal. (Verstraete and Vlaeminck, 2011)
During the nitrification, NH_4^+ is oxidized to NO_2^- and further to NO_3^-. Nitrification is also performed via biological processes and even in the same tank as the biodegradable organic matter removal. Thus, aeration also takes place during this process. NH_4^+ needs to be removed because of, among others, its toxicity to fish and to control eutrophication. In biological denitrification NO_3^- is reduced to NO, N_2O and N_2. This is, for instance, also performed to protect the receiving waters from eutrophication. Denitrification usually happens in an anoxic tank. However, other ways of biological N removal exist. (Tchobanoglous et al., 2003)
The fact that N_2O can be formed is important to note. Law et al. (2012) reviewed a number of articles concerning wastewater treatment technologies. (In addition to the technology that will be studied in this thesis, some other technologies were included in their review as well.) The N_2O emission factor, which is the amount of N_2O-N emitted relative to the N load imposed on the wastewater treatment plant (WWTP), for full-scale plants - reported by the articles reviewed by them - varied substantially, ranging from 0 to 25%. This is of particular importance. Modelling results of de Haas and Hartley (2004) indicate that, at emission factors of 1 to 5%, the N_2O emissions in a typical WWTP with biological nutrient removal could account for half or more of the total greenhouse gas (GHG) emissions. (Law et al., 2012) conclude that the large variation in N_2O emissions among the investigated plants was probably due to the different configurations and operational conditions applied. This could

imply that N_2O emissions from a WWTP can be reduced through proper plant design and operation. It might in addition also be interesting to note that, according to results of Ahn et al. (2010), N_2O emissions in aerated zones - where nitrification takes place - were higher than those in non-aerated zones - where denitrification takes place.

P removal is also done to control eutrophication and in particular because P is a limiting nutrient in most freshwater ecosystems. It can be achieved via chemical treatment using aluminium or iron salts, but successes in full-scale biological P removal since the 1980s have encouraged further use of this technology. During the latter treatment P is incorporated into cell biomass which is subsequently removed from the process as a result of sludge wasting. (Tchobanoglous et al., 2003)

These extensions to the original activated sludge systems created a need for new infrastructure and added to the energetic and sometimes chemical requirements of the treatment process. Hence, nowadays activated sludge systems have a high electricity demand and environmental footprint (Verstraete and Vlaeminck, 2011). See Figure 1.1 for a basic example of an activated sludge system with biological N removal.

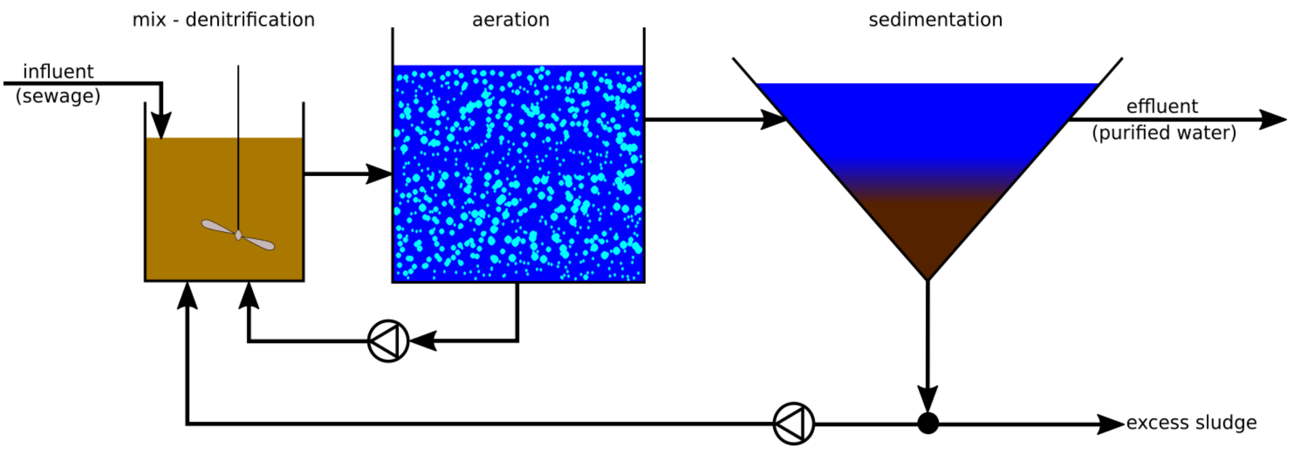


Figure 1.1: Scheme of a basic activated sludge system with biological N removal. Redrawn and modified from VITO (2010b)

Since it is argued that the energy consuming aeration needed for the aerobic treatment of wastewater is one of the causes of environmental impacts generated by activated sludge systems, it is important to note that anaerobic biological wastewater treatment also exists. Major advantages of this technology are the following: Energy recuperation is possible since the organic pollutants are partly converted into highly energetic biogas. It has, furthermore, a low amount of sludge production. Note that sludge production was already mentioned to bear considerable amounts of environmental impacts. Major disadvantages of this technology, on the other hand, are the following: Organic compounds and nutrients are not thoroughly removed and hence persist in the effluent. This leads to the need for additional treatment, for instance aerobic treatment, of the effluent. In addition, the optimal operating temperature of this process is between 30-37 °C. The influent must hence be heated in most cases. (VITO, 2010a) Since both advantages and disadvantages exist, this already indicates that a thorough environmental analysis is needed if one aims to select the most environmentally friendly solutions.

1.1.3 Moving towards optimal wastewater treatment plants

In the last decade, a different view on wastewater and its treatment has emerged: instead of considering the water contaminated with organics and nutrients, it is recently regarded more as a potential source of energy and recovered resources, such as nutrients. Water reuse is in addition also considered. A "wastewater treatment plant" could thus become a "water and resource recovery facility (WRRF)". (De Mulder, 2014; Blom, 2013; Corominas et al., 2013a; Holmgren et al., 2015; McCarty et al., 2011) Resource recovery could alleviate the environmental impacts of wastewater treatment, if the impacts of the processes needed for the recovery are less than the avoided impacts of the processes otherwise used to obtain these resources. This, again, stresses the need for a thorough environmental analysis.

In conclusion, WWTPs based on activated sludge systems remediate wastewater and thereby reduce environmental impacts, which helps safeguarding freshwater resources. In their turn, they however induce other environmental impacts. To truly achieve sustainable management of our freshwater resources, minimizing these induced impacts is imperative. This could for instance be obtained by optimizing existing technologies, modifying or extending existing technologies (e.g. with resource recovery) or using alternative technologies for wastewater treatment.

1.2 Modelling of wastewater treatment plants

1.2.1 Why use models and what is modelling?

Previous paragraphs showed that optimizing existing systems might reduce the occurring problems. It is however technically difficult to evaluate multiple optimization strategies at full-scale (Corominas et al., 2013b). An alternative to full-scale experimenting is the use of models. These are cost-effective tools for the evaluation of for instance control strategies (Gernaey et al., 2014). Other typical goals when modelling WWTPs are analysis of consequences of upgrading or retrofitting (Nopens, 2015), getting insight into plant performance, evaluating new plant design, and supporting management decisions (Henze et al., 2008a). Thus, by modelling a WWTP, optimization strategies and modifications can be analysed without the need for cumbersome full-scale experiments. Modelling is in addition a tool that speeds up scenario analysis (see further).

According to Nopens (2015), two important goals can be distinguished when mathematically modelling biosystems: (1) system analysis and (2) system optimization.

Modelling for system analysis

This first case typically concerns new or poorly understood systems which are often classically researched in a real lab environment. Such experimental analysis provides knowledge about the system. However, specifically for biosystems, this is often very time consuming because biosystems are quite slow systems. This limits the number of experimental runs. (Nopens, 2015)
Modelling can provide a solution here. The system under study can be translated into a mathematical model, a set of equations that (should) describe(s) the system. This set of equations can subsequently be solved, typically numerically, which is known as simulation or virtual experimentation, the counterpart of the real lab experiment. The advantage of simulation is its speed, i.e. the simulation time is shorter than the real time. In other words, the simulation of a model for e.g. 1 day is faster than 1 day, often in the order of minutes. (Nopens, 2015)
It should however be noted that moving from reality to virtual reality does not imply that experimental data collection is no longer required. In the application of models for system analysis, one typically defines a set of candidate models, which can be regarded as hypotheses of how a certain system behaves. When a hypothesis is withheld, by comparing with experimental data, one has gathered knowledge through virtual experimental analysis. (Figure 1.2 A).) (Nopens, 2015)

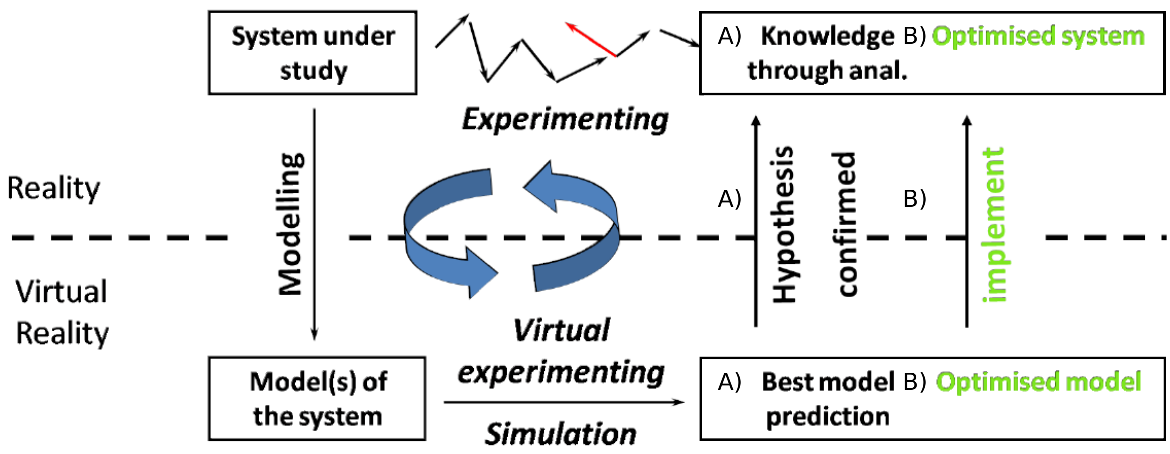


Figure 1.2: Modelling for system analysis (A) or for system optimization (B). Modified from Nopens (2015)

Modelling for system optimization

In this second type of modelling, one assumes to already have a good model of the system under study. Here, the emphasis lies on using the model to improve or optimize the system. Also in this case, the main advantage lies in the computational power, i.e. the large number of scenarios that can be computed in a short time frame. A similar analysis could take years when performed in a real experimental environment. The use of models thus greatly enhances the search for optimal designs and operational strategies for a specific system. (Figure 1.2 B).) (Nopens, 2015)
However, an important property of any model that should not be forgotten about is the fact that it will always be an approximation of reality, no matter what complexity it has. The obtained optimal solution should thus subsequently be implemented and tested in the real world for its validation. (Nopens, 2015)

1.2.2 How to model wastewater treatment plants?

Typical wastewater treatment plant configuration

Before summarizing which processes are typically described mathematically when modelling a WWTP, it might be useful to get an idea about which of them are of importance. Therefore, a typical configuration of an activated sludge process used for biological carbon and nutrient removal is given in Figure 1.3. This kind of process is probably still the most used in the world and will be the object under study in this thesis.
The treatment can be broken down into a couple of steps, according to Nopens (2015):

- Primary treatment: This step aims at removing pollutants that would hamper the secondary biological removal step. In the influent works, the raw influent from the sewer enters the plant. To remove large debris, these works include screens. Other steps that are often present are sand and grease removal. Often, also a primary settler is included. Its function is to remove suspended solids.

- Secondary treatment: this step contains bioreactors filled with activated sludge, a consortium of micro-organisms that remove carbonaceous, nitrogenous and phosphorus organic and dissolved pollution sources from the wastewater. The final step here is the water-sludge separation, often performed in settlers. Sludge collected from primary treatment and secondary treatment is recently increasingly sent to on-site anaerobic digestion (AD) units for sludge reduction purposes and energy recovery under the form of biogas.

- Tertiary Treatment: If effluent constraints are not met or if the effluent is to be upgraded for reuse, an additional step might still be required.

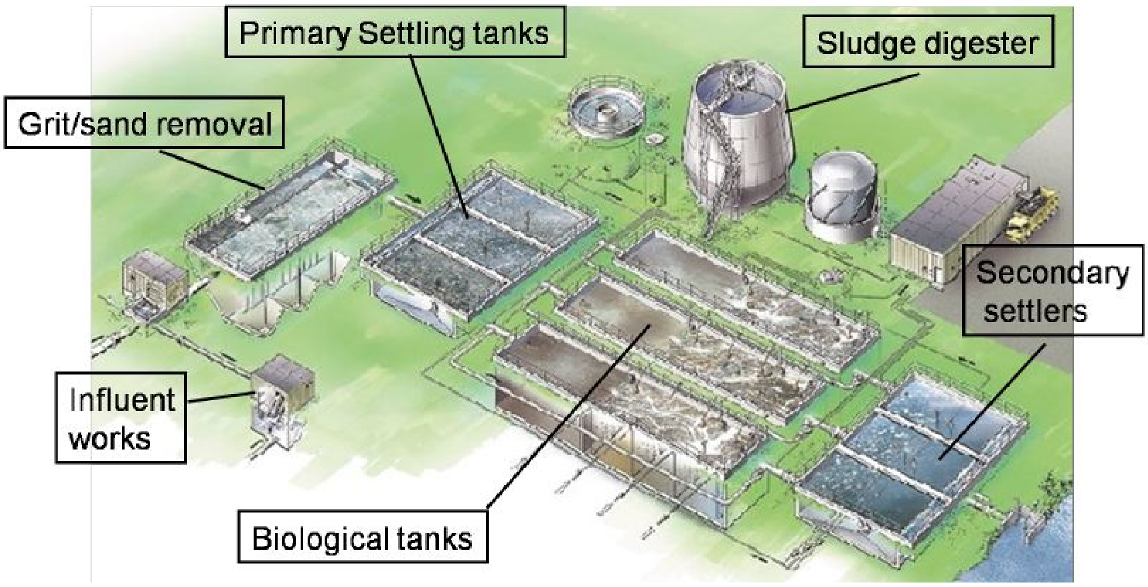


Figure 1.3: Schematic of a typical WWTP configuration including primary and secondary treatment (Nopens, 2015)

In-depth information about wastewater treatment can be found in Tchobanoglous et al. (2003).

Processes to be modelled

When considering the WWTP configuration in Figure 1.3 and the different steps in the treatment, it is not hard to imagine what processes should be modelled. Firstly, wastewater is flowing through a series of reactors and settlers. Therefore, the hydraulic behaviour of the different reactors and settlers and the mixing behaviour of the reactors have to be modelled. The biological processes in the biological reactors and the separating process in the settlers also need to be modelled. Additionally, as can be seen in Figure 1.1, part of the biological reactors is aerated. This aeration process also needs to be modelled. (Nopens, 2015) Finally, the AD can also be modelled (Batstone et al., 2002a,b).
Regarding the models describing the biological processes, it might be interesting to note that several of these have been developed for over the past 30 years. The International Water Association (IWA) has, through dedicated Task Groups, established a Scientific and Technical Report that summarizes models over which a scientific consensus existed at some point in time. The described models are the so-called family of Activated Sludge Models. (Nopens, 2015) Four such models have been presented: Activated Sludge Model No. 1 (ASM1), Activated Sludge Model No. 2 (ASM2), Activated Sludge Model No. 2d (ASM2d) and Activated Sludge Model No. 3 (ASM3) Henze et al. (2000, 2008b). These

models still form the basis for the majority of WWTP modelling studies carried out today.

Short description of some models for important processes

As described above, different processes need to be modelled to construct a proper WWTP model. Hence, an entire model of a WWTP is composed of the different process models, which are thus submodels of the entire plant model (Rieger et al., 2013). Software exists wherein these models are already implemented, e.g. WEST (product of MIKE Powered by DHI, `http://www.mikepoweredbydhi.com`). The following gives a short description of some important process models. The described process models are either used in the WWTP model in this thesis, or form the basis of the process models used in this thesis.

In the case of continuous flow through systems, 2 possible ways of dealing with hydraulics are constant volume reactors or variable volume reactors (Nopens, 2015; Rieger et al., 2013). In the model used in this thesis, the biological reactors are modelled as constant volume reactors (Amerlinck, 2015). This has the following mathematical meaning:

$$\frac{dV}{dt} = 0 = Q_{in} - Q_{out} \Rightarrow Q_{in} = Q_{out} \tag{1.1}$$

where V is the total volume of all the substances in the reactor, and Q_{in} and Q_{out} are the total flow rates of all the substances entering and leaving, respectively, the reactor (Nopens, 2015).

Modelling of the mixing behaviour is needed to simulate the dispersion of dissolved and/or particulate compounds in the liquid phase, or in other words, how concentration changes propagate through the system. There are 2 ideal types of mixing behaviour (Figure 1.4), which can be considered as extremes of possible mixing behaviour: (Nopens, 2015)

- In plug flow, no mixing occurs.
- In a continuous stirred-tank reactor (CSTR), complete mixing instantaneously occurs.

However, in reality, reactors will show a mixing behaviour in between these 2 extremes. A proper and rigorous description of mixing behaviour can be achieved through the use of the advection-dispersion equation. This equation, however, is a partial differential equation, which is not easy to solve. Therefore, an easier approximate approach to simulate mixing behaviour can be used in reactor engineering: the tanks-in-series approach. (Nopens, 2015) In this approach, 1 reactor is represented as a series of CSTRs (Figure 1.5) (Tchobanoglous et al., 2003). By increasing the number of CSTRs, the mixing behaviour will gradually change from the behaviour in a CSTR to the behaviour in a plug flow reactor

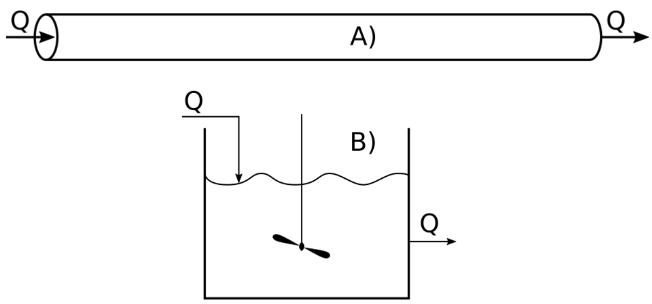


Figure 1.4: Different types of ideal continuous reactors: A) plug flow reactor and B) CSTR. Q means flow rate. Redrawn and modified from Nopens (2015).

(Nopens, 2015).

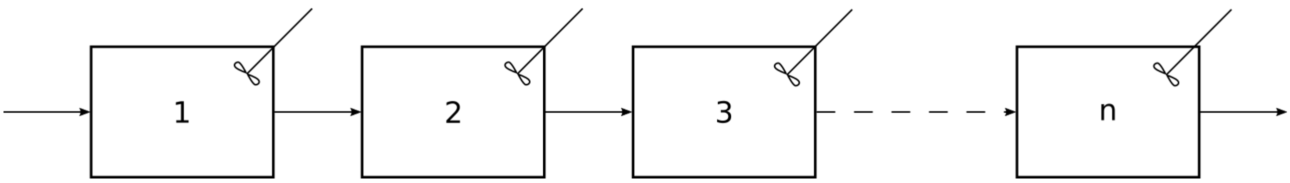


Figure 1.5: Illustration of tanks-in-series approach, where n CSTRs have been used. Redrawn from Nopens (2015).

ASM2d is mathematical model that allows dynamic simulations of biological processes for removal of chemical oxygen demand (COD) (carbon compounds), N, and P in activated sludge systems. It hence consists out of a system of ordinary differential equations (ODEs). It also allows the simulation of 2 chemical processes that may be used to model chemical precipitation of P. It is a minor extension of ASM2, which on its turn is an extension of ASM1. (Henze et al., 2000)
The mathematical model contains 19 state variables and describes 21 processes, 19 biological processes and 2 chemical processes. As a result of these processes, concentrations of the state variables will change as a function of time. Examples of processes are:

- Nitrifying organisms grow aerobically, thereby transforming NH_4^+ to NO_3^-. This thus models the nitrification.

- Heterotrophic organisms can grow aerobically. They thereby consume soluble carbon compounds and produce more particulate biomass. They can also grow anoxically, thereby transforming NO_3^- to N_2, which thus models the denitrification.

- Metal-hydroxides, which may introduced into the system by adding metals, result in the formation of metal-phosphate precipitate out of inorganic soluble P compounds.

Note that the transfer of compounds from the soluble phase to the particulate phase, results in the fact that these compounds can subsequently be separated from the water with gravitational settlers. (Henze et al., 2000)
Since the 21 processes of ASM2d are in fact biochemical and chemical processes, the equations modelling these processes have to describe the stoichiometry and the kinetics related to these reactions. The stoichiometric part of the equations was set up based on the principle of conservation of mass, electrons, and net electrical charge. The kinetics are mainly based on Monod kinetics and first-order kinetics. (Henze et al., 2000)

Regarding aeration, it is important to note that ASM2d, as described by Henze et al. (2000), contains the DO concentration as a state variable. However, it only contains O_2 consuming processes. Hence, an additional O_2 supplying term has to be added to the DO equation in ASM2d, in order to add O_2 to the simulated system. Modelling of such a term can be done based on an extension of the work of Redmon et al. (1983) and Boyle et al. (1994) by Rosso et al. (2005). The most important feature of this modelling, is that it exists out of mathematical equations, containing a correlation between the air flow rate provided to the reactor and the rate at which O_2 is supplied to the reactor.

The approach described by Tay (1982), can be used to model a primary sedimentation tank (PST):

$$\frac{S_0 - S}{S_0} = \frac{t_r}{T_A + t_r} \tag{1.2}$$

Where S_0 [mg L^{-1}] is the suspended solids concentration in the PST influent, S [mg L^{-1}] the suspended solids concentration in the effluent, t_r [min.] the actual mean retention time of the suspension flowing through the PST (Heinke et al., 1980), and T_A [min.] the half-removal time. The latter is a measure of the settleability of the solids and can be obtained by a regression analysis of experimental data.

The processes in a secondary secondary sedimentation tank (SST) can for instance be modelled as described by Takács et al. (1991). According to this approach, the settler is modelled in 1 dimension only, namely its height and it is discretized in a number of layers (Figure 1.6). The mathematical modelling is based on solids fluxes in these layers and on a mass balances of the solids in each layer. The solids flux due to gravitational settling, in addition, is defined as the product of the solids concentration,X , and the settling velocity of the solid particles, v_s. An equation to calculate v_s is also described by Takács et al. (1991).

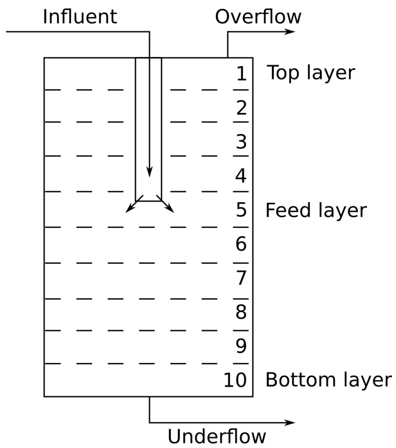


Figure 1.6: Redrawn and modified from Takács et al. (1991). Schematic representation of the discretization in layers of a settler, according to the modelling approach of Takács et al. (1991). Note that the settler will be modelled in 1 dimension only, its height. Hence, the settler will be considered as homogeneous in the other dimensions.

1.3 Life cycle assessment

Thus far, it became clear that improving the environmental performance of wastewater treatment is desirable. Modelling is in addition a tool that can speed up scenario analysis to achieve this. However, to select the proper measures to be taken, a thorough analysis of the environmental consequences is needed and life cycle assessment (LCA) is a tool that facilitates this analysis, which will become clear in the following.

1.3.1 Introduction to life cycle assessment

The increased awareness of the importance of environmental protection and the possible environmental impacts associated with products or services, has increased interest in the development of methods to better understand and address these impacts. One of the techniques being developed for this purpose is LCA. (ISO, 2006a) Note that from now on in this thesis, the term product can either mean product or service.

The eventual outcome of an LCA is a quantification of the environmental impact of a product (e.g. use of resources and environmental consequences of emissions) throughout its life cycle and the interpretation of these results. The concept "life cycle" of a product symbolizes the fact that everything from raw material acquisition through production, use and final disposal should be included into the

analysis (i.e. “cradle to grave”, Figure 1.7). (ISO, 2006a,b)
The life cycle is modelled by composing a so-called product system. This is a collection of the required unit processes in the life cycle (e.g. production processes and transport) with their quantified respective in- and outputs (e.g. energy, raw materials, and emissions to the environment). A unit process is the smallest process considered for which in- and outputs are quantified. The product system also includes so-called elementary flows and product flows. An elementary flow is a material or energy drawn from or emitted to the environment, without - respectively - previous or subsequent human transformation. A product flow is a product flowing to or entering from another product system. A product system is delimited by a system boundary, which specifies which unit processes are part of the product system under consideration. (ISO, 2006a,b) In Figure 1.7 a simplified example of a product system is given.
According to the widely adopted ISO standards, an LCA consists of 4 steps: goal and scope definition, life cycle inventory (LCI) analysis, life cycle impact assessment (LCIA), and life cycle interpretation. Below, the most important aspects of these 4 phases will be described. (ISO, 2006a,b)

Before continuing, it has to be noted - for the sake of clarity - that the term modelling is also used in the literature to describe certain aspects related to LCA (see for example ISO (2006a,b); Corominas et al. (2013a), and Zang et al. (2015)). LCA can thus in fact be considered as the modelling of the environmental impacts of a product. When in this thesis is said that dynamic WWTP modelling will be coupled to LCA, this could thus in fact be stated as the coupling of 2 models.

Goal and scope definition

In the description of the goal, it should be stated what the reasons for carrying out the LCA and its intended application are. (ISO, 2006a,b)
The description of the scope should contain, among others, the following elements: the product or - in case of comparative studies - the products under study, the functional unit (FU), the system boundary, impact categories selected (see description of life cycle impact assessment) and assumptions. The scope of an LCA may vary to a large extent depending on the subject and the intended use of the study. This means that the level of detail and thoroughness can vary significantly between different LCA studies. (ISO, 2006a,b) Furthermore, a description of all unit processes included in the product system should be given and a process flow diagram that outlines all the unit processes in the product system, including their interrelationships, should be drawn. (ISO, 2006a,b; De Meester, 2017)
The FU defines a certain quantification of the product, or its function, under study. The primary purpose of the FU is to provide a reference to which all other inputs and outputs are scaled. If for example 1 kg of meat is the FU of a certain product system, all energy requirements of the product

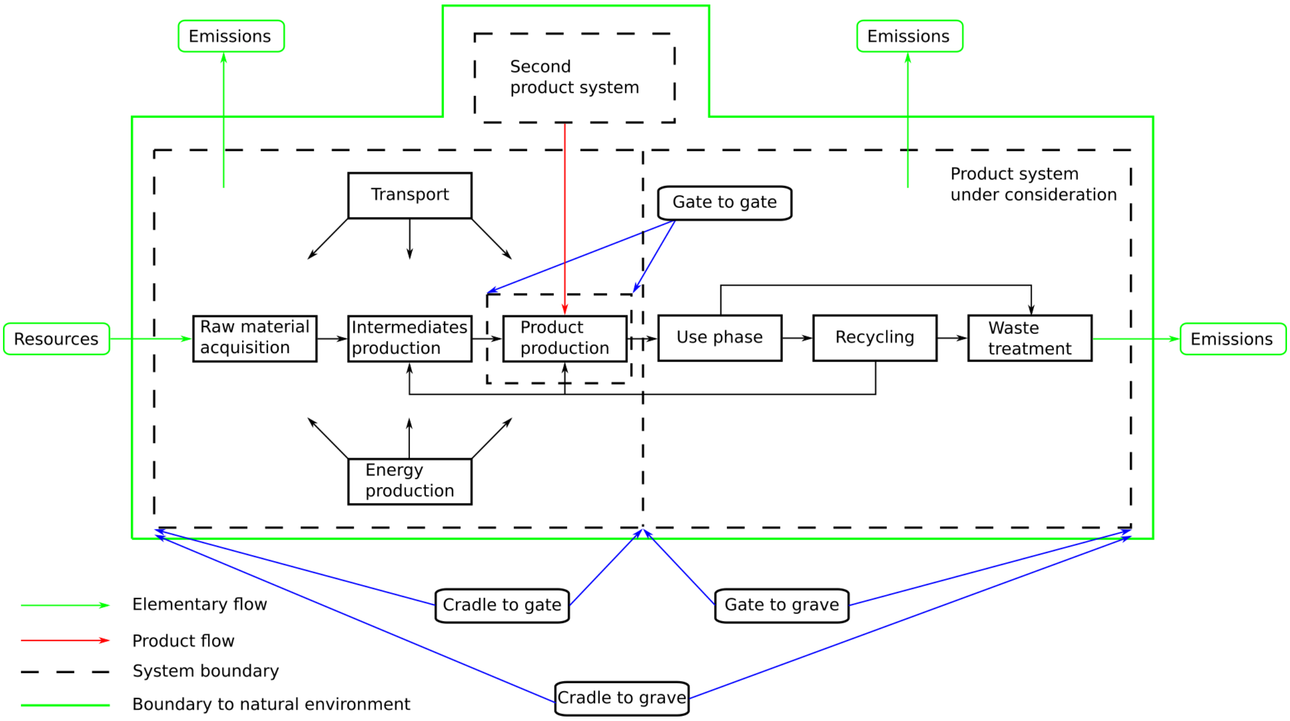


Figure 1.7: Based on both ISO (2006a) and (Masoni and Zamagni, 2011). Simplified example of a product system. The second product system is added to illustrate the concept of a product flow. The concepts cradle to grave, gate to gate, cradle to gate, and gate to grave are also depicted. The blue arrows indicate the corresponding system boundary for each of these concepts. Note that if the system boundary is chosen such that it corresponds with the cradle to gate concept, the flow between "Product production" and "Use phase" is in fact a product flow.

system should be expressed as the amount of energy needed to produce this 1 kg of meat. (ISO, 2006a,b)
Regarding the system boundary, the product system should ideally be composed in such a manner that in- and outputs at its boundary are elementary flows, since these form the basis of the quantification of the environmental impacts (see description of life cycle impact assessment). However, due to data and cost constraints this might not be possible. (ISO, 2006a,b)

Life cycle inventory analysis

LCI analysis involves the compilation and quantification of relevant in- and outputs of the product system under study and its composing unit processes (see Figure 1.8). For those data that may be significant for the conclusions of the study, data quality should be indicated. When reporting this data quality, the following items should for instance be specified: time when the data were collected and an estimate of the uncertainty of the data. (ISO, 2006a,b)

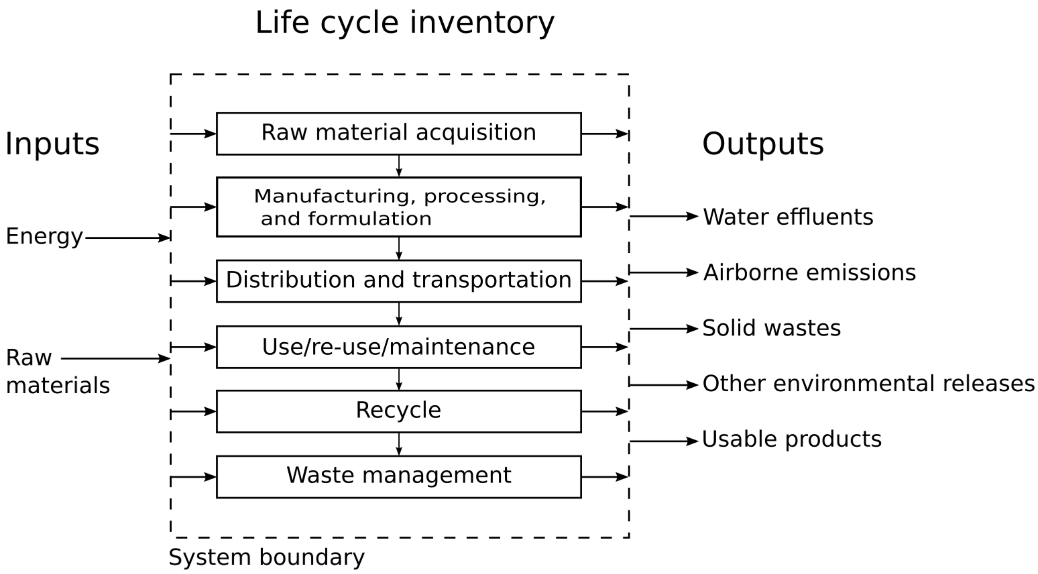


Figure 1.8: Conceptual schematic of an LCI analysis. Modified and redrawn from Schaubroeck and Dewulf (2015)

LCI data can be gathered by measurements at plants, i.e. primary data. Average or generic data can also be gathered, i.e. secondary data. (JRC-IES, 2010b) Secondary data is typically retrieved from databases (JRC-IES, 2010b), such as the ecoinvent database (`http://www.ecoinvent.org/`). With respect to primary and secondary data, a product system can be divided in a fore- and background system: For the foreground system, primary data should be used as much as possible, while secondary data is used for the background system. (JRC-IES, 2010b) The foreground system typically consists out of processes directly related to product under consideration, e.g. the use phase and the product production (Figure 1.7). The background system typically consists out of auxiliary processes, e.g. electricity production (Figure 1.7). Data might also be obtained through process models (JRC-IES, 2010b). In this thesis, data will primarily be gathered through process modelling.

Life cycle impact assessment

LCIA exists out of 2 phases. An overview of LCIA is shown in Figure 1.9. In the first phase, elementary flows related to the product system under study - that were identified in the LCI analysis - are assigned to impact categories. The latter are classes representing environmental issues of concern. For instance, emissions of certain amounts of various GHGs will each be assigned to the impact category climate change. This is also known as classification. (ISO, 2006a,b) See Table 1.1 for some examples of impact categories.

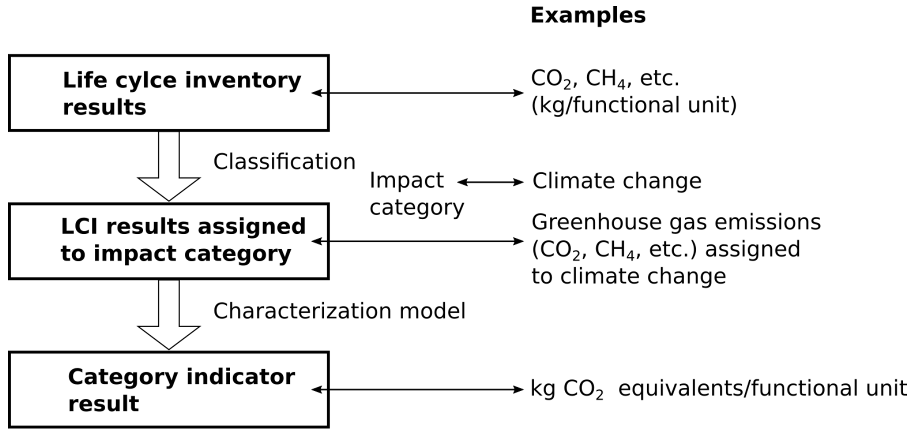


Figure 1.9: Modified and redrawn from ISO (2006b). Conceptual schematic representation of LCIA.

Table 1.1: Examples of LCA impact categories defined by (Goedkoop et al., 2013).

Impact categories
Climate change
Freshwater eutrophication
Freshwater ecotoxicity
Ozone depletion
Human toxicity
Natural land transformation
Mineral resource depletion

Subsequently, results have to be calculated, which is known as characterization. Therefore, for each impact category a category indicator is selected, which is a quantifiable representation of an impact category. E.g., for climate change radiative forcing can be used. (ISO, 2006a,b) According to the

LCIA method ReCiPe, radiative forcing is expressed as kg CO_2-equivalent (Goedkoop et al., 2013), which might seem a bit confusing. However, radiative forcing [W m^{-2}] is a measure of the influence a factor has in altering the balance of incoming and outgoing energy in the Earth-atmosphere system (IPCC, 2007). If the amount of radiative forcing caused by the emission of a certain amount of CO_2 - $1.4 \cdot 10^{-2}$ W m^{-2} ppm^{-1} - is taken as reference (Forster et al., 2007), radiative forcing can indeed be expressed as kg CO_2-equivalent. One obstacle however remains to calculate the final result: all LCI results assigned to a specific impact category, e.g. climate change, have to be converted into a common unit and summed. To convert LCI results into a common unit, characterization factors - which are derived from a characterization model - are used. (ISO, 2006a,b) For instance, the ReCiPe method uses the IPCC CO_2 equivalence factors - described by (Forster et al., 2007) - as characterization factors, to convert various GHGs to the common unit kg CO_2-equivalent. In this case, the characterization factors are defined as global warming potential (GWP), and their unit is kg CO_2 (kg gas)$^{-1}$, e.g. the GWP of CH_4 is 25 kg CO_2 (kg CH_4)$^{-1}$ (Goedkoop et al., 2013; Forster et al., 2007). From the above, the essence of the climate change characterization model used by ReCiPe also becomes clear: It calculates radiative forcing caused by the emission of a certain amount of all the relevant substances and expresses these results relative to the value of CO_2 (Goedkoop et al., 2013; Forster et al., 2007). Finally, the category indicator result can be calculated. According to the ReCiPe LCIA method, the category indicator result for the impact category climate change would be kg CO_2-equivalent emitted per FU (Goedkoop et al., 2013). In Figure 1.10, a schematic representation of characterization for the impact category climate change is shown.

Note that the use of characterization factors implies a linear relationship between LCI results and category indicator results, although this relation can be far from linear in reality (Schaubroeck and Dewulf, 2015). The latter is usually not considered in LCIA methods (JRC-IES, 2011).

Above, ReCiPe is referred to as an LCIA method. Various LCIA methods exist and they can be defined as a collection of characterization models to calculate results for a set of corresponding impact categories (Hauschild et al., 2013). ReCiPe (Goedkoop et al., 2013) can serve as an example. It comprises 18 impact categories at midpoint level (see further) - of which some examples are given in Table 1.1, 3 endpoint impact categories (see further), and the corresponding characterization models. A spreadsheet with all the characterization factors for all relevant substances for the respective impact categories is provided on the ReCiPe website (`http://www.lcia-recipe.net/`).

The starting point of the development of ReCiPe, was actually the integration of 2 former LCIA methods: CML 2002 (Guinée et al., 2002) - which focuses on midpoint impact categories - and Eco-indicator 99 (Goedkoop and Spriensma, 2001) - which only contains endpoint impact categories. According to JRC-IES (2010a), the difference between midpoint and endpoint impact categories can be explained as follows (see also Figure 1.11): An impact pathway links LCI data to so-called areas of protection. A category indicator result can be calculated for different locations on this impact pathway. Charac-

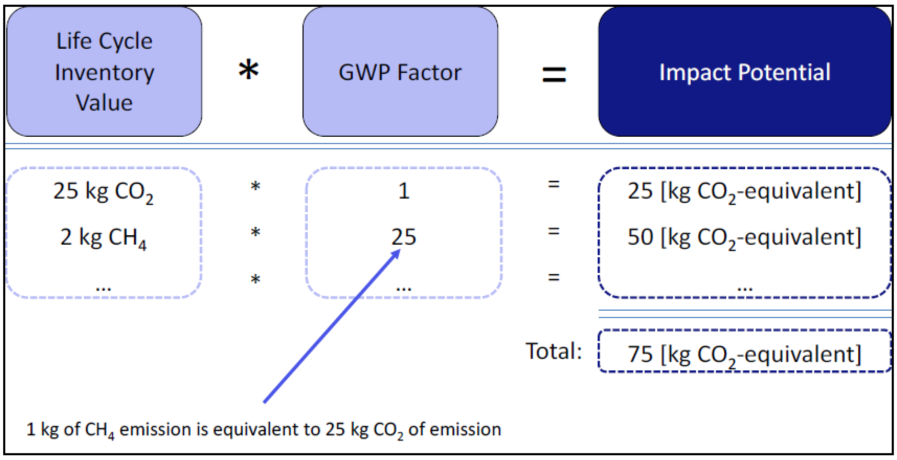


Figure 1.10: Example of the application of characterization factors - in this case GWPs of the concerning GHGs - to calculate category indicator results. The impact of CH_4 and CO_2 emission is characterized through multiplication with the respective characterization factors of CH_4 and CO_2 for the climate change impact category. The category indicator result is the total amount of kg CO_2-equivalent. (Masoni and Zamagni, 2011)

terisation at the endpoint level requires modelling all the way to the impact on the entities described by the areas of protection, e.g. on human health, the natural environment, and natural resources. Impact categories at the midpoint level are defined at the place where a common mechanism for a variety of substances within that specific impact category exists. For example, climate change impacts involve a series of steps, starting with the release of GHGs, and ending with impacts on humans and ecosystems. There is a point where the GHGs have an effect on the radiative forcing. GHG emissions have a pathway that is different before that point, but identical beyond that point. Therefore, radiative forcing provides a suitable indicator for the midpoint impact category of climate change.
An important conclusion regarding midpoint and endpoint is the following: Conversion of midpoint to endpoint results should be based, as far as possible, on a solid scientific foundation. This, hence, diminishes the fact that value choices tend to be included in the often difficult comparison of various midpoint results. On the other hand, for impact categories such as climate change, the consequences cannot be fully modelled all the way to the endpoint at this time, which thus introduces uncertainties in the conversion of midpoint to endpoint. Hence, it is useful to retain both midpoint and endpoint insights. JRC-IES (2010a)

Classification and characterization are usually performed through the aid of software, e.g. SimaPro (`https://simapro.com`). In these programs, different LCIA methods can be chosen. The software

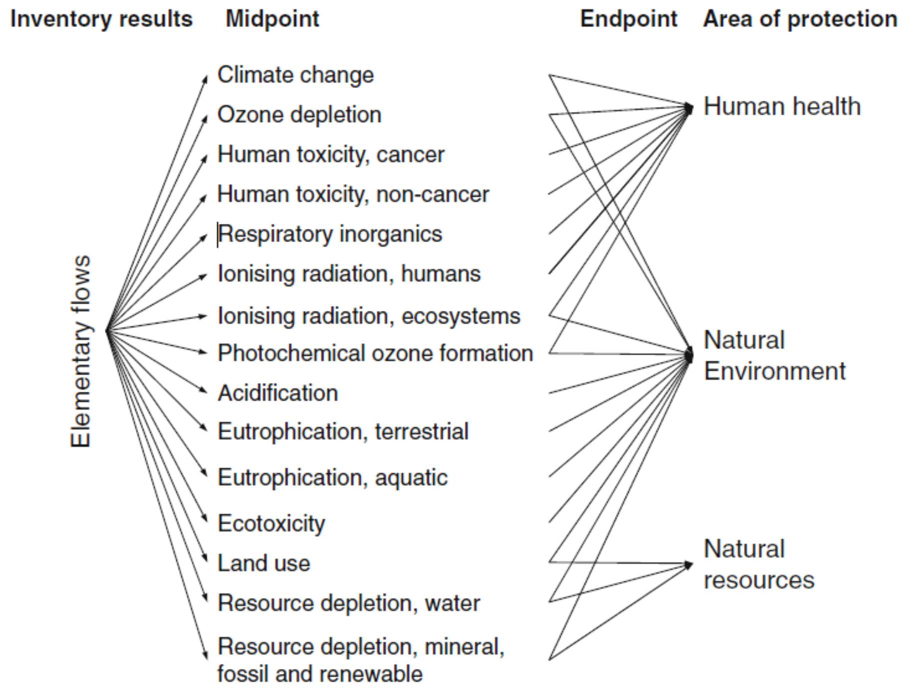


Figure 1.11: (Hauschild et al., 2013) Schematic representation of the conversion of LCI results to impact categories at midpoint level, and subsequently to endpoint level.

can also be linked to the aforementioned databases, that provide complete datasets on a wide variety of processes - such as electricity production - which can be used in the background system. The LCA practitioner can enter his LCI results and the software calculates the result.

A final remark regarding LCIA is, that the selected impact categories should reflect a comprehensive set of environmental issues related to the product system being studied, taking the goal and scope into consideration. In addition, this selection has to be justified. (ISO, 2006a,b)

Life cycle interpretation

In the life cycle interpretation, the findings from the LCI and the LCIA are summarized and discussed. In addition, conclusions and recommendations - for instance for decision-making - should be stated. This should all be done in accordance with the goal and scope definition. (ISO, 2006a,b)

1.4 Life cycle assessment for wastewater treatment plants

Within the field of wastewater treatment, LCA was already applied in the 1990s. Since then, more than 40 studies have been published in international peer-reviewed journals using an array of databases, system boundaries and LCIA methods. (Corominas et al., 2013a). It is therefore interesting to summarize some important aspects of previous LCA studies applied to WWTPs, because this will probably lead to an appropriate selection of methodologies to use in this thesis.

First of all, it is important to note that one of the widely used ways of presenting the results is taking a reference scenario for which the impacts are calculated. The impacts of the other scenarios are then compared to the reference scenario. In such a way induced and avoided impacts can be calculated for each scenario. (Corominas et al., 2013a)

1.4.1 Selecting an LCIA method

As mentioned above, different LCIA methods exist. Hauschild et al. (2013) published an elaborate review on LCIA methods and they state that none of the methods reviewed by them has true universal acceptance. One solution they propose, is to combine the best characterization models from different LCIA methods. They do, however, state that this approach leads to loss in consistency between characterization at midpoint and characterization at endpoint. They say that this consistency is only ensured when midpoint and endpoint models are developed to serve within the same framework, as is the case for several of the more recent LCIA methods, such as ReCiPe and LIME. As is to be expected, it is more or less impossible to draw a single conclusion from the summary of their analysis (in their supporting information), but ReCiPe doesn't seem like a bad choice.

1.4.2 Selecting important impact categories in wastewater treatment and identification of important impact generating processes and items

It is first of all important to note the following: Both Zang et al. (2015) and Corominas et al. (2013a) reviewed a number of WWTP LCA studies. Results from these studies indicate that when impact categories related to eutrophication and toxicity are reduced by increasing treatment, for instance to comply with lower nutrient limits for the effluent, environmental emissions linked to energy and chemical use increase. Thus, the improvement of local water quality is at the cost of regional/global effects stemming from energy and chemical production. (Zang et al., 2015)

Generally speaking, typical impact categories used for analysing wastewater treatment are: eutrophication, climate change, human toxicity, terrestrial ecotoxicity, freshwater ecotoxicity, marine ecotoxicity, acidification, photochemical oxidant formation, and ozone layer depletion (Zang et al., 2015; Corominas et al., 2013a). Emerging indicators are water use and land use Zang et al. (2015). Ozone layer depletion and abiotic depletion (which includes fossil energy and material depletion) were not found to be significant decision-making drivers in the studies where they were used, according to (Corominas et al., 2013a). Below, some important aspects regarding these impact categories will be discussed.

Eutrophication is an important impact category to consider when analysing WWTPs (Zang et al., 2015). This is mainly related to the emissions of N and P - and to a lower extent of organic compounds - to water (Gallego et al., 2008). However, for coastal WWTPs air emissions of NO_x and NH_3 from the biological reactors can cause marine eutrophication, due to atmospheric N deposition. It is furthermore widely assumed that freshwater eutrophication and marine eutrophication should be considered separately, since P is typically the limiting nutrient in freshwater, whereas N is more commonly limiting in marine waters. (Zang et al., 2015) However, results of Elser et al. (2007) contradict this paradigm and indicate that both ecosystems might be rather similar in terms of N and P limitation.

Climate change is also an important impact category. Direct GHG emissions from WWTPs include N_2O from the biological wastewater treatment (denitrification) and CH_4 from the anaerobic wastewater and/or sludge treatment process, with N_2O being of particular importance. (Zang et al., 2015) CO_2 emissions from the aerobic treatment process are - according to IPCC (2006) - not to be included in the inventory, because they are considered as biogenic. However, Griffith et al. (2009) indicate that 25 % of the dissolved organic carbon in WWTP effluent is fossil carbon, which is likely derived from petroleum-based household products such as detergents and pharmaceuticals.

Toxic impacts have gained increased attention when LCAs of WWTPs are performed. Important contributors to aquatic ecotoxicity (both freshwater and marine) are toxic contaminants in the effluent and fossil-based electricity consumption. Important contributors to human toxicity are fossil-based electricity, chemical production, and sludge incineration. (Zang et al., 2015) In addition, Munoz et al. (2008) quantified the potential environmental impacts of wastewater effluent containing priority pollutants - e.g. heavy metals and chlorinated solvents, and pharmaceuticals and personal care products of a specific WWTP. The results indicate that all of these might be of importance, especially the pharmaceuticals and personal care products. It has to be noted however, that using different LCIA models can lead to large discrepancies in the results of toxic impact categories (Zang et al., 2015; Renou et al., 2008; Pizzol et al., 2011).

Water use is an emerging indicator. There is however almost no freshwater use during the processes in WWTPs, although water loss from the total incoming influent might occur due to evaporation from open water surfaces and the water bound in exported sludge. (Zang et al., 2015)

1.4.3 Most important processes and items to include into the system boundaries

Subsection 1.4.2 listed some important contributors to the environmental impacts of WWTPs. Hence, conclusions regarding which items certainly have to be included into the system boundaries can already be drawn from this (e.g. chemical use and direct GHG emissions).
In addition, Zang et al. (2015) conclude that energy consumption, wastewater effluent, and sludge disposal are the main contributors to these impacts.
It is furthermore possible that the construction phase of capital goods has also an important contribution. Hence, capital goods should not be excluded from the system boundaries without a proper justification. (Corominas et al., 2013a)

1.4.4 Functional units applied in wastewater treatment LCA

The most used FU in the studies reviewed by Corominas et al. (2013a), is a certain volume of wastewater treated. However, they argue that this FU is not representative, if differences in influent quality or the removal efficiency between the analysed scenarios exist. To take this into account, some of the studies reviewed by them used a certain amount of organic pollutant treated or a certain amount of kg PO_4^{3-} equivalent treated. In addition, 9 % of the analysed studies use the life-span of the plant as FU. Finally, 1 study considers 10 years of operation within the FU. Zang et al. (2015) also mention the difference between the use of a FU expressed as volume of water treated and one expressed as amount of pollutant removed.

1.4.5 Clear examples of the usefulness of life cycle assessment for wastewater treatment plants

This section could be concluded with 2 examples of WWTP LCA studies with remarkable results that demonstrate the usefulness - and maybe even the necessity - of applying LCA in decision making. However, due to page limit guidelines, the reader is referred to the appendix (A.1) for these examples.

1.5 Previous coupling of (dynamic) modelling and life cycle assessment

It has become clear that water pollution is a serious problem and that WWTPs based on biological activated sludge processes diminish this problem, but at the same time cause environmental impacts themselves. LCA is a tool to thoroughly analyse environmental impacts, and its usefulness in analysing

WWTPs has already been demonstrated. Modelling is in addition a tool that can speed up the search for alternative and/or optimal WWTPs, but a thorough environmental analysis is not part of the modelling results. Indeed, coupling WWTP modelling to LCA extends the modelling results with an environmental dimension. This therefore speeds up the search for more environmentally friendly solutions. It results, in addition, in the fact that a thorough environmental analysis can be incorporated in the phase where it is decided which future measures will be taken, instead of first carrying them out and merely analysing what the consequences are. This all seems very interesting indeed, and there are a number of articles in the literature where the coupling was already made (see further).

As in any modelling exercise however, one has to be aware of the fact that modelling results are never perfectly accurate. Acceptable average relative deviations of WWTP modelling results from actual measurements are 5-20% for steady state simulations and 10-40% for dynamic simulations. (Nopens, 2015) This stresses the fact that models can assist in decision making, but the chosen measure(s) should be tested in the real world to validate the model.

1.5.1 Steady state modelling coupled to life cycle assessment

In steady state, no changes over time occur, thus all model outputs - e.g. nitrate concentration in the WWTP effluent - will be scalars. Scalars are also the inputs that are expected in the LCI analysis phase of an LCA. Thus, in this case the coupling is rather straightforward.

Steady state WWTP simulations were coupled to LCA or simplified LCA by Ontiveros and Campanella (2013); Alvarez-Gaitan et al. (2016); Rahman et al. (2016); Guo et al. (2016); Fang et al. (2016); Rodriguez-Garcia et al. (2014); Steele et al. (2014); Wang et al. (2012); Foley et al. (2007) and Meneses-Jacome et al. (2015). It should be noted that not all "materials and methods" sections in the mentioned articles are as clear as they should be and it was hence not always clear whether steady state or dynamic simulations were used. Examples of the analysed scenarios are: different alternatives of biological nutrient removal, where the reference scenario was the performance of a conventional plant without nutrient removal (Ontiveros and Campanella, 2013), and the impact of decreasing nutrient limits (Rahman et al., 2016).

1.5.2 Dynamic modelling coupled to life cycle assessment

In steady state, no changes over time occur. However, influent flows in WWTPs are highly dynamic (Nopens, 2015; Henze et al., 2000). It should thus not come as a surprise that various aspects of WWTPs also vary with time and in dynamic simulations these variations in time are indeed simulated.

Two major dynamic aspects of the influent flow of municipal WWTPs are the following: Firstly, a diurnal pattern can be recognised because of the typical water consumption pattern of people. Two peaks can be observed, one in the morning and one in the evening, because most people are then at home and awake. Secondly, in the case of combined sewer systems, rain fall events can cause peaks in the influent flow of 6 to 10 times the average flow rate at dry weather. (Nopens, 2015)
As is to be expected, also concentrations of pollutants like COD, N, and P show dynamic behaviour and they do not necessarily all behave in exactly the same way (Rieger et al., 2013).

Dynamic WWTP simulations were coupled to LCA by Corominas et al. (2013b); Bisinella de Faria et al. (2015); Meneses et al. (2016, 2015); Flores-Alsina et al. (2010) and Hadjimichael et al. (2016), and to a simplified LCA by Mouri et al. (2013). Examples of the analysed scenarios are: WWTP control strategies (Meneses et al., 2016, 2015; Flores-Alsina et al., 2010) and nutrient removal strategies (Corominas et al., 2013b).

Since variations in time are simulated by dynamic simulations, the model output for each simulated process variable is a vector. This is already less straightforward to use as input data for the LCA, since those are typically expected to be scalars. An easy way to deal with this, is calculating the average values and using those as input data. However, then all information regarding the temporal dynamics, as simulated by the dynamic model, will be lost in the final LCA result.
Corominas et al. (2013b); Meneses et al. (2016) and Meneses et al. (2015) clearly indicate that scalars are used as input data for the LCA. Thus some sort of average was calculated, but the calculations are not explicitly mentioned. Bisinella de Faria et al. (2015) nicely illustrate how they integrated the simulation results over the simulation time to get the total amounts. The input data for the LCA are eventually expressed as amount per m^3 treated water, which is their FU. Hence, results were averaged out over the amount of treated water. Flores-Alsina et al. (2010) and Mouri et al. (2013) are not clear about the input data for the LCA, but it is likely that scalars are also used since the LCA results are scalars. Hadjimichael et al. (2016) simulated a period of 10 years. Their input data for the LCA are totals for this period. Thus, none of the mentioned studies incorporated the temporal dynamics of the model output into the LCA results.

It is also interesting to note that Bisinella de Faria et al. (2015) present a good argument to use dynamic instead of steady state simulations. They compared both cases. The impacts for all impact categories calculated through the results of the former were higher than the latter (one of these results is shown in Figure 1.12), because the simulation results were strongly influenced by influent perturbations. Hence, if these simulation results accurately describe the real world, the use of steady state simulations will result in an underestimation of environmental impacts. These results, in addition, agree with conclusions of Guo et al. (2012). They state that the average value of N_2O emissions under dynamic influent conditions cannot be simulated by a steady state model subjected to a similar influent quality. This highlights the usefulness of dynamic simulations.

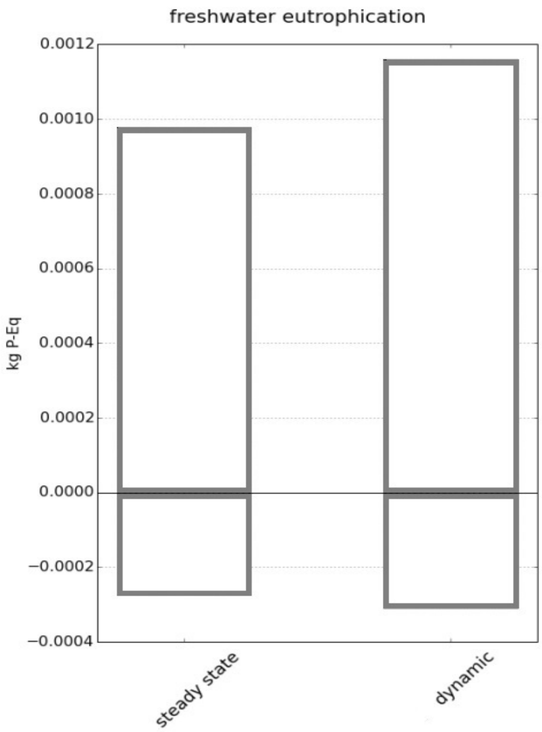


Figure 1.12: Modified from Bisinella de Faria et al. (2015) (figure retrieved from their supplementary data). Result for the impact category freshwater eutrophication when comparing a steady state and a dynamic simulation. The negative part of the graph refers to avoided impact.

The wastewater treatment plant of Eindhoven

At this point it is already interesting to note that the WWTP of Eindhoven, located in the southeast of the Netherlands, will be the object under study in this thesis, since the aforementioned authors, Hadjimichael et al. (2016), actually coupled dynamic modelling (DM) to LCA for the very same WWTP. Therefore, some important aspects of their study will be summarized below.

In their study, the system boundaries were expanded to contain the entire catchment, the sewer system with its combined sewer overflows (CSOs), the WWTP and the effluent receiving river section within the catchment boundaries. The results were in fact obtained through an integrated model that is made-up through the integration of 3 separate models: one for the catchment and sewer system, one for the WWTP, and one for the river section. In this way a more integrated analysis of the entire urban wastewater system was performed. It was for instance possible to include the environmental impacts of CSO events and to assess their importance in the environmental impacts of the urban wastewater system.

Since the effluent receiving river section was also modelled, it was possible to quantify the emissions of NH_4^+ to water as concentrations in the actual river section. P loads emitted to the river section were on the other hand estimated based on empirical measurements. In this manner, the purification capacity of the receiving water was taken into account in the estimated emissions and this is a nice illustration of a site-specific assessment of the impact category eutrophication.

The FU was 10 years of system operation treating approximately 546,550,190 m^3 of wastewater in total. The total contribution of CSO events to the NH_4^+ and P emissions appeared to be a small part of the overall emissions (respectively 1.2% and 7.7% for the reference scenario). This was attributed to the fact that the total CSO volume was less than 4% of the WWTP effluent volume over 10 years. However, it can be expected that CSO events cause peaks in these emissions. Since the dynamic aspects of the model output are not incorporated into the LCA results, as mentioned before, the effects of these peaks are averaged out over time. It is thus in this way not possible to analyse the severity of these peaks, although their consequences might be more serious than just increasing the emissions with such a small average amount. It might thus be interesting to incorporate the temporal dynamics of the model output into the LCA results.

1.6 Objectives of this research

Its has become clear that our freshwater resources need to be safeguarded. The most widely used technologies to treat wastewater are WWTPs based on biological activated sludge processes. However, they cause considerable environmental impacts themselves. LCA is a tool to analyse those impacts and can thus assist in the search for optimal or alternative solutions. A WWTP model is furthermore a tool that can speed up scenario analysis and/or alleviate the problem that modifying full-scale installations merely for experimenting is technically difficult and expensive. If these models are coupled to LCA, a thorough environmental analysis of the investigated scenarios can assist in the decision making phase, where it is decided which technologies will assist in building a sustainable future. This seems very interesting indeed and the coupling of modelling and LCA was already performed in a number of articles.

There are, in addition, indications that dynamic WWTP modelling results give a more accurate description of reality than steady state modelling results. Dynamic models were also already coupled

to LCA, but - to the best of the author's knowledge - the dynamic aspect of the modelling results was not yet incorporated into the LCA results.
It will therefore be the main goal of this thesis to incorporate the dynamic aspect of WWTP modelling results into the LCA results and to analyse if this is actually useful. For this purpose, first 2 scenarios will be analysed: one with only dry weather conditions and one with dry and wet weather conditions, as is to be expected in reality. These scenarios were chosen, since it is to be expected that they will result in a significant difference in dynamic WWTP (model) behaviour and therefore illustrate whether or not it makes sense to incorporate the dynamic aspect of the modelling results into LCA studies. Another goal will be the following: investigate whether or not dynamic LCA can lead to selecting additional scenario(s), that have the potential to improve the environmental performance of the WWTP under study. The model used in this thesis is a model of the Eindhoven WWTP, located in the southeast of the Netherlands.

CHAPTER 2

Materials and methods

2.1 System description: The Eindhoven wastewater treatment plant

As mentioned before, the focus of this thesis is the Eindhoven WWTP, located in the southeast of the Netherlands. It has a treatment capacity of 680,000 person equivalent (PE), where 1 PE is defined as 150 g COD per day. In 2013, the average influent load was 62,694 kg COD day^{-1}. (Blom, 2013) In Figure 2.1 an aerial overview of the Eindhoven WWTP is shown.

2.1.1 The water line

All information about the Eindhoven WWTP in this subsection (2.1.1) and subsection 2.1.2, was retrieved from a process manual written by Telkamp et al. (2009), unless stated otherwise.

The maximal hydraulic capacity of the primary treatment, including the primary settlers, is 35,000 m^3/h and that of the biological treatment and secondary settlers is 26,250 m^3/h. The effluent is discharged into the river "Dommel" and part of it is used as process water. A simplified schematic of the water line is provided in Figure 2.2.

The first influent treatment steps

Sewage enters the WWTP, flowing gravitationally from the sewer into 3 receiving cellars. From these cellars, the influent flows gravitationally to and through coarse screens, where large solids are removed. Then, it is pumped up in the influent pumping station. After pumping, the influent flows through finer screens, again removing solids.
Subsequently, the influent is aerated in a mixing ditch (not shown on the schematic of the water line).

Figure 2.1: (Telkamp et al., 2009) Aerial overview of the Eindhoven WWTP.

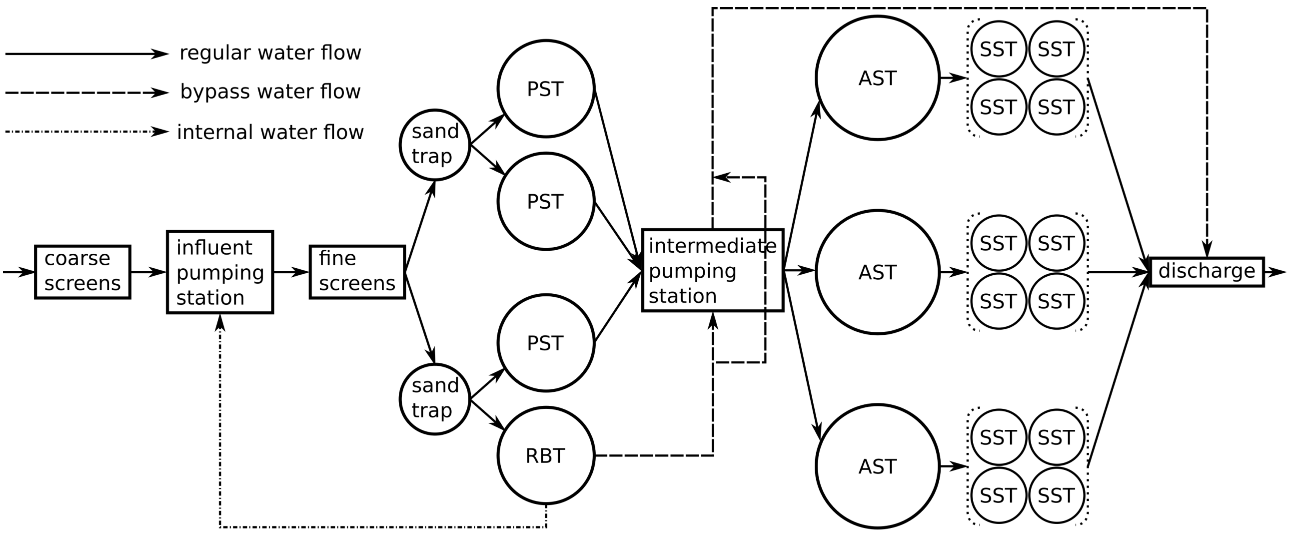


Figure 2.2: Redrawn from Telkamp et al. (2009). Simplified schematic representation of the water line of the Eindhoven WWTP.

It then flows through 2 sand traps, from which sand is removed mechanically after which the sand is washed with WWTP effluent.

Primary sedimentation tanks (PSTs)

Subsequently, the influent flows through 3 circular PSTs. Each PST has a diameter of 60 m, and a water depth next to the wall of 2.5 m. They are equipped with a rotating bridge that is connected to a scraper in order to collect sedimented sludge at the center, where the sludge is extracted through pumps. The PSTs are also equipped with an installation that removes the floating layer formed out of lighter compounds such as oils and fats.

Intermediate pumping station

The presedimented influent flows to an intermediate pumping station, from where it is pumped to three parallel activated sludge tank (AST) lanes. P is removed biologically in the next step, but $Al_2(SO_4)_3$ solution (see Table 2.1) is dosed for additional P removal in the intermediate pumping station. This results in the formation of $AlPO_4$. The most important parameter of the dosing flow controller is the setpoint for the PO_4^{3-} concentration in the effluent: 0.7 mg P L^{-1}.

Table 2.1: Characteristics of the Al product dosed at the Eindhoven WWTP (Telkamp et al., 2009). *wt*% means weight percent.

Product	Supplier	Description	Al content
$Al_2(SO_4)_3$	Fuji	Waste product [a,b]	3.0 *wt*%

[a] However, more than only the transportation cost is paid for this product (Flameling, 2016).
[b] Transported to the Eindhoven WWTP as liquid waste product and dosed without dilution (Flameling, 2016).

Activated sludge tanks (ASTs)

Subsequently, the presedimented influent is treated biologically in 3 identical ASTs, for removal of N, P, and organic compounds. The WWTP of Eindhoven has the modified University of Cape Town process configuration (Tchobanoglous et al., 2003). Each AST is composed of 3 rings and a cascade distribution system. The inner ring is anaerobic, the middle ring is anoxic, and the outer ring is partly aerated. In the text below, the inner, middle, and outer ring will be referred to as the anaerobic, anoxic, and aerated part respectively. See Figure 2.3 for a schematic of the ASTs and Table B.1

for some technical AST characteristics.

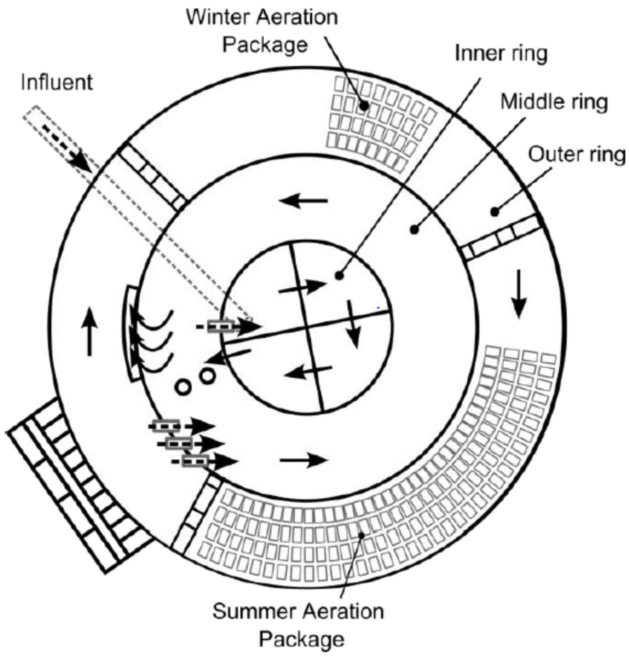


Figure 2.3: The circular modified University of Cape Town configuration of the ASTs at the Eindhoven WWTP (Amerlinck, 2015). The arrows indicate the flow direction of the water and the rectangular structure at the lower left is the cascade distribution system. The inner ring is the anaerobic part, the middle ring the anoxic part, and the outer ring the aerated part. The barred arrows crossing the walls of the rings, represent recirculation A and B. (Telkamp et al., 2009)

Presedimented influent enters the ASTs via the anaerobic part. Next, the water/sludge mixture flows to the anoxic part and subsequently to the aerated part. Then it flows to the SSTs via the cascade distribution system. Sludge from the underflow of the SSTs is recycled back to the anoxic tank (return activated sludge (RAS)). From the anoxic part, internal recirculation of water/sludge mixture with a low level of NO_3^- takes place to the anaerobic part (recirculation A). Through recirculation B, NO_3^- rich internal recirculation takes place from the aerated part to the anoxic part. For both recirculation A and B, pumps are installed.

In the anaerobic part no O_2 or NO_3^- is present. The anaerobic part in each AST, contains 4 stirrers and is composed of 4 compartments. In the anoxic part, no free oxygen is present, but bound oxygen under the form of NO_3^- is. The anoxic part in each AST contains 2 flow generating propellers. The aerated part contains 6 flow generating propellers per AST.

The aerated part is aerated by plate aerators that are arranged in 2 distinct units: a big "summer package" and a smaller "winter package". The needed airflow is generated with compressors.

Secondary sedimentation tanks (SSTs) and effluent discharge

The water/activated sludge mixture is subsequently separated in 12 circular SSTs, 4 for each AST. The SSTs have a diameter of 52 m. They are equipped with a system to remove the scum layer, a rotating sludge clearing bridge, and a RAS pump.

Finally, the effluent flows gravitationally into an effluent ditch and further into the Dommel.

Rain buffer tank

A rain buffer tank (RBT) of 8,750 m^3 is located next to the 3 PSTs. When rain weather peaks of more than 26,250 m^3/h occur, it is filled with 2 Archimedes screws. After usage of the RBT, suspended solids from the sewage might have sedimented there. To remove those, the RBT is equipped with a flushing system.

2.1.2 The sludge line

In Figure 2.4, an overview of the sludge line is visible. From the pipes bringing the RAS from the SSTs to the ASTs, waste sludge is extracted. The extracted sludge is also known as secondary sludge and this is carried out with 1 pump per AST.
The secondary sludge is sent to 2 gravitational sludge thickeners. The sludge thickener overflow water is directed back to the intermediate pumping station. A pump is located after each thickener to pump the sludge to the next stage. Each thickener is also equipped with a stirrer that operates continuously. The thickened sludge is then sent to a mixing tank. If needed, effluent is added for dilution, to ensure that the sludge has the right dry matter content for transportation to the sludge treatment facility (STF) (see further). The mixing tank is also equipped with a stirrer.
The thickened sludge flows from the mixing tank to a buffer tank, which is equipped with a constantly operating stirrer. Sludge leaves the buffer tank via an underflow.
Waste sludge is not treated at the Eindhoven WWTP, but pumped to the STF in Mierlo. This takes place through two 7 km pipes. The dry matter content of sludge leaving the WWTP is controlled in order to facilitate the transportation through the pipes. To achieve the transport, 4 pumps are present (1 for redundancy) to pump the primary sludge (from the PSTs). To pump the secondary sludge to Mierlo, 2 are pumps present. In each of the 2 pipes for sludge transport, primary and secondary

sludge is mixed together. At Mierlo, the sludge is dewatered further (partly) through centrifugation. The centrate is sent back to the Eindhoven WWTP through the sewer system. A third pipe is used to pump effluent, which will be used as process and flushing water, from the WWTP to Mierlo. From Mierlo, the partly dewatered sludge is transported to the sludge incineration facility (SIF) in Moerdijk (Blom, 2013), at 100 km distance, where it is incinerated.

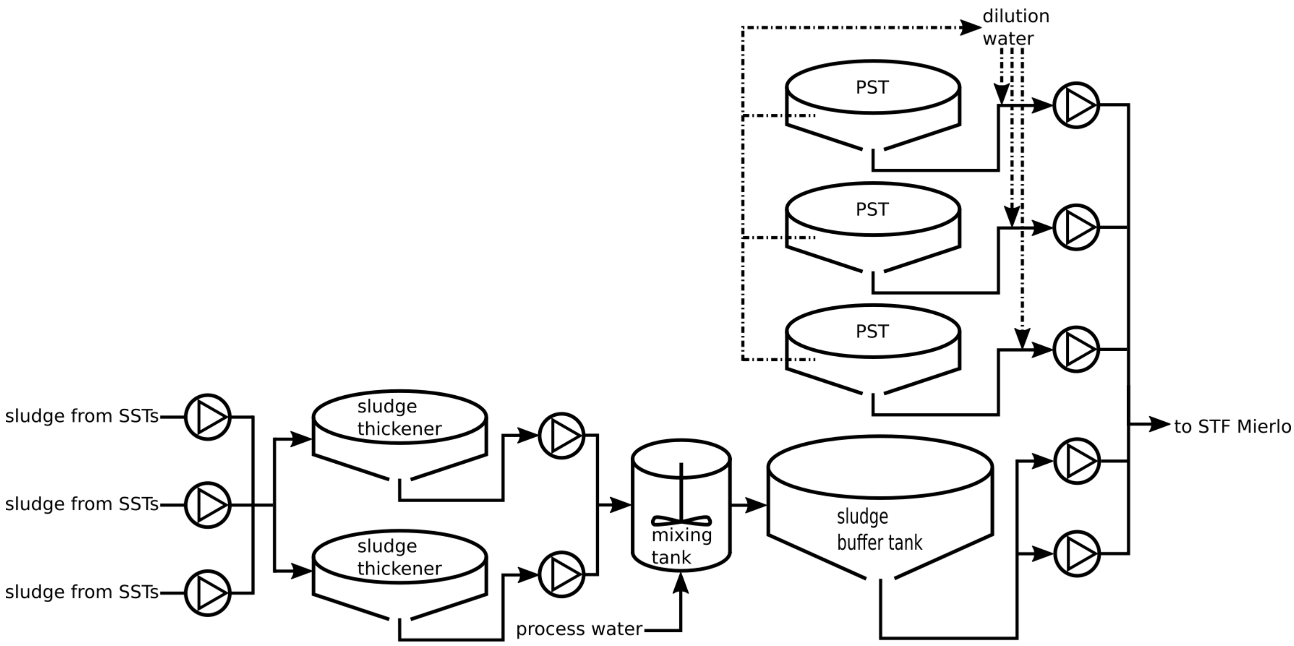


Figure 2.4: Redrawn from Telkamp et al. (2009). Simplified schematic representation of the sludge line of the Eindhoven WWTP.

2.2 Model of the wastewater treatment plant of Eindhoven

Some clarifications on the used symbols for units: In many cases, the fundamental dimensions of physical properties are used, such as in Table B.3. In that case, note the following physical properties and the abbreviations of their fundamental dimensions: physical properties: [mole mass length time] ([n M L T]). In other cases, actual units are used. In case actual units are used, L stand for liter: example of units: [gram (liter)$^{-1}$] ([g L^{-1}]).

2.2.1 Overview of the whole plant model

The Eindhoven WWTP model is implemented in the software WEST (2016 version, product of MIKE Powered by DHI, `http://www.mikepoweredbydhi.com`). Multiple versions of the model were created (Amerlinck, 2015). No written description of the version used in this thesis, created by De Mulder (2017), exists. The previous version was calibrated with data from 2013 and it is described by Amerlinck (2015). In addition, the current version was validated with data from 2013. It is infeasible to thoroughly describe the changes made by De Mulder (2017) within the scope of this thesis. Hence, only the most important differences between the current and the previous version will be described briefly.
An overview of the model as implemented in WEST, can be found in Figure 2.5. A short description of all the blocks in this figure can be found in Appendix B.2.1. It is important to note that the 3 separate lanes of the biological treatment are modelled as 1 lane, with its volume equal to the entire volume of the plant. In addition, the mixing behaviour of the ASTs is modelled by using the tanks-in-series approach: In the model, the anaerobic part is represented by 4 CSTRs in series, the anoxic part by 2, and the aerated part by 6. (Amerlinck, 2015)

2.2.2 Modelling of the hydraulics

As can be seen in Table B.2, the hydraulic behaviour of the tanks where the biological reactions occur - the anaerobic, anoxic, and aerobic tanks - is modelled with the fixed volume reactor approach. (Amerlinck, 2015)

2.2.3 Biokinetic model

The ASM2d model (Henze et al., 2000) forms the basis of the biokinetic model of the Eindhoven WWTP model (Amerlinck, 2015). An important extension is the inclusion of a particulate inorganic fraction (Wentzel et al., 2002; Amerlinck, 2015), because this results in an extra state variable, X_{Ii}, added to the standard state variables in ASM2d. X_{Ii} [M(TSS) L^{-3}] is the concentration of particulate inorganic inert material (expressed in grams total suspended solids (TSS)). In Table B.3 all state variables of the Eindhoven biokinetic submodel are described. In Table B.4 they are shown with their respective conversion factors, which illustrates their mass composition. The meaning of the state variables and their mass composition is important for the classification in the LCA part of this thesis (see Chapter 2.5.4). Note that X_{MeOH} - metal-hydroxides - and X_{MeP} - metal-phosphate - are state variables normally used for chemical P removal. This process is however modelled in another way in

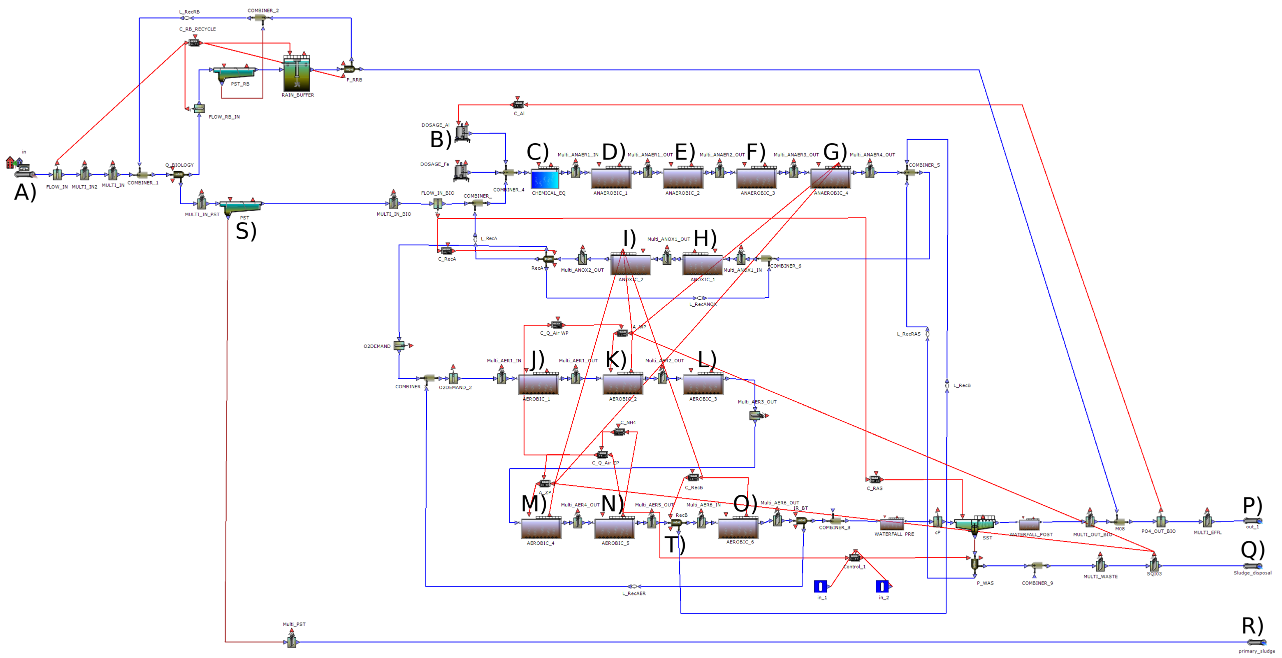


Figure 2.5: Partial layout of the Eindhoven WWTP model, showing the most important components. Furthermore, the blocks relevant for this thesis are: A) in B) DOSAGE_Al C) CHEMICAL_EQ D), E), F) and G) ANAEROBIC_1, 2, 3, and 4 respectively H) and I) ANOXIC_1 and 2 respectively J), K), L), M), N), and O) AEROBIC_1, 2, 3, 4, 5, and 6 respectively P) out_1, Q) Sludge_disposal, R) primary_sludge, S) PST, and T) RecB. (See Table B.2 for a short description of these blocks.)

the Eindhoven model (Subsection 2.2.4). These state variables were not removed from the model, but they have no functionality and can thus be ignored in the context of this thesis.
Besides, the biokinetic reaction equations are only implemented in the biological tanks (ASTs) in the whole plant model. These are reactors D) to O) in Figure 2.5. Hence, it is only there that CO_2, N_2O, and CH_4 are assumed to be formed and emitted.

2.2.4 Modelling of chemical phosphate removal

Regarding chemical P removal through precipitation of PO_4^{3-}, it is important to note that the available processes in ASM2d (Henze et al., 2000) are unused, simply because the compounds that are used for this are not dosed. Hence, the concentrations of the concerning state variables (should) remain zero. Amerlinck (2015) explains how chemical P removal is modelled. The important aspects for this thesis are the following: $Al_2(SO_4)_3$ (alum) is dosed in the block DOSAGE_Al (Figure 2.5). The amount that is dosed there, is expressed as mass of Al. The precipitation reactions only occur in the block CHEMICAL_EQ (Figure 2.5). The state variable S_{PO_4} [M(P) L^{-3}], which consists primarily out of ortho-phosphates (Table B.3), is affected by this in the following manner: The outflowing mass of S_{PO_4} is equal to the inflowing mass minus the mass that disappeared through precipitation. The precipitate has the following composition: $Al_{1.2}H_2PO_4(OH)_{2.6}$. For every calculation in this thesis, S_{PO_4} will be considered as existing only out of PO_4^{3-}. The formed precipitate, and hence its mass, is incorporated into the state variable X_{Ii} [M(TSS) L^{-3}]. X_{Ii} is the concentration of particulate inorganic inert material and due to the precipitation process, its P content varies. The mass of the formed precipitate is also added to the state variable X_{TSS} [M(TSS) L^{-3}], which is the concentration of the total suspended solids. The mass of Al that is incorporated into the precipitate is subtracted from the available $Al_2(SO_4)_3$ (whose concentration is expressed as [M(Al) L^{-3}]).

2.2.5 Influent

The used influent data is obtained through online measurements, performed in 2013, of the influent of the Eindhoven WWTP. Outliers were removed and big gaps were filled according to the methodology described by De Mulder et al. (2017). The time span used in this thesis runs from November 16 to December 8 (2013), further referred to in terms of days in the year, i.e. day 320 to 342. From day 320 to 332, normal dry weather conditions occur, with no large peaks in the influent volumetric flow rate. From day 332 on, also rain weather conditions occur, with some large peaks in the influent volumetric flow rate (Figure C.1).

2.2.6 Adaptations, settings, and other relevant model aspects as used in this thesis

All dynamic simulations in this thesis were initialized by first running a simulation for 250 days with average dry weather influent values (day 320 to 332), to drive the model to steady state. The values of the state variables obtained in this manner served as starting point for the dynamic simulations.
The simulation with dry weather conditions was performed with the influent data from day 320 tot 332. All simulations with both dry and wet weather conditions were performed with influent data from day 320 to 342. (See Section 2.3.)
WEST was set to write out the simulation results every 2 seconds and interpolate between the variable step size ODE solver output to obtain results at the specified time points. All variables used for the LCA calculations will be briefly described in Section 2.5.3. Besides, some unformatted WWTP model results were also written out to facilitate scenario analysis (Table 2.2).
The underflow of the PST (S) in Figure 2.5) was connected to a (virtual) sensor (MultiSensor, see Table B.2) in order to quantify primary sludge production.

Table 2.2: Unformatted WWTP model results used in this thesis.

Variable	Unit
Influent COD mass flow rate	[M(COD) T^{-1}]
Influent volumetric flow rate	[L^3 T^{-1}]
Influent TN mass flow rate	[M(N) T^{-1}]
Influent TP mass flow rate	[M(P) T^{-1}]
Influent TKN mass flow rate	[M(N) T^{-1}]
Volumetric flow rate generated by recirculation B pump[a]	[L^3 T^{-1}]
Influent PO_4^{3-} mass flow rate	[M(P) T^{-1}]
DO concentration in AEROBIC_4[b]	[M(O_2) L^{-3}]

[a] T) in Figure 2.5.

[b] M) in Figure 2.5.

In all MultiSensor blocks that were used to write out data, i_{N,S_I} was set to 0.033 g N (g COD)$^{-1}$ and i_{N,X_I} to 0.02 g N (g COD)$^{-1}$ (see Table B.4), in accordance with the settings in the "<Root>" (which can be viewed in WEST by clicking on the white background of the model).
As model for the SST, the Takács model (Takács et al., 1991), was used. Modelling results, related to the Takács model, for the influent data used in this thesis were calibrated and are thus realistic, despite reported shortcomings of the Takács model during rain weather conditions (Torfs, 2015).
The WWTP model delivers results for cumulative electricity usage, more specifically pumping, mixing, and aeration energy [kWh]. A "cost" block was added (not shown on any Figure for simplicity), to which various blocks that consume electricity can be connected. The cost block sums the individual energy uses. See Table 2.3 for which components were connected.

Table 2.3: Connections of blocks to the cost calculator block in the Eindhoven WWTP model. (See Table B.2 and Figure B.1 for a description of these blocks. (Cost calculator block not described or shown there.)

Calculated item in cost block	Connected item
Aeration energy [kWh]	AEROBIC_1 to 6
Mixing energy [kWh]	ANAEROBIC_1 to 4, ANOXIC_1 and 2, and AEROBIC_1 to 6
Pumping energy [kWh]	Q_BIOLOGY, PST_RB, P_RRB, DOSAGE_Al, RecA, RecB, IR_BT, SST, and P_WAS

For scenario 6. (see Section2.3), a feed-forward controller was added to control effluent PO_4^{3-} peak emissions (Figure 2.6). In the model, a feedback controller was already installed. The latter measures the effluent PO_4^{3-} concentration and alters the Al dosing flow rate (i.e. the control action). Its lower setpoint is 0.4 mg L^{-1} PO_4-P and its upper setpoint 0.7. Its minimum control action is dosing 0 m^3 d^{-1} Al solution. The added feed-forward controller measures influent PO_4^{3-} mass flow rates. For flow rates below $9 \cdot 10^5$ [g PO_4-P d^{-1}], the minimum control action of the effluent PO_4^{3-} controller is unaltered. For values equal or higher than this number, the minimum control action is set to 60 m^3 d^{-1} Al solution. The idea here is to only increase Al dosing if influent PO_4^{3-} mass flow rate peaks are detected. In addition, the lower setpoint of the effluent PO_4^{3-} concentration controller was altered from 0.4 to 0.2 mg L^{-1} PO_4-P in scenario 6. This was done for the following reason: due to the increased dosing rate at influent peak events, overall effluent PO_4^{3-} emissions were in fact higher due to a rebound effect. The intention was however to retain the overall emissions and to lower them when peak events occurred. By lowering the lower setpoint, this seemed to be achieved to some extent.
In scenario 5. (Section 2.3), it was the intention to increase overall PO_4^{3-} removal, thus not only the emission peaks. For this purpose, only the lower and upper setpoint of the effluent PO_4^{3-} concentration controller were altered. They were set to 0.2 and 0.5 mg L^{-1} PO_4-P respectively.

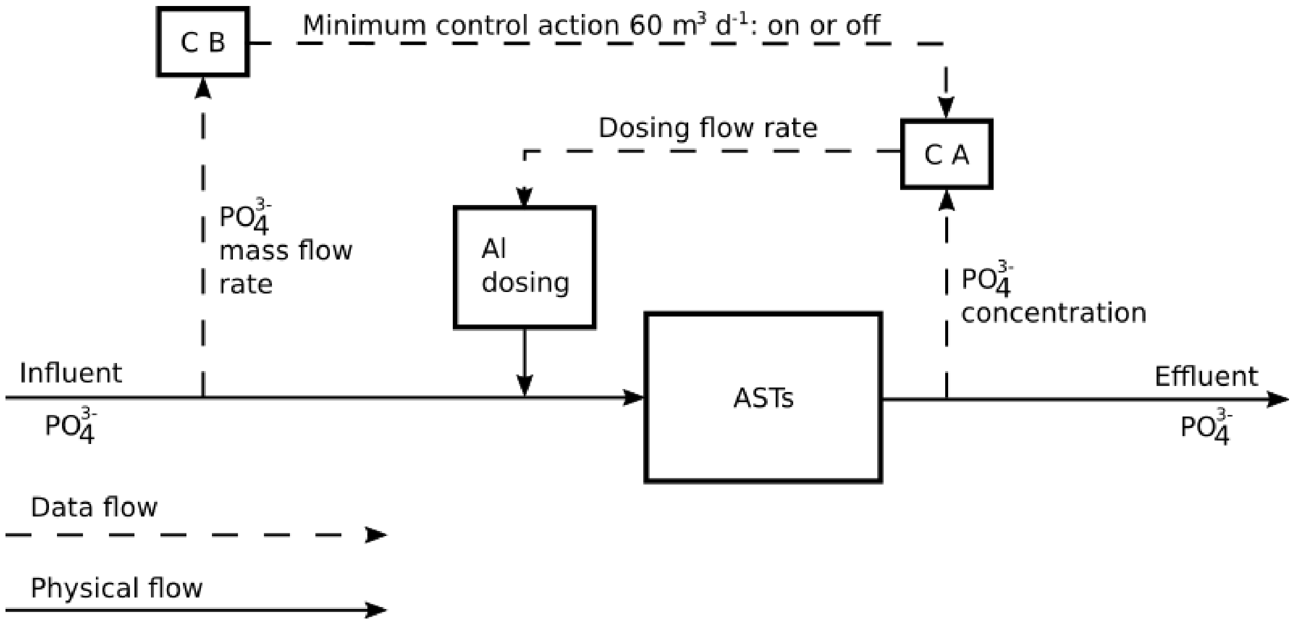


Figure 2.6: Schematic of the added feed-forward controller for scenario 6. (see Section 2.3). C A: effluent PO_4^{3-} concentration controller. It was already available in the model. C B: feed-forward controller to lower peaks in effluent PO_4^{3-} mass or mass flow rate emissions. See text for more specifications.

2.3 Scenarios

The analysed scenarios in this thesis are:

1. Steady state simulation with dry weather conditions, i.e. with average dry weather influent values (day 320 to 332). The simulation was run for 250 days. The last 21 days were used for the LCA calculations. It was verified that the system was in steady state during the used time span: all micro-organism biomass concentrations were constant in time in the used time span.

2. Steady state simulation with dry and wet weather conditions, i.e. with average influent values for the influent data containing both dry and wet weather conditions (day 320 to 342). The rest of the specifications are the same as for scenario 1.

3. Dynamic simulation with influent data only containing dry weather conditions, thus without large peaks in the influent volumetric flow rate (day 320 to 332). The whole simulation (12 days) was used for the LCA calculations.

4. Dynamic simulation with influent data containing both dry and wet weather conditions (day 320 to 342). Thus, large peaks in the influent volumetric flow rate occurred. The whole simulation (22 days) was used for the LCA calculations.

5. Similar to scenario 4, but with increased overall PO_4^{3-} removal: lowered lower and upper setpoint of the effluent PO_4^{3-} concentration controller, see Section 2.2.6.

6. Similar to scenario 4, but with a feed-forward controller added to only lower effluent PO_4^{3-} emissions peaks (see Section 2.2.6 and Figure 2.6).

7. Similar to scenario 4, but with the lower and upper setpoint of the aerobic reactor 5 (N) in Figure 2.5) TSS concentration controller changed from 3350 and 3450 to 3850 and 3950 g m^{-3} respectively. Before running a dynamic simulation, a steady state initialization with the new TSS setpoints was performed.

Note the following: It is not the intention to compare all scenarios to each other. 1 will be compared to 3, 2 to 4, and 3 to 4. Finally 4, 5, 6, and 7 will be compared to each other. In addition, the ideas for scenario 5. and 6. were developed during the interpretation of the dynamic LCA results (see Subsection 3.5.1).

2.4 Python™ scripts

A Jupyter notebook (`http://jupyter.org/`. Anaconda version 4.2.0 (64-bit) customized, `https://www.continuum.io/`) that uses the Python™ programming language (version 3.5.2, `https://www.python.org/`) was developed. This notebook is accompanied by a Python™ script containing additional functions. The notebook serves as interface between the Eindhoven WWTP model and the LCA calculations. It also performs additional conversions and calculations where needed as well as much of the LCA calculations. Some aspects of the notebook belong in the sections "Life cycle inventory analysis" (2.5.3) and "Life cycle impact assessment" (2.5.4) and can be found there. In this section, the most important concepts of the notebook will be clarified. The notebook and script can be downloaded and viewed here (although with some displaying errors): `https://github.com/TomLauriks/dynamic_WWTP_model_plus_LCA`. It is well documented and provided with clarifications for the interested reader.

2.4.1 The scripts as interface between the Eindhoven model and LCA calculations

Simulations can be performed with the Eindhoven model and results be can written out as text files (with .txt extension). These results can be read in into the notebook.

In Subsection 2.2.3 and 2.2.4, and Table B.3, many important state variables of the Eindhoven model can be found together with their units. These units all represent concentrations. In Table 2.2 it is visible that for the influent, also the volumetric flow rate is available. In fact, the volumetric flow rate going in and out of every unit in the model (Figure 2.5) - if applicable - is available. Hence, all concentrations can be converted into mass (or molar) flow rates. Since LCA calculations typically require emitted or consumed masses, these mass flow rates are converted to masses emitted or consumed in a certain time interval in the notebook. Note that the Eindhoven model provides the possibility to write out mass flow rates going in and out of units, for instance ASTs or the SST, in many cases (see for instance Table 2.2). Mostly, these are directly used for the calculations in the notebook. In the cases where mass flow rates are not available, mass flow rates going into and out of a unit are calculated by multiplying the respective volumetric flow rates and concentrations.
Emitted or consumed masses in a certain time interval, can be calculated from mass flow rates in the following manner:

$$\int_{t_1}^{t_2} \frac{dm}{dt} dt = \int_{t_1}^{t_2} dm = m(t_2) - m(t_1) \tag{2.1}$$

where m [M] is mass, and t [T] is time. This integration is approached numerically in the following manner: Let F [M T^{-1}] denote a mass flow rate, then integration occurs according to:

$$\int_{t_{start}}^{t_{\text{end}}} F dt \approx \sum_{i=1}^{N} \frac{F(t_i) + F(t_{i-1})}{2} \cdot \Delta t_i \tag{2.2}$$

where N is the number of time intervals, Δt_i, into which the integrated time span, $t \in [t_{\text{start}}, t_{\text{end}}]$, is divided. In fact, every integration of variables over time in the notebook (see further), occurs similar to this formula, thus by replacing F by the concerning variable(s).

2.4.2 Calculations of some missing aspects in the model that are relevant for the LCA calculations

Electricity consumption

As described in Subsection 2.2.6, a cumulative electricity usage of the WWTP [kWh] can be obtained from the Eindhoven model. However, the results thus obtained, gave untrustworthy outcomes. As this issue remained unresolved within the time frame of this thesis, model results for total cumulative electricity usage of the WWTP are replaced by a linear increasing range as a function of time: In 2013, the total electricity usage of the Eindhoven WWTP was 12,210,411 kWh (Blom, 2013), or 33453.18 kWh d^{-1} (which is also equal to 0.387 kWh s^{-1}). (These data do not include electricity for sludge pumping to Mierlo.) If a simulation is for instance performed for 12 days (note that every 2 seconds a data point is generated by WEST), then electricity usage is increased with 0.387 kWh s$^{-1} \cdot 2$ s $= 0.774$ kWh every 2 seconds until 33453.18 kWh d$^{-1} \cdot 12$ d $= 401,438$ kWh is reached.

Calculation of CO_2 emissions

CO_2 is not a state variable in ASM2d (Henze et al., 2000). Therefore, the production of CO_2 is calculated according to a mass balance that was composed for loss of carbon compounds - due to oxidation to CO_2 - in the biological tanks (reactors D) to O) in Figure 2.5). Furthermore, carbon compounds have the units [M(COD)] in ASM2d (See Table B.3) and the atomic composition of one of the substrates for bacterial growth, S_F, is unknown. Hence, its carbon content is unknown and the exact stoichiometry for the transformation of substrate to biomass and CO_2 cannot be obtained. Therefore, the obtained mass loss is converted to CO_2 emissions with the following conversion factor: 0.86 kg CO_2 (kg COD oxidized)$^{-1}$ (Kim et al., 2015).

Note that the biological tanks are modelled as fixed volume CSTRs. The mass balance for loss of carbon compounds in a time interval $[t_1, t_2]$ in each biological tank in the model can be constructed as follows (see also Figure 2.7):

$$\begin{aligned}
\frac{d(VC(t))}{dt} &= Q(t)C_{in}(t) - Q(t)C(t) - \frac{dm_{out}(t)}{dt} \\
dm_{out}(t) &= Q(t)C_{in}(t)dt - Q(t)C(t)dt - VdC(t) \\
\int_{t_1}^{t_2} dm_{out}(t) &= \int_{t_1}^{t_2} Q(t)C_{in}(t)dt - \int_{t_1}^{t_2} Q(t)C(t)dt - \int_{t_1}^{t_2} VdC(t) \\
m_{out}(t_2) - m_{out}(t_1) &= \int_{t_1}^{t_2} Q(t)C_{in}(t)dt - \int_{t_1}^{t_2} Q(t)C(t)dt - V(C(t_2) - C(t_1))
\end{aligned} \tag{2.3}$$

where V [L^3] is the (constant) volume of all the substances in the reactor, t [T] is time, Q [L^3 T^{-1}] is the total flow rate of all substances going in and out of the reactor, C_{in} and C [M(COD) L^{-3}] are the concentrations of degradable carbon compounds going in and out - respectively - of the reactor, and m_{out} [M(COD)] is the mass of carbon compounds oxidized and thus leaving the reactor as CO_2. Note that if a variable is dependent on time, this is explicitly shown.

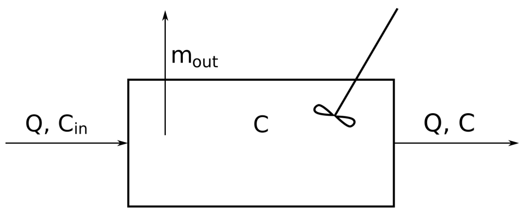


Figure 2.7: CSTR where biodegradable carbon compounds flow in and out in a flow with a total flow rate Q and with a concentration C_{in} and C [M(COD) L^{-3}] respectively. Mass loss of these compounds occurs, as they are partly oxidized to CO_2, which escapes the reactor. m_{out} represents the mass of carbon compounds that is oxidized [M(COD)].

The total mass of COD oxidized [M(COD)] in all the biological tanks in a time interval $[t_1, t_2]$ can subsequently be calculated by adding together Equation 2.3 for each individual biological reactor:

$$\begin{aligned}
\mathrm{COD}_{\mathrm{oxidized,total}} &= \sum_{i=1}^{N} (m_{out,i}(t_2) - m_{out,i}(t_1)) \\
&= \sum_{i=1}^{N} \int_{t_1}^{t_2} Q_i(t)C_{in,i}(t)dt - \sum_{i=1}^{N} \int_{t_1}^{t_2} Q_i(t)C_i(t)dt - \sum_{i=1}^{N} V_i(C_i(t_2) - C_i(t_1))
\end{aligned} \tag{2.4}$$

where N is the total number of biological tanks (reactors D) to O) in Figure 2.5).
Equation 2.4 can be simplified substantially. The terms containing the integrals represent the mass that went in or out a certain reactor in the considered time interval. In Figure 2.5 can be seen that in many cases, the mass that goes out a reactor, is equal to the mass that enters the subsequent

reactor. Hence, a lot of these terms cancel out. The following equation demonstrates which of these terms remain and hence how the total COD mass oxidized in a time interval $[t_1, t_2]$ is calculated. The conversion of COD oxidized to CO_2 emitted $[M(CO_2)]$ with the conversion factor is furthermore also demonstrated:

$$\begin{aligned}
&\mathrm{COD}_{\text{oxidized,total}} = \int_{t_1}^{t_2} Q_D(t)C_{in,D}(t)dt - \int_{t_1}^{t_2} Q_G(t)C_G(t)dt + \int_{t_1}^{t_2} Q_H(t)C_{in,H}(t)dt - \\
&\int_{t_1}^{t_2} Q_I(t)C_I(t)dt + \int_{t_1}^{t_2} Q_J(t)C_{in,J}(t)dt - \int_{t_1}^{t_2} Q_N(t)C_N(t)dt + \\
&\int_{t_1}^{t_2} Q_O(t)C_{in,O}(t)dt - \int_{t_1}^{t_2} Q_O(t)C_O(t)dt - \sum_{i=1}^{N} V_i(C_i(t_2) - C_i(t_1)) \\
&\text{total } CO_2 \text{ mass produced biology} = \mathrm{COD}_{\text{oxidized,total}} \cdot 0.86
\end{aligned} \tag{2.5}$$

N_2O and CH_4 emissions

N_2O and CH_4 emissions are not part of the Eindhoven model results and are obtained by using emission factors:

- $N_2O_{\text{emitted}} = 0.01 \cdot \mathrm{TKN}_{\text{influent}}$ [kg N_2O], where $\mathrm{TKN}_{\text{influent}}$ [kg N] is the mass of Kjeldahl N in the influent.
- $CH_{4,\text{emitted}} = 0.007 \cdot \mathrm{COD}_{\text{influent}}$ [kg CH_4], where $\mathrm{COD}_{\text{influent}}$ [kg COD] is the mass of COD in the influent.

Both factors were obtained from VROM (2008).

In addition, in the notebook it can be chosen to base the emission factor for N_2O on the total Kjehldahl nitrogen (TKN) load on the ASTs - instead of on the one in the influent - since N_2O emissions mainly originate from the activated sludge units (Kampschreur, 2010).

Taking into account the amount of P in the effluent as a result of P precipitation

P that is precipitated is incorporated into the state variable X_{Ii} (see Subsection 2.2.4). However, this P is not taken into account in the Eindhoven model total phosphorus (TP) calculation. Therefore, an approximation is used to quantify the final fate of this P.

First, the rate at which mass of P is precipitated is determined in the same way as in the model of reactor C) in Figure 2.5:

$$F_{PinX_{Ii}} = F_{S_{PO,in}} - F_{S_{PO}} \tag{2.6}$$

where $F_{PinX_{Ii}}$ [M(P) T^{-1}] is the rate at which P is precipitated and hence incorporated into X_{Ii}, $F_{S_{PO,in}}$ [M(P) T^{-1}] the mass flow rate of inorganic soluble phosphorus going into the reactor, $F_{S_{PO}}$ the mass flow rate going out the reactor.

Subsequently, $F_{PinX_{Ii}}$ is integrated to obtain the mass of P incorporated into X_{Ii} in a time interval $[t_1, t_2]$. This mass is partitioned over the effluent and sludge discharge by multiplying it with the ratio of X_{Ii} mass that went out through the effluent in the whole simulation time span and the sum of the X_{Ii} masses that went out through the effluent and the secondary sludge discharge (P) and Q) in Figure 2.5) in the whole simulation time span:

$$\text{precipitated P mass in effluent} \approx \int_{t_1}^{t_2} F_{PinX_{Ii}} dt \frac{\int_{t_{start}}^{t_{end}} F_{X_{Ii},effluent} dt}{\int_{t_{start}}^{t_{end}} F_{X_{Ii},effluent} dt + \int_{t_{start}}^{t_{end}} F_{X_{Ii},sludge} dt} \tag{2.7}$$

where $F_{X_{Ii},effluent}$ and $F_{X_{Ii},sludge}$ [M(TSS) T^{-1}] are the mass flow rates of X_{Ii} in the effluent and secondary sludge discharge respectively, and t_{start} and t_{end} are the simulation start and end time.

PO_4-P is precipitated as $AlPO_4$ and it can be argued whether or not it makes sense to incorporate this into the P emissions, since $AlPO_4$ is insoluble in water (PubChem, 2017). However, bacteria exist that can dissolve insoluble phosphates (Ayyakkannu and Chandramohan, 1971). Hence, the precipitated phosphate will be regarded as available for biota.

Approximation of the produced sludge mass

In Figure 2.4 can be seen that secondary sludge is thickened after the SSTs. However, in Figure 2.5 it can be seen that these thickeners are not present in the Eindhoven model. Hence, the mass composition (water content) of secondary sludge as needed in an LCA is probably not well simulated in the Eindhoven model. Furthermore, primary and secondary sludge are pumped through the same pipes to Mierlo. Therefore the following approximation is made: The mass flow rate of TSS is assumed to be equal to the dry matter mass flow rate of the sludge. TSS mass flow rates are added together for primary and secondary sludge. This mass of TSS is assumed to be incorporated into a suspension with 97.7 $wt\%$ water, since the average dry matter content of the Eindhoven sludge in 2013 (primary and secondary) was 2.3 $wt\%$ (Blom, 2013). Note that in the Eindhoven model, sludge mass is also quantified only based on TSS mass.

Relevant results obtainable from the Eindhoven model and the above described modifications

In Figure 2.8, a conceptual overview is given of relevant results obtainable from the Eindhoven model and the above described modifications. In the description of the system boundary (Section 2.5.1), a more detailed figure will be given that compares the description of the actual WWTP with the data that can be obtained through the model.

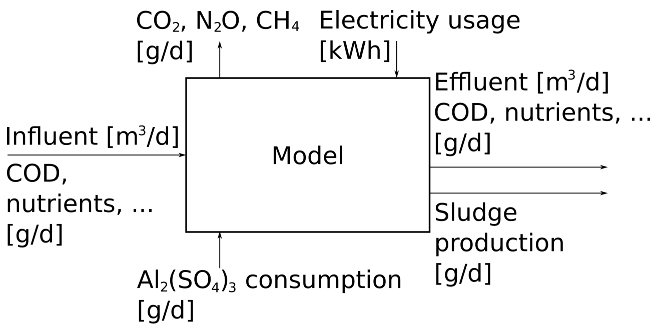


Figure 2.8: Conceptual overview of relevant results obtainable from the Eindhoven model and the modifications of its outputs described in Subsection 2.4.2

2.4.3 Calculating classic and dynamic LCA results

As can be seen in Figure 1.10 and the concerning Subsection (1.3.1), emitted masses (or used masses of resources) are converted into environmental impacts in the LCIA phase of LCA. In Subsection 2.4.1 it is described how, through integration, mass flow rates - obtainable as WWTP model output - are converted to emitted masses in a certain time interval. In the notebook, it can be chosen whether classic or dynamic LCA is performed. Both options are based on the emitted masses obtained through integration.

In classic LCA, for every impact category 1 result is obtained. This is achieved in the notebook as follows: For a certain simulation, the emitted masses of pollutants and consumed masses of resources are obtained for the whole simulation time span through integration (as also performed by Bisinella de Faria et al. (2015)). Thus, for every substance, 1 result is obtained. Through LCIA (see Section 2.5.4), these results are converted into a single outcome for the concerning impact categories. Subsequently, the value of the FU is calculated, which is also achieved by integrating the concerning variable over the whole simulation time span. For instance, if the FU is volume of influent that entered the (virtual) WWTP, the influent volumetric flow rate is integrated. (See Section 2.5.1 for more info on the available FUs.) Finally, the results for the impact categories are divided by the value of the FU. (See Figure 2.9.) Note that since electricity usage is cumulative, at the end of the simulation the total electricity usage is obtained. As FU, 1 day of WWTP operation can also be chosen (see further). In this case, the value of the FU is equal to the simulation end time minus the simulation start time.

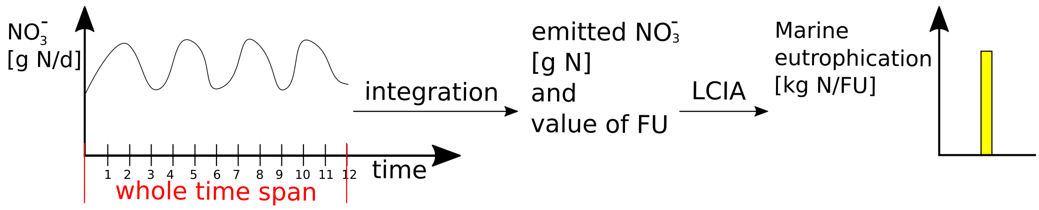


Figure 2.9: Illustration of how in the notebook WWTP model results - in this figure the mass flow rate of NO_3^- in the effluent - are converted into classic LCA results, i.e. a single score for specific impact categories.

If the option dynamic LCA is chosen in the notebook, a time series of results for every impact category is obtained. This is achieved in the notebook as follows: The simulation time span is divided into smaller time intervals. Integration occurs in each of these time intervals, thus in each of the considered time intervals the emitted/consumed masses and the value of the FU are calculated. Through LCIA, emitted and consumed masses are converted into results for the concerning impact category in each of these time intervals. The impact category result in each time interval is divided by the value of the FU in that time interval. Thus time series are obtained and every value in such a time series, is a result for the environmental impact (per FU) generated in the time interval between the previous and current point in time that is displayed on this time series (See Figure 2.10). Again electricity usage and increase of time are cumulative. For both, the values in the considered time intervals are calculated by: value at end of time interval minus value at beginning of time interval.
In this thesis, all dynamic LCA results were obtained by dividing the whole simulation time span into time intervals of (approximately) 2 minutes. (Except the last time interval, which is automatically equal to the remaining simulated time.) By choosing 2 minutes as time interval, the dynamics of emitted and consumed masses followed the dynamics of the mass flow rates that caused them very well. This effect seemed desirable for cause and effect interpretation purposes. Two minutes therefore seemed appropriate.
The thus obtained time series are also converted into histograms in the notebook (see Figure 2.11). The number of bins in these histograms is set equal to the square root of the number of observations, rounded to the nearest integer. On certain histograms, the arithmetic mean, $\bar{x}$, is displayed.

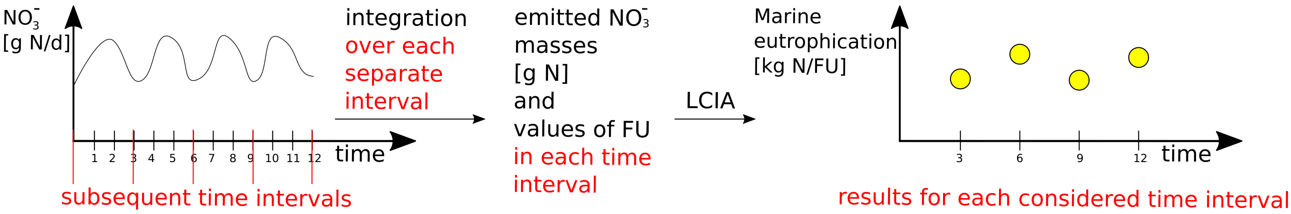


Figure 2.10: Illustration of how in the notebook WWTP model results - in this figure the mass flow rate of NO_3^- in the effluent - are converted into dynamic LCA results, i.e. a time series of results for specific impact categories.

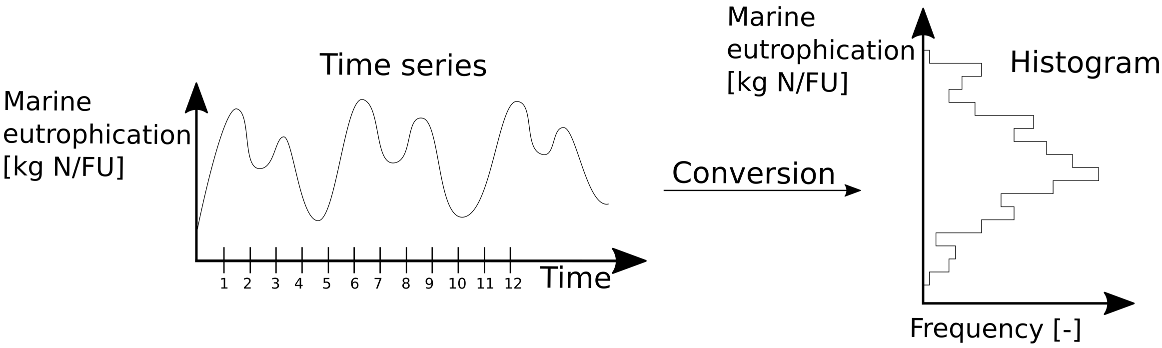


Figure 2.11: Illustration of the concept of converting time series into histograms. Note that the times series in this thesis in fact exist out of discrete results in time, while the one here is depicted as continuous.

2.5 LCA aspects

The performed LCA was based on the ISO 14040/14044 guidelines (ISO, 2006a,b). According to the ISO guidelines, an LCA consists out of 4 steps into which various aspects should be included: goal and scope definition, LCI analysis, LCIA, and life cycle interpretation. (See Subsection 1.3.1.)

2.5.1 Goal

The goal of this thesis was already elaborately stated in Section 1.6. As mentioned, the main goal is to incorporate the dynamic aspect of WWTP modelling results into the LCA results and to analyse if this is actually useful. Thus, the main goal is not to have the best data quality and most complete inventory.

Therefore, the scenario analysis results should be perceived as indications for future research, rather than strong arguments for decision making.

2.5.2 Scope definition

A description of the analysed scenarios was already given in Section 2.3.

System boundaries

The system boundaries were the same for all scenarios. They don not include the sewer system or any aspect related to the WWTP infrastructure, since these are considered as the same for all scenarios. The foreground system consists of emissions of the GHGs CO_2, N_2O, and CH_4, effluent emissions, $Al_2(SO_4)_3$ dosing, sludge mass generation, and operational electricity usage. The background system is composed of transportation, electricity production, $Al_2(SO_4)_3$ powder production, and sludge treatment. The influent is considered as a waste product and no impact related to its generation is attributed to the WWTP (ISO, 2006b), for instance the extraction of fresh water from the natural environment. The latter is debatable, since the ReCiPe methode does not take polluting water into account in the impact category water depletion (WD). It would thus make more sense to close the water mass balance of the product system and calculate the actual water use, but due to lack of data this was not possible.

The system boundaries are visualized in Figure 2.12. This figure also gives an overview of some important aspects of the actual WWTP that should certainly be considered, which data were retrieved from the WWTP model, which data are missing, and which data were calculated from the WWTP model output but with assumptions or supplemented with additional data. Important remarks about the figure: Data related to electricity consumption is depicted as if it was provided by the model. However, data about electricity usage - except for sludge pumping to the sludge drying facility - was retrieved from an environmental report (see Subsection 2.4.1), because the model output for electricity usage gave untrustworthy results. It seemed however more interesting for future research to already compare the description of the most important power consumers of the actual WWTP to the data provided by the model, in case the electricity usage modelling would work correctly. With mixing/flow generating energy is meant the energy used by the flow generating propellers (Section 2.1.1). The fact that the propellers provide both flow and mixing, is not explicitly modelled. However, the carrousel behaviour of the ASTs is taken into consideration in the model (Amerlinck, 2015), which means that the flow behaviour is mimicked and thus generated (by the pumps, which was visually checked). It is therefore assumed that mixing, pumping, and “flow generating energy” are incorporated into the energy modelling results in a realistic manner.

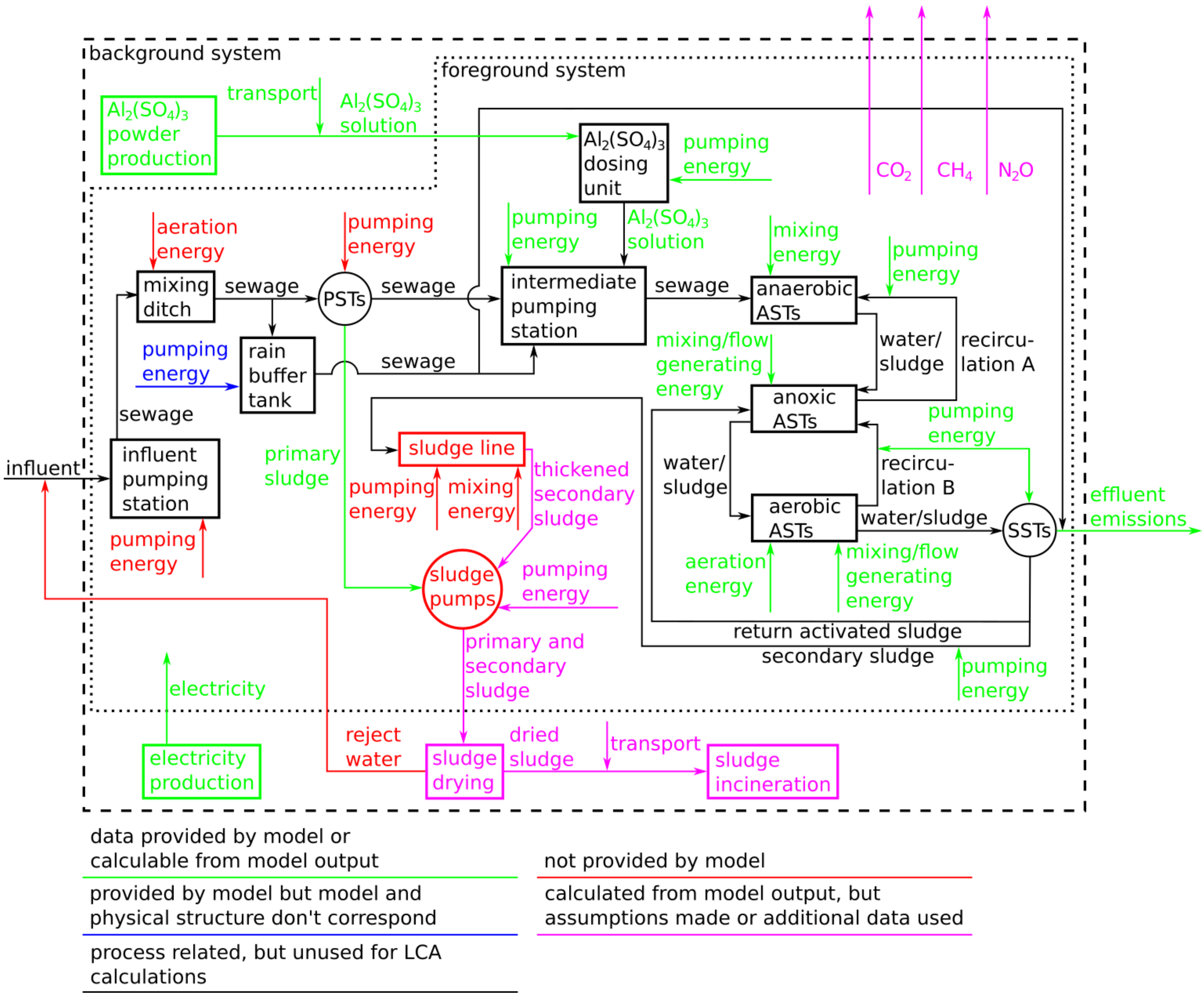


Figure 2.12: Schematic overview of the foreground and background system of all scenarios in this thesis. An overview is also given of data provided by or calculable from the model output (green), missing data (red), data of which the quality needs to be checked (blue, the RBT in the real WWTP is filled with 1 pumping system, but it is modelled with 3 pumping systems), and data of which the quality needs improvement or serious improvement (purple). Note that data related to electricity consumption is depicted as if it was provided by the model. However, data about electricity usage - except for sludge pumping to the sludge drying facility - was retrieved from an environmental report (see Subsection 2.4.1).

Available functional units (FUs)

In the notebook, a couple of FUs can be chosen: 1) no scaling, 2) 1 m^3 influent, 3) 1 kg COD in the influent, 4) 1 kg TP in the influent, 5) 1 kg total nitrogen (TN) in the influent, 6) 1 kmol TN + TP in the influent, and 7) a day of WWTP operation. Thus, for option 2) to 7), the environmental impacts are divided by the value of the concerning variable in the considered time interval(s). For option 1), absolute impacts are calculated in the considered time interval(s). The FUs mass of nutrients or COD removed could also be chosen and are probably more relevant but are not straightforward to apply and/or calculate from the WWTP model output. Next to the classic function of the FU, it is the intention of the provided FUs to analyse their influence on the LCA results.

2.5.3 Life cycle inventory analysis

Since the classification and characterization have been performed to a substantial extent by the author himself (see Subsection 2.5.4), it has to be noted that determining the relevance of LCI data was mainly based on analysing for which of the emissions - for which data was available - characterization factors exist in the ReCiPe LCIA method.
It also has to be noted that this is - partially - not a “classic” LCA. In case a “dynamic” LCA is performed, for every variable in Table 2.4 - the LCI - a time series is obtained. Even for the shortest simulation, these are composed of 8641 data points. Therefore, only an LCI of the 7 scenarios will be given for a classic LCA. In addition, only the LCI for the FU a day WWTP operation will be given. Since the values of the used FUs are available in this document, LCIs related to other FUs could be calculated from the available information. Besides, the interested reader could reproduce/extract more information from the notebook if needed. It can be downloaded and viewed here (although with some displaying errors): `https://github.com/TomLauriks/dynamic_WWTP_model_plus_LCA`.
In addition, all conversions, units, and calculations are thoroughly described in the notebook. Therefore, the description of conversions and calculations will be kept as brief as possible in this section.

Table 2.4: LCI - for a classic LCA (see Subsection 2.4.3) - of the 7 analysed scenarios: 1. steady state (SS) dry weather, 2. SS dry and wet weather, 3. dynamic (dyn) dry weather, 4. dyn dry and wet weather, 5. lower maximum setpoint for the effluent PO_4^{3-} concentration controller (dyn), 6. feed-forward controller for reduction of effluent PO_4^{3-} mass flow rate peaks (dyn), and increased TSS concentration in the biological reactors (dyn). The FU is day WWTP operation in all cases in this table. AcOH stands for acetic acid.

Scenario	1	2	3	4	5	6	7
	SS dry	SS dry+wet	dyn dry	dyn dry+wet	dyn PO_4^{3-} setpoint	dyn PO_4^{3-} peaks	dyn TSS
Inputs through influent							
Influent volume [m^3]	1.08e5	1.26e5	1.08e5	1.26e5	1.26e5	1.26e5	1.26e5
COD [kg COD]	6.42e4	6.76e4	6.42e4	6.76e4	6.76e4	6.76e4	6.76e4
TN [kg N]	6.21e3	6.60e3	6.21e3	6.60e3	6.60e3	6.60e3	6.60e3
TP [kg P]	1.24e3	1.32e3	1.24e3	1.32e3	1.32e3	1.32e3	1.32e3
Effluent emissions							
PO_4^{3-} [kg PO_4^{3-}]	2.16e2	2.37e2	2.79e2	2.97e2	2.37e2	2.67e2	2.93e2
non-PO_4-P [kg P]	1.19e1	1.45e1	1.24e1	1.61e1	1.71e1	1.70e1	1.74e1
NO_3^- [kg NO_3^-]	2.35e3	3.25e3	2.62e3	3.75e3	3.95e3	3.80e3	3.46e3
non-NO_3-N [kg N]	2.60e2	2.90e2	2.82e2	4.10e2	5.40e2	5.21e2	3.93e2
AcOH [kg AcOH]	3.14	3.45	4.00	7.49	1.32e2	1.08e2	9.18
water [kg water]	9.86e7	1.15e8	9.92e7	1.16e8	1.16e8	1.16e8	1.16e8
Greenhouse gases							
Biogenic CO_2 [kg CO_2]	1.11e4	1.16e4	1.11e4	1.16e4	1.16e4	1.16e4	1.19e4
Fossil CO_2 [kg CO_2]	1.61e3	1.68e3	1.60e3	1.67e3	1.67e3	1.67e3	1.71e3
Biogenic CH_4[a] [kg CH_4]	4.02e2	4.24e2	4.02e2	4.24e2	4.24e2	4.24e2	4.24e2
Fossil CH_4[b] [kg CH_4]	4.72e1	4.97e1	4.72e1	4.97e1	4.97e1	4.97e1	4.97e1
N_2O [kg N_2O]	6.21e1	6.60e1	6.21e1	6.60e1	6.60e1	6.60e1	6.60e1
Electricity consumption							
Total[c] [kWh]	3.35e4	3.35e4	3.35e4	3.35e4	3.35e4	3.35e4	3.35e4
Chemical dosing							
$Al_2(SO_4)_3$ powder[d] [kg $Al_2(SO_4)_3$]	5.25e3	5.59e3	5.72e3	5.98e3	7.55e3	6.41e3	6.17e3
Transport [tkm]	1.52e3	1.62e3	1.65e3	1.73e3	2.18e3	1.85e3	1.79e3

Continued on next page

Table 2.4 – continued from previous page

Scenario	1	2	3	4	5	6	7
	SS dry	SS dry+wet	dyn dry	dyn dry+wet	dyn PO_4^{3-} setpoint	dyn PO_4^{3-} peaks	dyn TSS
Sludge treatment							
Waste sludge [kg sludge]	1.25e6	1.41e6	1.06e6	1.21e6	1.21e6	1.21e6	1.35e6
Sludge pumping electricity[e] [kWh]	4.23e2	4.76e2	3.59e2	4.11e2	4.11e2	4.11e2	4.58e2
Transport [tkm]	1.25e4	1.41e4	1.06e4	1.21e4	1.21e4	1.21e4	1.35e4
Incinerated sludge [kg sludge]	1.06e5	1.20e5	9.03e4	1.03e5	1.03e5	1.03e5	1.15e5

[a] Originating from biogenic carbon sources.

[b] Originating from fossil carbon sources.

[c] With total electricity usage is meant the total electricity for pumping, mixing, and aeration as mentioned in Table 2.3. (Data however obtained as described in Subsection 2.4.2.) This excludes the pumping electricity for sludge treatment.

[d] Mass of $Al_2(SO_4)_3$ powder was used to calculate impacts of production. Mass of $Al_2(SO_4)_3$ solution (not explicitly shown, but calculable from the data in Table 2.1) was used to calculate amount of transport [tkm].

[e] Not included in "total electricity consumption".

Some clarifications on the foreground system data will now follow. In Table B.3 and B.4, the meaning, units, and mass compositions of the biokinetic submodel state variables can be found. In addition, by adding virtual sensors (MultiSensor in Table B.2) at any place in the model, the volumetric flow rate and concentrations of COD [M(COD) L^{-3}], TP [M(P) L^{-3}], and TKN [M(N) L^{-3}] can be obtained. Quantification of effluent emissions will now be clarified. S_{PO_4} [M(P)] was assumed to consist entirely out of PO_4^{3-}. Its mass was added together with the estimated $AlPO_4$ mass [M(P)] in the effluent due to P precipitation (Subsection 2.4.2). Units were converted from [M(P)] to [M(PO_4^{3-})] by applying molar masses. To obtain non-PO_4-P, the mass of S_{PO_4} [M(P)] was subtracted from the TP mass [M(P)]. S_{NO_3} [M(N)] was assumed to consist entirely out of NO_3^-. Its unit was converted to [M(NO_3^-)]. Non-NO_3-N [M(N)] was in fact TKN [M(N)]. It was verified that in this manner, all N was indeed quantified. S_A [M(COD)] was assumed to consist entirely out of acetic acid. Its unit was converted to [M(acetic acid)] by applying the stoichiometric relations from the following equation: $CH_3COOH + 2O_2 \longrightarrow 2CO_2 + 2H_2O$. To quantify water, it was assumed that the volume of the effluent was equal to the volume of effluent water, which is also the way this is calculated in the WWTP model.

Data quality of effluent emissions is good, since the WWTP model is in fact a calibrated model. It should however be noted that modelling results are never perfectly accurate (Section 1.5).
Important aspects of the GHG emission quantifications are the following: The calculated CO_2 emissions were divided into fossil and biogenic emissions. From Tseng et al. (2016) was derived that a reasonable number for the fraction of fossil carbon in the activated sludge processes off-gases is 0.126. Biogenic CO_2 emissions were not taken into account in the impact category climate change (CC), in accordance with (IPCC, 2006) guidelines. Data quality on CO_2 emissions is estimated to be moderate: it is based on a mass balance that gave results which seemed to be correct (see Section B.3.1). However, a conversion factor retrieved from the literature was still needed to convert mass of COD oxidized to mass of CO_2 formed. CH_4 emissions were also divided into fossil and biogenic emissions, since ReCiPe distinguishes both (see further). After taking the fraction of industrial wastewater in the 2013 Eindhoven influent (Blom, 2013) into consideration and careful analysis of data of (Tseng et al., 2016) and Law et al. (2013), a fraction of 0.105 of the CH_4 emissions that originates from fossil carbon sources seemed a reasonable number. In all scenarios, the emission factor for N_2O was based on the TKN in the influent. Data quality of CH_4 and N_2O emissions is very bad. From Foley et al. (2011) can be deduced that a generic N_2O emission factor is certainly inadequate and that a generic CH_4 emission factor is probably inadequate.
The method of calculating electricity consumption was already explained (Subsection 2.4.2). Note that total electricity consumption in Table 2.4 does not include the electricity required for sludge pumping to Mierlo. The data quality is good, however total electricity consumption does not show dynamic behaviour.
Regarding chemical dosing (see also Subsection 2.2.4), the data quality of dosed $Al_2(SO_4)_3$ is good. Unit conversion from [M(Al)] to [M($Al_2(SO_4)_3$)] was applied. The latter mass was used to quantify the impacts of the background process $Al_2(SO_4)_3$ powder production (see further). Mass of $Al_2(SO_4)_3$ was converted to mass of $Al_2(SO_4)_3$ solution with the data in Table 2.1 to calculate $Al_2(SO_4)_3$ transport. The $Al_2(SO_4)_3$ solution is transported 55 km, which is derived from Hadjimichael et al. (2016). Water use as a result of buying and dosing $Al_2(SO_4)_3$ solution, was not attributed to the Eindhoven WWTP, since this is in fact a waste product and the Eindhoven WWTP would probably use effluent water to dissolve $Al_2(SO_4)_3$ powder if the latter would be purchased instead of the $Al_2(SO_4)_3$ solution waste product.
Finally, important aspects of sludge treatment are the following: Calculating waste sludge mass was already described in Subsection 2.4.2. The data quality on the dry matter mass is good. Calculation of the water content is probably based on a good approximation. Data was obtained from the Eindhoven WWTP about sludge pumping to Mierlo. The data contained the current usage [A] of a sludge pump and the volumetric flow rate of sludge, in time intervals of 1 minute for approximately 5 days and 7 hours (data from 2017). Some values of the data were missing. Missing data were replaced by values

of previous time points, since the data did not vary much. The current usage was multiplied with 330 V to obtain the power usage. Both power usage and flow rate were numerically integrated over the whole time span to calculate total volume of sludge pumped and energy used. A density of 1 kg L^{-1} was assumed for the sludge. The total energy usage was divided by the total pumped sludge mass to obtain an estimate for kWh (kg sludge pumped)$^{-1}$: 3.39e-04 kWh (kg sludge)$^{-1}$ (see Appendix 1 of the notebook for actual calculations). This number was multiplied with the waste sludge mass to obtain an estimate for pumping energy. This data quality could probably be improved. As background processes (see further), a process for sludge drying and for sludge incineration were used. The drying process dries sludge from a dry matter content of 5 $wt\%$ up to 92 $wt\%$. Thus, per kg dried sludge 0.9456 kg water is removed. The incineration process incinerates sludge with 73 $wt\%$ dry matter. Thus, for drying 97.7 $wt\%$ dry matter sludge to 73 $wt\%$, per kg sludge 0.9148 kg water is removed. It was assumed that the environmental impacts of the drying process could be scaled by the amount of water removed. Thus, to calculate the amount of sludge to be treated by the drying process, the following conversion factor was used: $\frac{\text{kg sludge background process}}{0.9456\text{kg water}} \frac{0.9148\text{kg water}}{\text{kg WWTP sludge}} = 0.9674 \frac{\text{kg sludge background process}}{\text{kg WWTP sludge}}$. The info on the drying process does not mention that treatment of reject water is included. Thus, the fact that the Eindhoven influent data also contains the reject water from Mierlo can be left unmodified. The background incineration process incinerates sludge with 73 $wt\%$ water. Thus, to calculate the amount of sludge that is to be incinerated out of the 97.7 $wt\%$ water sludge exiting the WWTP, the following conversion factor was used: $\frac{0.08518 \text{ kg } 73\ wt\% \text{ water sludge}}{\text{kg } 97.7\ wt\% \text{ water sludge}}$. Moreover, in reality, dewatered sludge at Mierlo is transported to the SIF at Moerdijk (Blom, 2013), which is 100 km from Mierlo. The SIF at Moerdijk receives the slugde with a dry matter content of 23 $wt\%$ (Sijstermans, 2016). Thus for every kg 97.7 $wt\%$ water sludge, only 0.1 kg 77 $wt\%$ water sludge is actually transported.
A concluding remark is at its place: As mentioned, the LCA results in the notebook are calculated and then divided by the value of the FU, due to the manner in which the notebook was constructed. This is justified, since all LCA calculations are linear. To be able to extract LCI data as shown in Table 2.4, in the notebook Appendix 2 was added. There, the values of the concerning variables are divided by the value of the FU.

Data for the processes of the background system were retrieved from the database ecoinvent 3 - allocation, default (`http://www.ecoinvent.org/`). The used processes are listed in Table 2.5. The nature of the background processes for production of $Al_2(SO_4)_3$ powder production, sludge drying, and sludge incineration does not correspond well with the situation in reality. It was unrealistic to incorporate the construction of a thorough LCI into the time frame of this thesis and at the same time investigate the usefulness of dynamic LCA. Therefore, the most adequate available processes in ecoinvent were chosen. Transport of the $Al_2(SO_4)_3$ was assumed to happen with a lorry. Transport of sludge from Mierlo to Moerdijk indeed happens with a lorry (Afman and Korving, 2013).

Table 2.5: Background processes, retrieved from the ecoinvent database (version 3 - allocation, default), used in this thesis.

Aluminium sulfate, powder {RER}| production
Electricity, medium voltage {NL}| market for
Transport, freight, lorry 16-32 metric ton, EURO6 {RER}| transport, freight, lorry 16-32 metric ton, EURO6
Raw sewage sludge {CH}| drying, sewage sludge
Raw sewage sludge {CH}| treatment of, municipal incineration with fly ash extraction

2.5.4 Life cycle impact assessment

For LCIA, the ReCiPe Midpoint and Endpoint (H) ((Goedkoop et al., 2013), `http://www.lcia-recipe.net/`), version 1.12, method was chosen. For the reason of this choice, see Subsection 1.4.1. In addition, as also mentioned in that subsection, the ReCiPe midpoint and endpoint models are developed to serve within the same framework and only then consistency between them can be ensured. Since using both midpoint and endpoint insights is useful - as explained in Subsection 1.3.1 - this is an additional argument for choosing the ReCiPe method. The (H) stands for hierarchical, and this ReCiPe version was chosen because it is based on scientific consensus in many of the choices regarding its modelling aspects (JRC-IES, 2011).
All ReCiPe impact categories - 18 midpoint and 3 endpoint - are calculated by the notebook and will be included into results and discussion (to the extent where they are relevant).

The ReCiPe characterization factors were exported from the SimaPro software (version 8.2.3.0 `https://simapro.com`). These factors were applied to characterize the impact of direct WWTP emissions (which are, amongst others, listed in Table 2.4). The matrix that resulted from the classification performed by the author and that is used for the characterization can be found in Table B.5, in case of the midpoint impact categories, and in Table B.7, in case of the endpoint categories. Clarification of all impact category units and their abbreviations used in this thesis can be found in the same section (B.4.1). Note the following about endpoint characterization: Endpoint characterization factors were used to calculate LCIA results for 16 of the 18 midpoint categories. These 16 impact categories contribute to the 3 ReCiPe endpoint impact categories. To calculate the actual endpoint LCIA results, the results of the contributing midpoint categories were added together.

Impacts for background processes (Table 2.5) are quantified in the notebook as follows: Impacts for the concerning processes were calculated with the SimaPro software. This was performed for production of 1 kg $Al_2(SO_4)_3$ powder, 1 kWh electricity, performance of 1 ton.km (tkm) transport, drying of 1 kg sludge, and incineration of 1 kg sludge. These impacts are multiplied by the LCI values of the respective items (see Table 2.4 and Subsection 2.5.3). These results are added together with the results obtained through the characterization factors to obtain total LCIA results. For contribution analysis, the individual results of sludge treatment, chemical dosing, electricity consumption (not including sludge pumping to Mierlo), and effluent plus GHGs emissions (not including biogenic CO_2 emissions) are also plotted on various resulting figures. See Table 2.4 for what is included in these aspects.

CHAPTER 3

Results and discussion

3.1 Introduction

For the sake of clarity, if time series are shown with flow rates [M T^{-1}] or [L^3 T^{-1}], then these are a function of time. If time series of emitted or consumed masses [M] or LCIA results (for units, see Subsection B.4.1) are shown, then every data point is a result for the interval between the concerning and the previous point in time.

The results will be discussed according to the following topics:

A. Discussion of the consequences of steady state versus dynamic WWTP modelling on LCA results.

B. What to use for decision making, a "classic" LCA result - i.e. a single score per FU - or an average "dynamic" result - i.e. the average of the time series of LCA results (where each individual data point is a result expressed per respective value of the FU).

C. Selecting relevant midpoint impact categories.

D. Discussion of how dynamic LCA is a valuable addition to classic LCA.

E. The functional unit in dynamic LCA and its influence on classic LCA.

F. A (modest) scenario analysis.

One of the goals of this thesis is to investigate whether or not dynamic LCA can help to select measures to be taken to improve the current environmental aspects of the Eindhoven WWTP. The considerations that led to the selection of scenarios 5. and 6. (see Section 2.3) are mainly explained in Subsection 3.5.1.

It will not be possible to display every result that can be generated with the notebook. Moreover, additional scenarios could be generated. The interested reader is again referred to the notebook for more information. It can be downloaded and viewed here (although with some displaying errors): `https://github.com/TomLauriks/dynamic_WWTP_model_plus_LCA`. (Some of the data sets needed for scenario generation could not be uploaded there due to copyright issues.)

Besides, plots of various variables are available in Appendix C.1 for scenarios 3. and 4. These plots are the WWTP model results listed in Table 2.2 and some intermediate results, i.e. emitted and consumed masses. These plots will be used to search for the causes of the impacts as calculated by the LCIA.

3.2 Steady state vs dynamic WWTP modelling for LCA

In this section, "classic" LCA results will be used, because it will be shown in the following sections that "dynamic" LCA is not very useful for scenario comparison.

In Figure 3.1, a comparison of LCIA results of scenarios 1. (steady state simulation with dry weather conditions) and 3. (dynamic simulation with dry weather conditions) is shown. These results were obtained after application of the FU a day WWTP operation. It can be seen that for exactly the same conditions, a dynamic and a steady state simulation lead to different midpoint results. It is not so that one of the 2 outcomes is consequently worse in terms of generated environmental impacts. Steady state is most of the times worse, but also sometimes better. This is true, even in the case of only dry weather, where the dynamic influent behaviour is less variable than the case of dry and wet weather (no large peaks in the influent volumetric flow rate and influent pollutant mass flow rates occur, see Figure C.1). The same result occurred in the case of dry and wet weather (result not shown). This is true while in both cases (dynamic vs steady state) the total volume, COD, TN, and TP mass in the influent per FU are exactly the same (see Table 2.4). In Appendix C.2 a mathematical deduction can be found that shows that the latter is always true.
It can be seen in Figure 3.1 that in the case of endpoint results, steady state is consequently worse. However, in Section 3.4.1 will be shown that climate change and fossil depletion contribute approximately 70 % to the endpoint results during the whole simulation time span (in case of a dynamic simulation and the same FU as in this section). In addition, it can be seen on Figure 3.1 that steady state scores worse on climate change and fossil depletion, which explains why it is consequently worse when considering endpoint results. This is of course not always true. Hence, the midpoint results

clearly demonstrate that using steady state or dynamic simulations can lead to remarkably different results - worse for some impact categories and better for other - for one and the same scenario. The fact that steady state and dynamic simulations can lead to different results is in accordance with observations of Bisinella de Faria et al. (2015) and Guo et al. (2012).

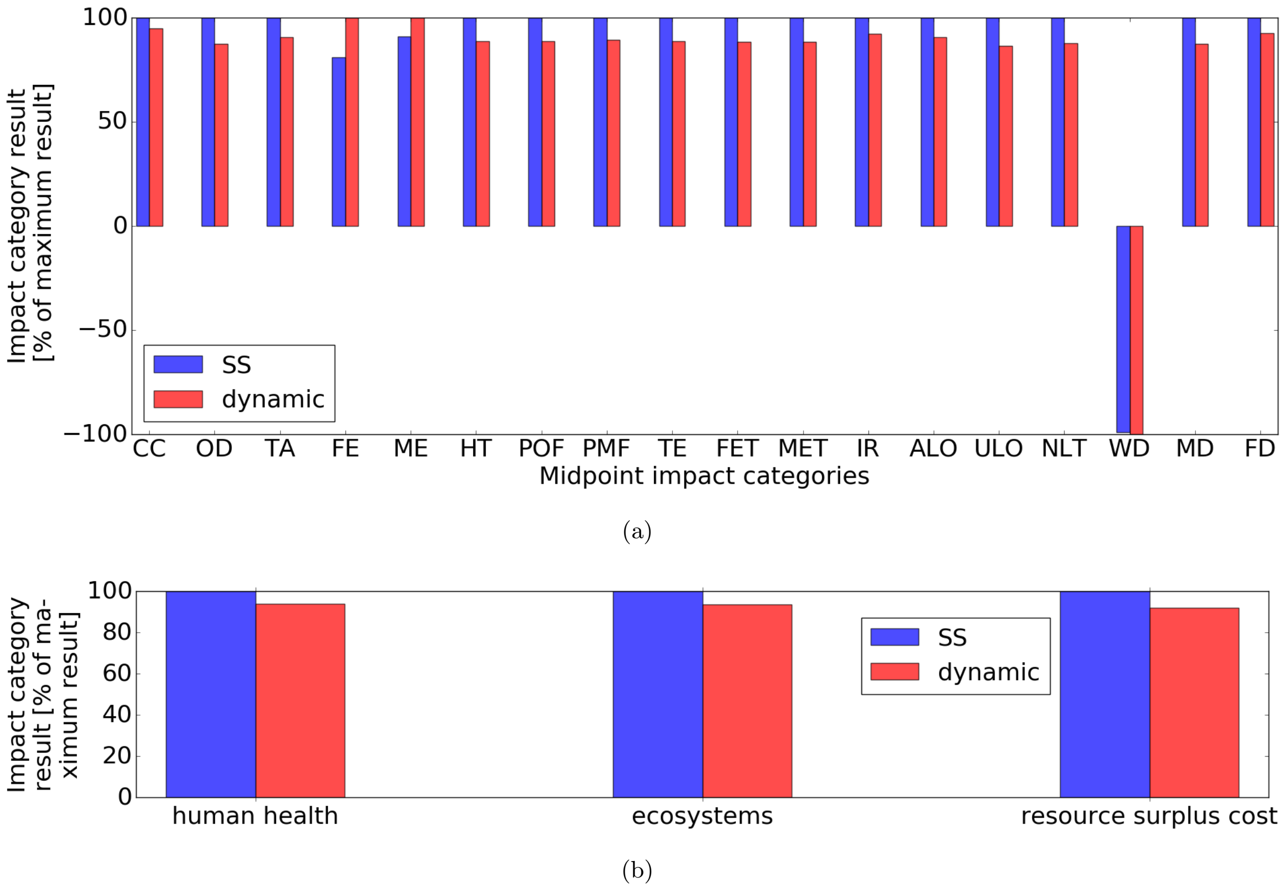


Figure 3.1: LCIA results for a classic LCA with the FU a day WWTP operation. (a) Midpoint impact categories. (b) Endpoint impact categories. Compared scenarios: 1. steady state (SS) simulation with dry weather conditions and 3. dynamic simulation with dry weather conditions. See Table B.6 for impact category abbreviations (or the abbreviations section.)

The cause of this can probably be found in the fact that the WWTP model contains non-linear relations, the ODE system of the biokinetic model is for instance not linear (Henze et al., 2000). Thus, it is likely that performing a simulation with average influent values does not result in total emissions that are the same as in a case where varying influent data - however on average exactly the same -

are used.
The fact that water depletion (which only takes into account the water discharged through the effluent) is the category where both show the least difference is an additional indication for this conclusion. Water does not participate in any of the biokinetic reactions (see notebook). It can only leave the system via the effluent and waste sludge. From Table 2.4 can be calculated that less than 1.2 % of the influent water left the system via sludge wastage in both cases. Furthermore, from Table 2.4 and Table 2.1 it can be calculated that $Al_2(SO_4)_3$ dosing introduced less than 0.3 ‰ of the total ingoing water mass in both cases. Thus, non-linear behaviour of water mass discharged through the effluent as a function of influent water mass is negligible.

These are strong arguments to use dynamic simulations. However, it should be taken into account that relative average deviations from measurements for dynamic simulations are in general larger than for steady state simulations (Section 1.5). It would therefore be good to check, in the future, how an LCA based on both steady state and dynamic simulations compares to an LCA based on actual measurements.

3.3 Classic vs average dynamic LCA results

In "classic" LCA, 1 result for every impact category - per total value of the FU - is obtained, see for example Figure 3.1. In "dynamic" LCA, as performed in this thesis, a time series of LCA results - each individual result expressed relative to the value of the FU in the concerning time interval - for every impact category is obtained, see for example Figure 3.2. From the latter figure it is clear that these results cannot directly be used for decision making in LCA, since it would be impossible to accurately distinguish which scenario has a greater impact for a certain impact category.

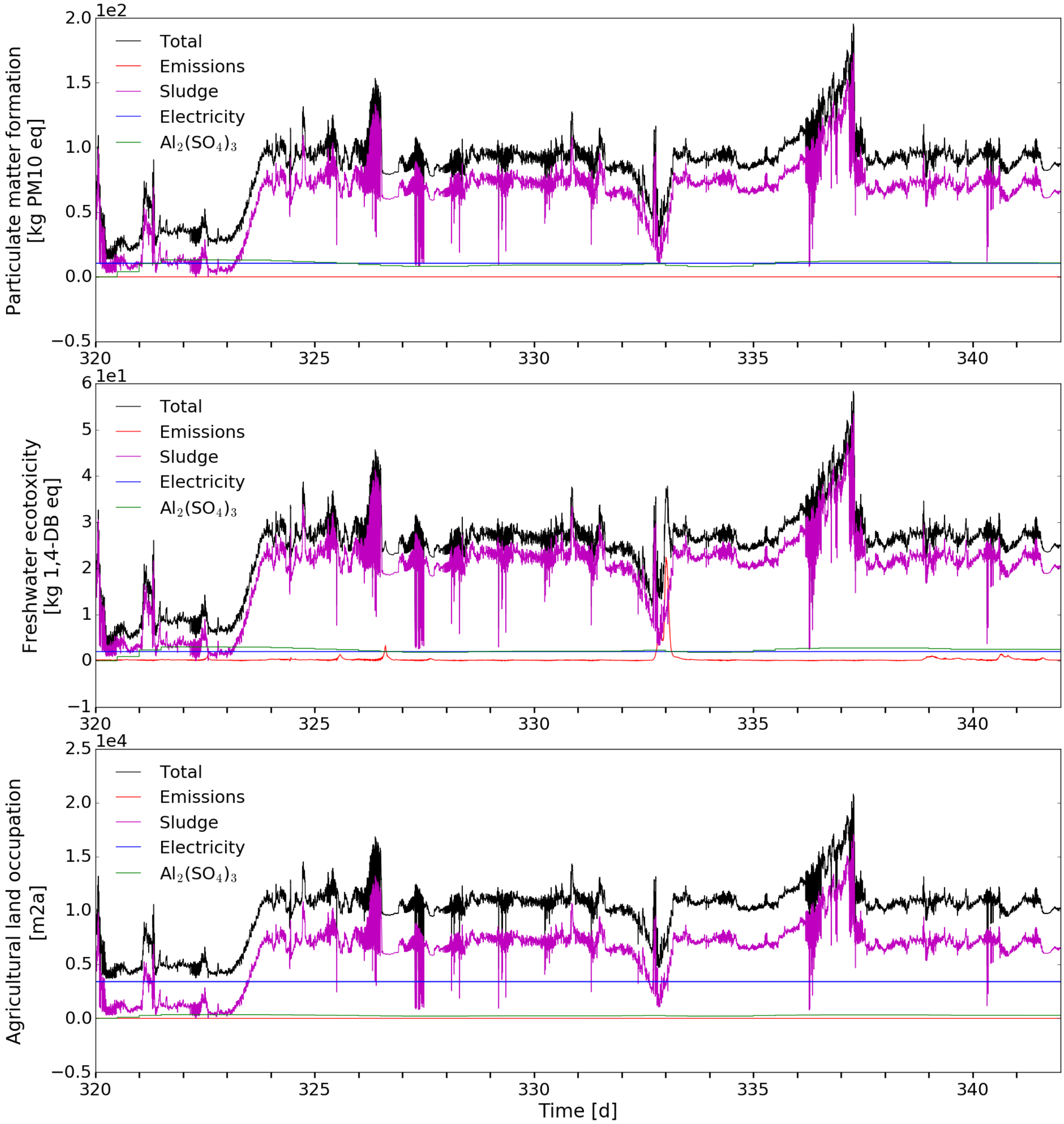


Figure 3.2: Time series of LCIA midpoint results as obtained through the described methodology (Section 2.4.3). Scenario: 4., FU: a day operation. For contribution analysis, total impacts are divided into 4 categories. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions. On the y axis, the concerning midpoint impact category can be seen.

Average results (arithmetic mean) of the time series can be calculated, which could indeed easily be compared. The time series of both mid- and endpoint impact categories are in the notebook also converted into histograms. For the total scores - thus not contributions as described in Figure 3.7 - average results are displayed on the histograms, see Figure 3.3. The average of these time series can be equal to the total result obtained through classic LCA, but this is not necessarily true. This is proven in Appendix C.3. In addition, a simple mathematical deduction is also made there, which proves that both are equal if the value of the applied FU is the same for all observations - thus at all time instants - in the dynamic case. It also indicates that a very varying value of the applied FU at the considered time instants will lead to different results. The extent of these differences will now be investigated.

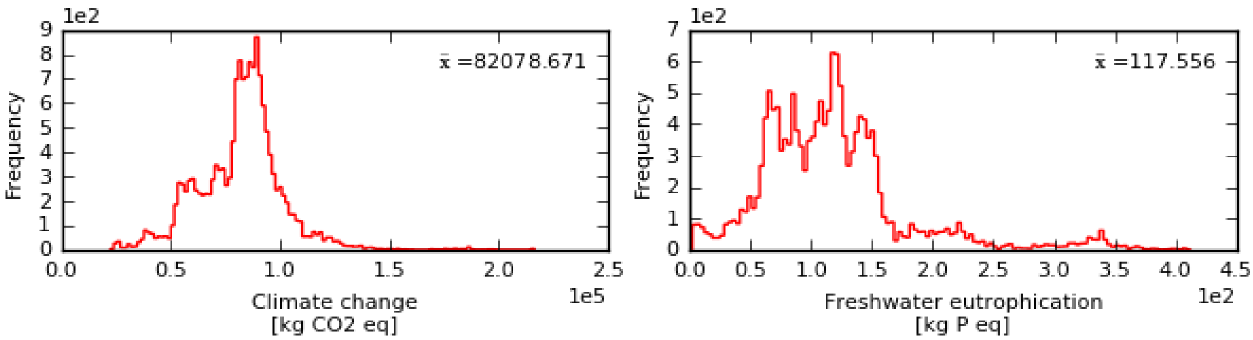


Figure 3.3: Histograms obtained from the conversion of the time series of total midpoint impact category results, shown in Figure 3.7. Displayed scenario: 4., FU: a day operation. The arithmetic mean, $\bar{x}$, of the concerning total impact category results is displayed on the graphs.

In Table 3.1 results are shown for scenario 4 for a classic LCA and for the average of the time series obtained through dynamic LCA. The FUs a day operation and kg COD in the influent were chosen. Subsequent time intervals in the case of dynamic LCA are always equal (except for the last one) and kg COD in the influent is very variable in the considered time intervals (which can be deduced from Figure C.1 (b)). It was therefore hypothesized, that for the former case results will be almost equal, and that for the latter case results can be different. In the table it can be seen that this is indeed true. In case of the highly variable kg COD influent, results in fact differ to a substantial extent. The maximum occurring difference is even 40 %.

Since it is the function of the FU to scale the impacts to a comparable quantity, it seems that calculating the total impact - within a specific impact category - divided by the value of the FU is more correct than calculating the arithmetic mean - within one specific impact category - of all impacts divided by the respective values of the FU. Therefore in this thesis, scenarios will be compared according to the classic approach and dynamic LCA will be used to obtain more information.

Table 3.1: Comparison of classic LCA results and the average of time series (Figure 3.7) as obtained through dynamic LCA. See the abbreviations section or Table B.6 for midpoint impact category abbreviations. The effect of choosing 2 specific FUs is investigated: a day WWTP operation and kg COD in the influent. Per FU and impact category, results are expressed as percentage of the maximum value.

	Functional unit: a day WWTP operation								
LCA type	CC	OD	TA	FE	ME	HT	POF	PMF	TE
Dynamic	100	100	100	100	100	100	100	100	100
Classic	100	100	100	100	100	100	100	100	100
	FET	MET	IR	ALO	ULO	NLT	WD	MD	FD
Dynamic	100	100	100	100	100	100	100	100	100
Classic	100	100	100	100	100	100	100	100	100
	Functional unit: kg COD influent								
	CC	OD	TA	FE	ME	HT	POF	PMF	TE
Dynamic	100	100	100	100	100	100	100	100	100
Classic	70	65	63	81	87	64	64	63	63
	FET	MET	IR	ALO	ULO	NLT	WD	MD	FD
Dynamic	100	100	100	100	100	100	100	100	100
Classic	65	64	61	62	65	64	89	65	60

3.4 Selecting relevant midpoint impact categories

3.4.1 Relevance of midpoints from contributions to endpoints

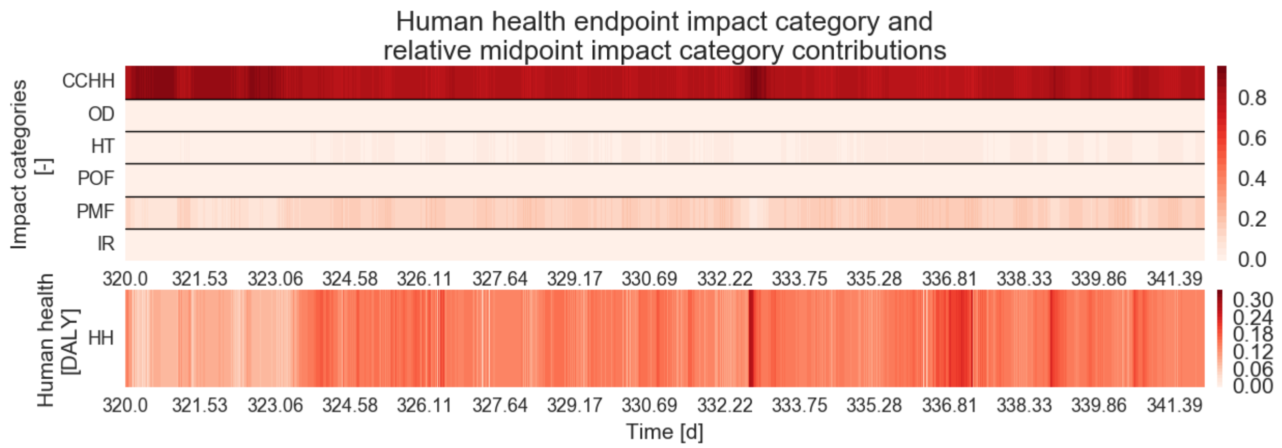
Conversion of midpoint to endpoint results should be based, as far as possible, on a solid scientific foundation JRC-IES (2010a). This will be exploited to get indications on the relevance of midpoint categories, from the extent to which they contribute to the endpoint categories. The reasoning behind this is that if the contribution of a midpoint impact category to a specific endpoint impact category is negligible in comparison with the contributions of the other midpoints, the concerning midpoint is less important to improve. For example, if all biodiversity is lost (endpoint category ecosystems) due to a specific emission, it does not make sense to not prioritize this problem. It should however be kept in mind that conversion of midpoints to endpoints also introduces uncertainties JRC-IES (2010a). The methodology described in this section should thus be conceived as providing good indications, rather than absolute certainties.

To investigate the extent to which midpoints contribute to endpoints, dynamic LCA - thus time series - will be used. For this purpose, the time series are visualized as heatmaps, which are colormaps (Figure 3.4). These figures are constructed in the following way: As described in Subsection 2.5.4, endpoint results were calculated by multiplying the emissions with the endpoint charactization factors, thus obtaining results for 16 midpoint categories that contribute to endpoint categories. For each endpoint category, results of contributing midpoint categories were summed. First, each individual endpoint time series was visualized as a heatmap. Next to each endpoint heatmap, the contributing midpoints are visualized as heatmaps. For every individual point in time, the latter are expressed in the following manner: they are scaled to the value of the concerning endpoint category and are thus expressed as a fraction of the total endpoint result at the concerning point in time.
Figure 3.4 shows results for scenario 4. This is the way the existing WWTP operates in conditions similar to reality, i.e. with both dry and wet weather conditions. It can thus be used as a base case that might be improved. The FU a day of operation is chosen, because for this analysis the absolute impacts are needed. By choosing time as the FU, only a correction is made for the case when the considered time intervals are not equal (note that only the last considered time interval can be different). In Figure 3.4 it can be seen that over the whole simulation time span, all endpoint impacts are almost entirely caused by the midpoints fossil depletion (FD) and climate change (CC). They should thus certainly be considered. Figure (a) indicates that the contribution of ozone depletion (OD) is negligible over the whole simulation time span (seems at most 3 % at any time instant), which is in accordance with conclusions of Corominas et al. (2013a) (see Subsection 1.4.2). Photochemical oxidant formation (POF) is also negligible (note that release of volatile organic compounds from the WWTP processes was not taken into account), as is ionising radiation (IR). particulate matter formation (PMF) and human toxicity (HT), are not always negligible. In Figure (b), only agricultural land occupation (ALO) contributes to a clear extent. Urban land occupation (ULO) and natural land transformation (NLT) sometimes contribute some percentages. Figure (c) shows that metal depletion (MD) should not be neglected. The fact that FD and MD seem important for this WWTP LCA, is not in accordance with general conclusions about the importance of impact categories by Corominas et al. (2013a).

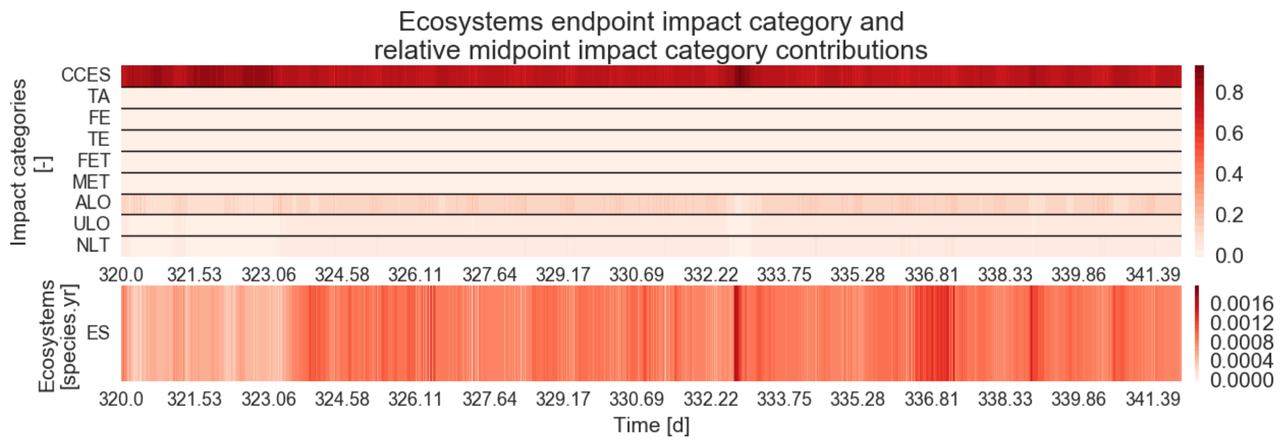
The observations that CC and FD have such a dominant impact should be interpreted with caution. Direct WWTP GHG emissions and sludge treatment contribute substantially to CC and FD respectively (Figure C.4). It was indicated that data quality of CO_2 emissions is moderate, data quality of

N_2O and CH_4 emissions is very poor, and data quality of sludge treatment is poor. The conclusions in this section might thus change substantially if data quality is improved. However, the methodology used in this section can clearly be used to get indications on the relevance of midpoint impact categories.

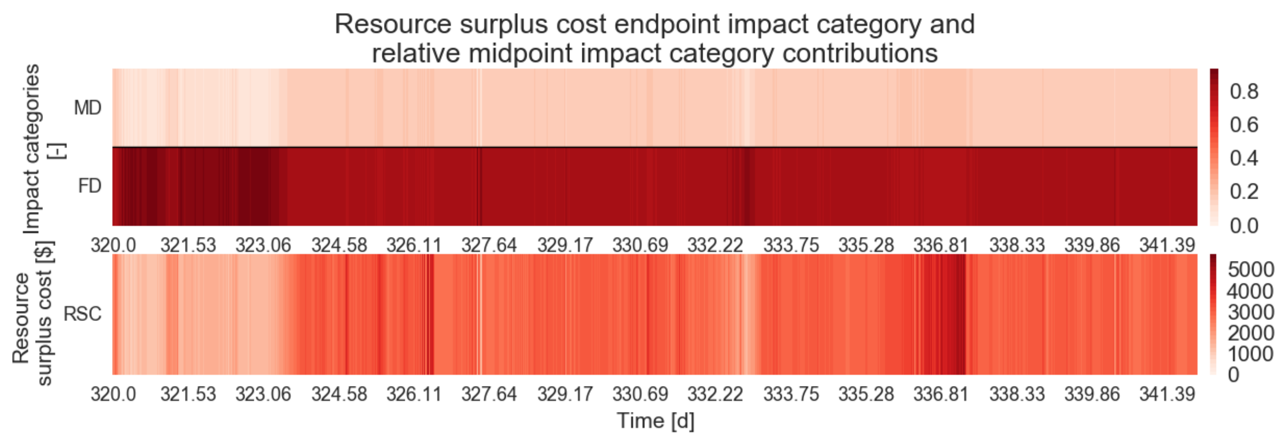
To apply the described approach, dynamic LCA is not necessarily needed. Making a bar chart of the midpoint to endpoint contributions in the case of a classic LCA would even be clearer. However, displaying the contributions as a time series (in heatmap form), provides insights in the dynamics. For instance, if emission peaks occurred in impact catgeories more related to local scales with possibly severe acute effects - such as freshwater eutrophication (FE), the heatmaps would provide indications on this, which could thus be included in selecting relevant impact categories.



(a)



(b)



(c)

Figure 3.4: Time series of endpoint impact category results (thus dynamic LCA), visualized as heatmaps. Scenario: 4., FU: a day operation. For abbreviations of midpoint categories contributing to endpoints, see Table B.8. For each individual point in time, the midpoints are expressed as the fraction to which they contribute to the concerning endpoint.

3.4.2 Making the selection

From the above it is clear that CC, FD, MD, ALO, and PMF should be considered. In addition, ULO and NLT will not be considered, because they are almost negligible. They are, furthermore, mainly dominated by sludge treatment (Figure C.4), of which data quality is not good.
Of all toxicity related categories, only freshwater ecotoxicity (FET) will be considered. The reason for this is that they are all dominated by impacts of sludge treatment (Figure C.4) and retaining them all will make the analysis needlessly complicated. In addition, direct WWTP emissions contribute to FET (in the form of fermentation end products, all assumed to be acetic acid) and it could be interesting to analyse the related dynamics. WD will not be considered, since a good quantification of water usage was not possible.
Futhermore, in Subsection 1.4.2 it became clear that FE and marine eutrophication (ME) should be considered. Moreover, FE is related to direct WWTP emissions, which might locally be severe. The fact that CC and FD dominate the endpoints is thus less relevant here, because these are related to a global scale. This is particularly relevant for the Eindhoven WWTP, since the effluent receiving water, the river "Dommel", is a relative small and sensitive river and the Eindhoven WWTP governing body, Waterboard the Dommel, sets it as a particular goal to reduce NH_4^+ concentration peaks and overall nutrient concentrations in the Dommel (Flameling, 2016).
In conclusion: CC, FE, ME, PMF, FET, ALO, MD, and FD will be considered.

3.5 Dynamic LCA as a valuable addition to classic LCA

3.5.1 Searching for impact causes

From the previous sections, it became clear that classic LCA should preferentially be used to compare scenarios. It also became clear that LCA in general can provide indications on the relevance of environmental impacts. These indications can be combined with specific goals of the instance for which the LCA is intended (Waterboard the Dommel, see Subsection 3.4.2). In contrast, dynamic LCA provides insights into the dynamics of environmental impacts. This might thus lead to identification of impact causes and provide indications on which aspects are best to improve, which will be investigated below.

It has to be noted that, for example, sludge treatment impacts are calculated in the notebook to coincide with the moment that the sludge is generated. This, of course, does not happen in reality. In the future, this aspect could be changed. This will however not be easy/always possible and it would make things more difficult to interpret.

First, the midpoint impact category time series will again be displayed as a heatmap (Figure 3.5). Despite the above selection of midpoint categories, all midpoint categories are displayed on this figure. In the final scenario analysis, only the selection will be used, but the intention of this figure is to demonstrate that the time series of all 18 ReCiPe midpoint categories can be shown in a clear and compact manner. The idea is to first investigate this figure to identify important aspects and then look at the time series plotted in more detail.

Figure 3.5 reveals that all categories but CC, FE, ME, and WD have very comparable time related dynamics. However, note that for FET an emission peak occurs around day 333 that does not occur in the other categories with comparable dynamics. It is also very clear that impact peaks occur in every impact category. To get more insight in the causes of all this, the more detailed time series plots can subsequently be analysed.

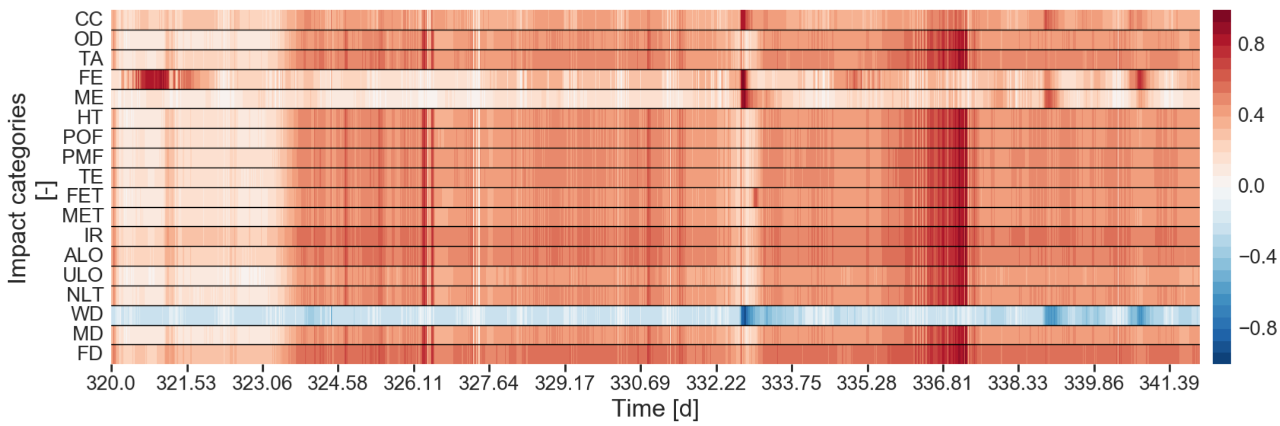


Figure 3.5: Heatmap of the time series of all midpoint impact categories. Each individual observation in an impact category is scaled to the maximum value that occurred in the concerning impact category. Scenario: 4., FU: a day operation. For midpoint impact category abbreviations and units, see Table B.6.

When looking at the more detailed plots of the time series in Figures 3.2 and 3.6, it can be seen that the dominant dynamics pattern is caused by sludge treatment, which dominates both dynamics and the impact (see also Figure C.4) in these categories. Note, however, that electricity production contributions are not to be neglected, certainly in FD and ALO. Note also that, as mentioned, sludge treatment data is of poor quality. Thus, these results should not be used for real life decision making at the Eindhoven WWTP. In case the data quality is assumed good, it can be concluded that sludge treatment is clearly causing much impact. Hence, the scenarios that could be investigated should clearly try to avoid more sludge treatment (i.e. sludge generation). Finally, also note the fact that

sludge treatment has a very low impact from day 320 to 322, which makes sense because in Figure C.2 (c) it can be seen that at that time almost no sludge is produced. This, on the other hand seems strange, because in this time span, influent COD (Figure C.1 (b)) and influent TSS mass flow rate (result not shown) do not seem to deviate much from average dry weather values and they are the main driving forces for sludge production.
Subsequently, it can be seen in Figure 3.2 that there is an impact peak in FET at day 333, caused by direct WWTP emissions. However, it is clear that remediating this peak will not have much effect on the overall score of this category. This will, on the contrary, probably increase impacts in other categories (Corominas et al., 2013a; Zang et al., 2015), which illustrates the added value of dynamic LCA: From a total impact perspective, the occurring emission peak is less important to improve. However, Waterboard the Dommel can still decide that it wants to take measures to prevent such emission peaks in the future, if they turn out to be the cause of water quality deterioration in the Dommel. If, on the other hand, it would be proven that these peaks are unimportant, other environmental aspects of the Eindhoven WWTP should be prioritized. Such considerations are not yet incorporated into the legislation, since effluent limits do not take into account the possibility of trade-offs. It is probably a good idea for policy makers to take these broader perspectives into account.
Next, FE - and thus impacts related to P emissions (Goedkoop et al., 2013) - can be seen on Figure 3.7. Impacts are clearly dominated by WWTP emissions, as is to be expected. Besides, in the first 2 days a large peak occurs, while the influent TP mass flow rate during that time interval does not show a large peak (Figure C.1). However, on Figure C.3 (b) it can be seen that during that time interval $Al_2(SO_4)_3$ dosing has not started yet, which explains the high P emission peak. This might also explain the fact that less sludge is formed, because $Al_2(SO_4)_3$ dosing increases sludge production. This, hence, demonstrates that dynamic LCA is able to visualize the dynamics of trade-offs in environmental technology. Other emission peaks are also visible. These peaks do coincide with influent TP mass flow rate peaks. Considering the specific goals of Waterboard the Dommel, remediating these emission peaks is desirable. It seems, in addition, that this might improve the overall score in this category to a substantial extent. It is however not a good idea to increase the overall control action of the $Al_2(SO_4)_3$ dosing controller (i.e. dosing flow rate), because this would lead to more (chemical) sludge production. This, again, highlights the added value of dynamic LCA: Impact peaks are indeed worthwhile to improve now, from a total impact perspective. In addition, care should be taken to avoid the possibility of large environmental trade-offs that will certainly occur if substantially more sludge will be produced. Therefore it is proposed to add a feed-forward control loop to measure the influent PO_4^{3-} mass flow rate and increase the Al dosing flow rate only if large peaks are detected (Figure 2.6). Measuring the mass flow rate is an important aspect here. It was noticed that influent P concentrations do not show large peaks, while mass flow rates do (result not shown). This occurs because flow rates of P and infuent volume increase in the same time spans (Figure C.1). In the sce-

nario analysis (Section 3.7), the effect of this will be compared to increasing the overall control action of this controller, to investigate the extent to which trade-offs would occur if the broader perspective provided by LCA would not be taken into account.

In Figure 3.7 also ME - and thus impacts related to N emissions (Goedkoop et al., 2013) - can be seen. Also here, emission peaks are visible that seem to contribute to a substantial extent. Thus, again, remediating them seems worthwhile from the total impact perspective. However, reducing NO_3^- emissions would require increasing the recirculation B flow rate. Reducing NH_4^+ emissions would require increasing aeration. Since the electricity usage related to these actions is not a result provided by the WWTP model at this time, it does not make sense to investigate this scenario in the context of this thesis. However, it would be a worthwhile addition.

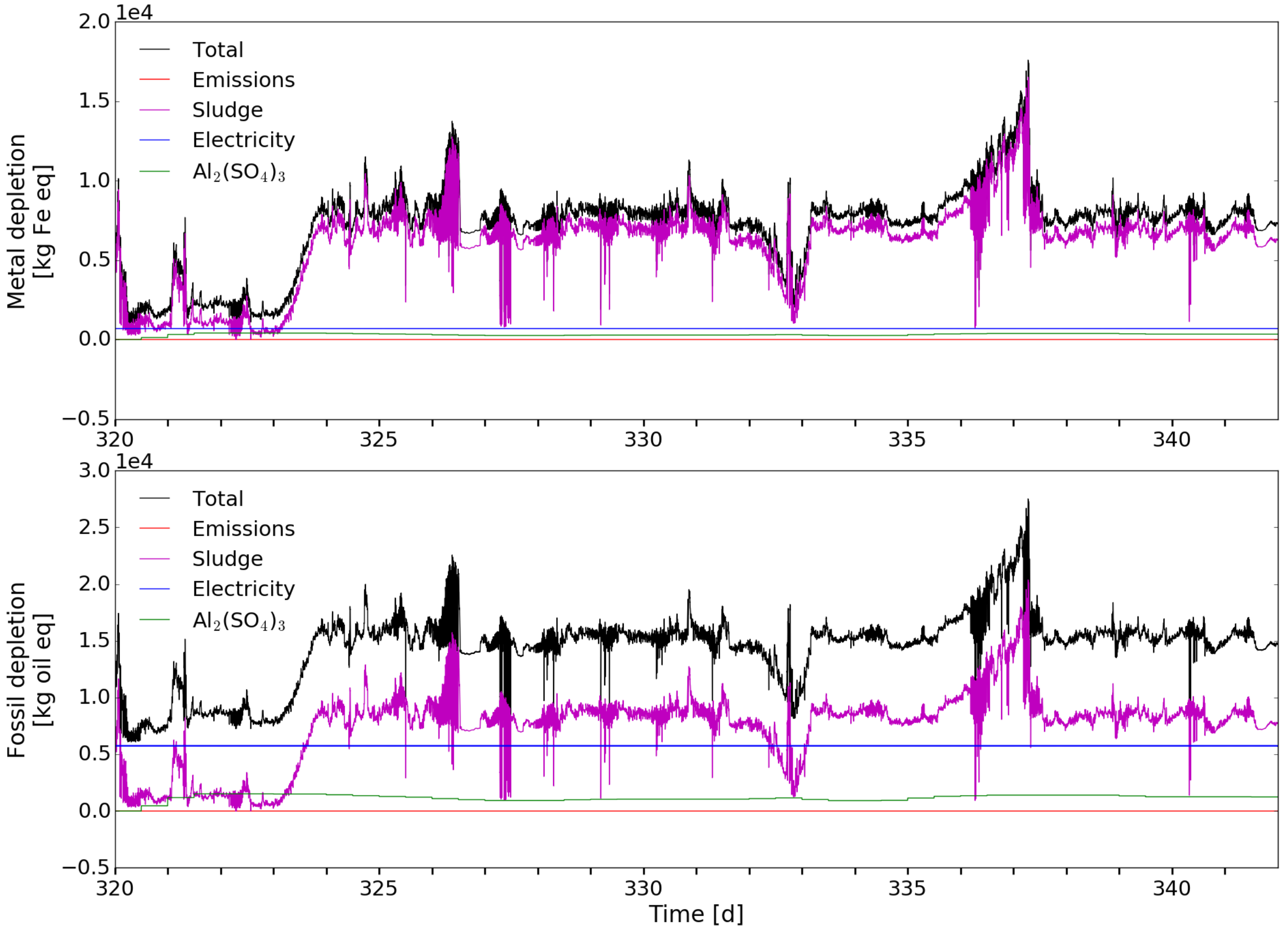


Figure 3.6: Time series of LCIA midpoint results. Scenario: 4., FU: a day operation. For contribution analysis, total impacts are divided into 4 categories. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions. On the y axis, the concerning midpoint impact category can be seen.

An additional change in the WWTP operational aspects that Waterboard the Dommel considers, is increasing the activated sludge concentration in the biological tanks (De Mulder, 2017). The effects of this are anticipated to be a lower sludge production. Steady state WWTP design equations indicate that an increased solids retenion time (SRT) leads to more TSS mass in the ASTs and hence a higher TSS concentration. An increased SRT can be obtained through lowering sludge wastage. (Henze et al., 2008a) It is in addition known from practical experience that net sludge production decreases with an increasing SRT. Mechanisms like maintenance energy requirements, endogenous respiration, and grazing by higher animals can be the cause of this. (Van Loosdrecht and Henze, 1999) Furthermore, if this indeed occurs, this means that more incoming COD will be oxidized to CO_2, instead of being discharged through the sludge. This will increase direct CO_2 emissions and the need for aeration. Again, the effect of increased energy consumption due to aeration is currently not modelled, which is indeed important when looking at FD in Figure 3.6 and CC in Figure 3.7. It is, however, also visible there that both sludge treatment and WWTP GHG emissions are the main contributors to CC (see also Figure C.4). Thus, despite the missing electricity data, increasing sludge concentration seems interesting for the modest scenario analysis in this thesis.

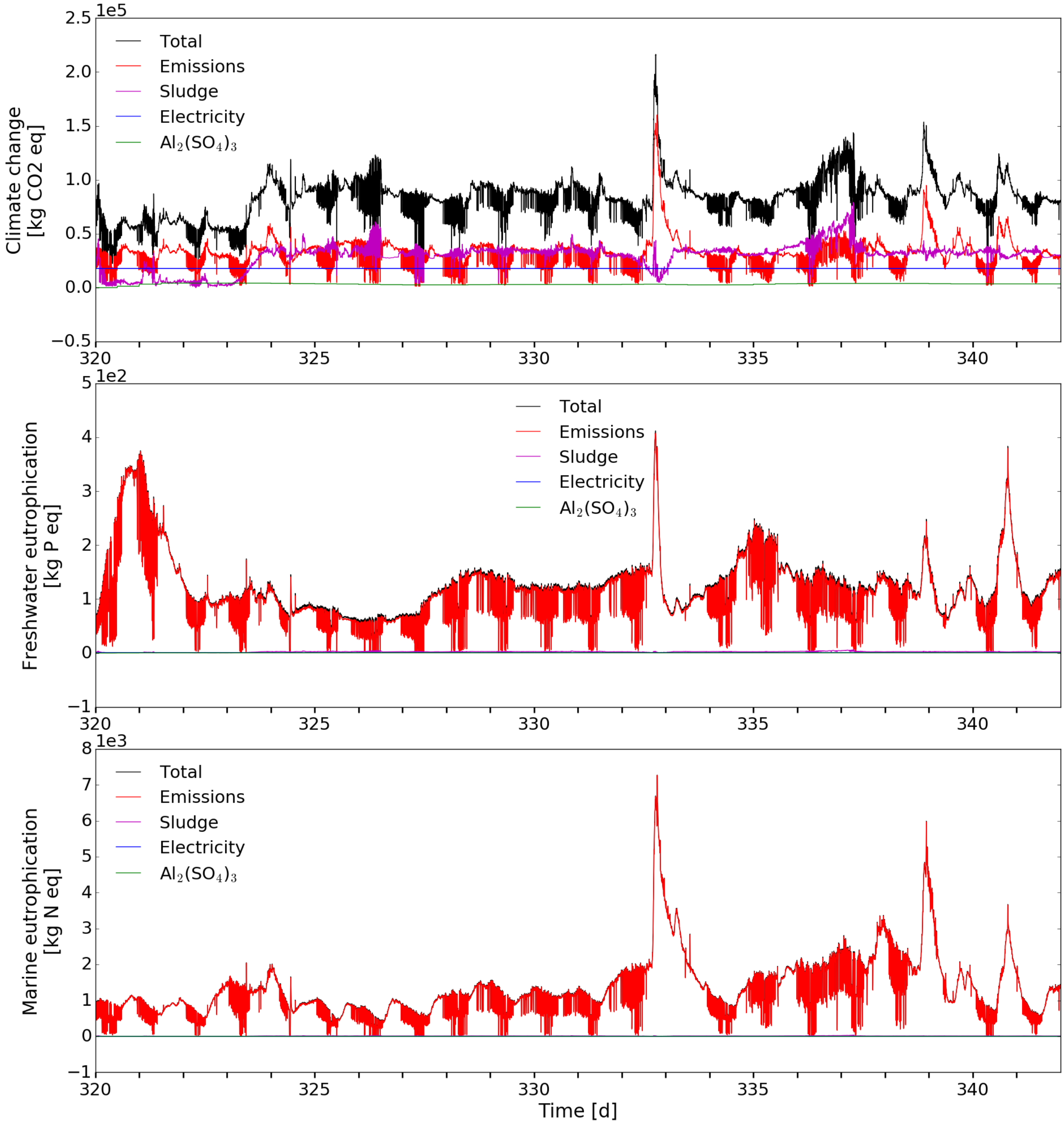


Figure 3.7: Time series of LCIA midpoint results. Scenario: 4., FU: a day operation. For contribution analysis, total impacts are divided into 4 categories. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions. On the y axis, the concerning midpoint impact category can be seen.

Due to time restrictions, a quantification of the percentage that emission peaks contribute to the total results of specific midpoint impact categories was not incorporated into the notebook. From the total impact perspective, this would be interesting to do in the future. Code could for instance be written that quantifies how much impact is generated due to emissions peaks - above a certain threshold value - in a specific midpoint impact category while performing dynamic LCA. The sum of these impacts minus the sum of what would be caused by the threshold impacts, could then be expressed as a percentage of the total impact that occurred in that midpoint category. In this way, it can be quantified - instead of the qualitative estimation performed above - how much can be gained from remediating emission peak causes in specific midpoint impact categories. This might lead to efficient measures to deal with causes of substantial environmental impacts.

3.5.2 Additional information for decision making

Finally, the emission peaks previously discussed can be an additional item to be included in the decision making phase. This is only relevant for emission peaks that can locally cause severe problems, for instance toxicity related impact categories and FE. However, it can be seen in Figure 3.2 that emission peaks in FET caused by direct WWTP emissions are not of particular relevance. Note, though, that NH_4^+ emissions are not incorporated into the ReCiPe FET impact category (see characterization factors, downloadable here `http://www.lcia-recipe.net/`). This is debatable since NH_4^+ is an important toxic pollutant in aquatic environments (EPA, 2013) and is of particular relevance for this specific case, the Eindhoven WWTP. On the other hand, N emissions are indeed incorporated in ME. However, it seems not very sensible to use this impact category as proxy for NH_4^+ and NO_3^- emissions, since it is not intended for this purpose. Hence, only FE is relevant, but ME will be included for illustrative purposes.
The severity of impact peaks in FE and ME can already be seen in Figure 3.7, but histograms could be a clearer way to display these events. To investigate the possible added value of this, the time series of FE and ME impacts of the direct WWTP emissions from Figure 3.7 were converted into histograms in Figure 3.8. It can be seen that impacts with a certain value occur in a high frequency, but also that clearly emission peaks occur, this in both impact categories. This is also visible on the time series. However, the 95th percentile gives an additional clear quantification of the severity of impact peaks to be expected in 5 % of the cases. This could indeed be used as an additional argument for decision making. If, for instance, during scenario analysis no clearly better options can be discriminated, maybe differences in impact peaks could provide the decisive argument.

To communicate results regarding the distribution of impacts to a non-scientific audience - e.g. management or stakeholder meetings, an even clearer way of displaying these results than histograms

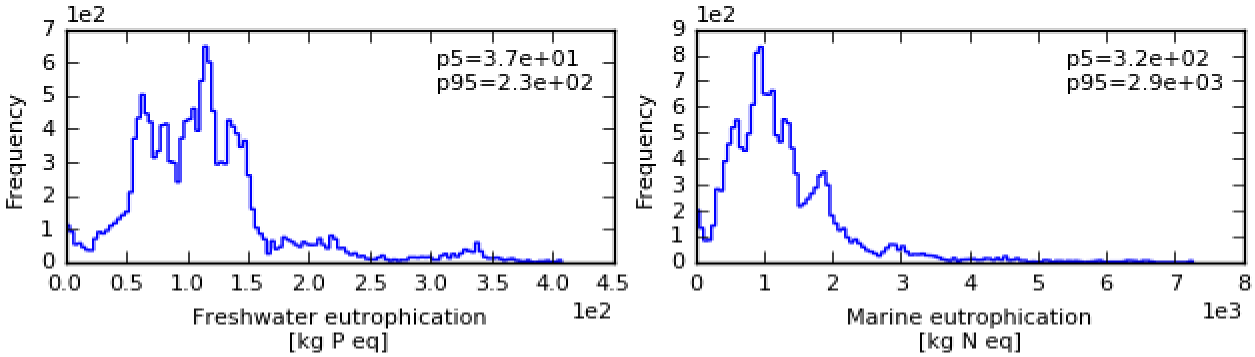


Figure 3.8: Histograms obtained from the conversion of the time series, shown in Figure 3.7, of the contributions of direct WWTP emissions to the concerning midpoint impact category results. Displayed scenario: 4., FU: a day operation. p5 and p95 are the 5th and 95th percentiles respectively.

might be necessary. For instance a bar chart, where some relevant percentiles are represented can be used (Figure 3.9). It was chosen to display the 50th percentile, because this is more representative for the most frequent impacts than the average due to the skewness of the distribution (see FE on Figure 3.8). From the bar chart, it is very clear that the statistical dispersion of FE impacts is high. In addition, it also gives an idea of the severity of peaks that can be expected in 5 % of the cases.

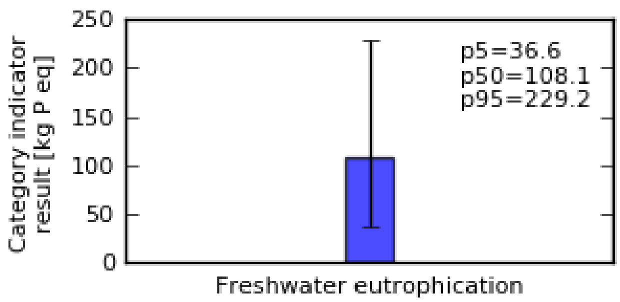


Figure 3.9: 5th percentile (p5), 50th percentile (p50), and 95th percentile (p95) of the time series, shown in Figure 3.7, of the contributions of direct WWTP emissions to the freshwater eutrophication results. Displayed scenario: 4., FU: a day operation. The bar represents p50, the bottom error flag p5, and the top error flag p95.

It has however to be noted that in Subsection 3.6.1 it will be shown that other FUs than operating time might be irrelevant in dynamic LCA. This limits the applicability of using dynamic LCA results in decision making as presented in this Subsection, 3.5.2, to case studies where operating time is sufficient as FU, i.e. where the scenarios are subject to very comparable conditions - for instance influent composition and effluent limits. However, subjecting 2 existing WWTPs to the same conditions, might be obtained through the use of WWTP models. This might even be more correct than applying a FU to the 2 investigated WWTPs operating under different conditions, since impacts probably do not scale linearly to the concerning FU (for instance amount of pollutants removed).

3.6 The functional unit

3.6.1 Functional unit for dynamic LCA

In previous the sections, it already became clear that scenarios should be compared by means of classic LCA results. Still, maybe FUs other than operating time could potentially be an added value in dynamic LCA.

Applying FUs in dynamic LCA might provide additional information. It should namely be the case that environmental impacts scale to some extent with variations in the FU (see also Subsection 3.6.2). This can be analysed in the following way: If as FU a variable is chosen that scales proportionally to the impacts at every time instant, then the impacts will become constant in time. Considering the non-linearity of the Eindhoven model, almost no variable will show this behaviour. However, even when impacts are a non-linear function of a certain variable, for instance kg COD removed, it is very likely that by applying it as FU, impacts will become more constant in time than when a less relevant FU is chosen. Thus, when a very influential variable is applied as FU, impacts will likely show a low variability. If at a certain moment in time still an impact peak occurs, another variable will probably be the cause of this.
One example will be given, because all results are fairly similar. The example will be the dynamic behaviour of CC LCIA results of scenario 4., with kg TN in the influent as FU. This FU is the most relevant in this case, because in Table 2.4 it can be seen that N_2O emissions are - over the whole simulation time - the most influential for CC caused by direct WWTP emissions and N_2O emissions are a fraction of influent TKN and thus completely follow the dynamics of influent TKN.
From Figure 3.10 it can be seen that large peaks occur in the total LCIA results near day 327 and 336. (All separate contributions to the total results are plotted on separate plots in Figures C.5 and C.6.) Such peaks do not occur in the CC LCIA results in Figure 3.7. The cause of this is the following: Figure 3.7 reveals that contributions of electricity and Al dosing stay constant in time at the

concerning time instants and that contributions of sludge treatment and WWTP emissions become smaller than electricity contributions and comparable to Al dosing contributions. It can also be seen in Figure C.1 that the influent TN load, becomes very low, which results in a low value of the FU in that moment. This explains the peaks in electricity and Al dosing contributions and thus the peak in the total impact (better visible on Figure C.5 and C.6). Since Al dosing is indeed a modelling result, it can be concluded that at this specific time instant the function N removal is not the cause of CC impacts (since Al is not dosed for N removal). This can, however, also be deduced from Figure 3.7, in a much easier way.
Next, it can be seen in Figure 3.10, that approximately all impact peak groups of the different contributions occur around the same time instants. Figure 3.7 shows that these events coincide with moments when emission impacts are low. This is also true for the emissions (Figure C.6), while N_2O emissions coincide with the FU dynamics. However, also CO_2 emissions are incorporated into direct WWTP emissions. It can be seen in Figure C.1 that the dynamics of influent COD and TN mass flow rates are a bit different. In addition, CO_2 emissions are likely a bit shifted in time, because they are a consequence of the biological reaction to influent COD dynamics (Figure B.2). This illustrates that it will probably be very hard to define a sensible FU for dynamic LCA (except for operating time), because it will be very hard to pinpoint the exact moment that a certain amount of pollutant is removed and link this to the processes responsible for the removal and thus generated impacts. In addition, in Appendix C.5, some considerations can be found on the FUs mass of nutrients or COD removed that could not be provided as option in the notebook. These considerations, provide additional arguments for this conclusion.

The conclusion is the following: All additional info that might be obtained from applying FUs in dynamic LCA is probably obtainable in other and much easier ways. In addition, it will be hard - or even impossible - to define sensible FUs in dynamic LCA. Thus, dynamic LCA will probably be limited to quantifying absolute impacts for a certain scenario (or impacts scaled to the operating time). However, this does not affect the ability of dynamic LCA to quantify the relevance of impact peaks in total impact category results for individual scenarios. This is thus not problematic for the above demonstrated potential of dynamic LCA to search for efficient measures to reduce environmental impacts (i.e. impact peak remediation, rather than overall decrease of emissions, which will likely cause larger trade-offs).

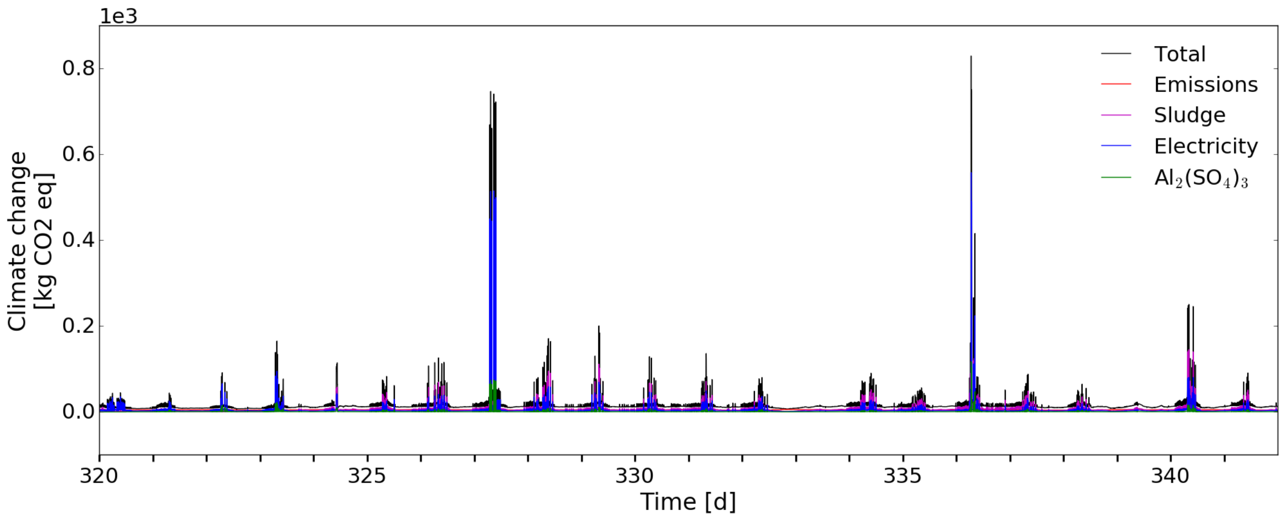


Figure 3.10: Time series of midpoint impact category results for CC. Displayed scenario: 4., FU: kg TN in the influent. For contribution analysis, total impacts are divided into 4 categories. Emissions include effluent and GHG emissions, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions. The legends on the graph show which contribution to the total result is plotted.

3.6.2 Influence of the functional unit

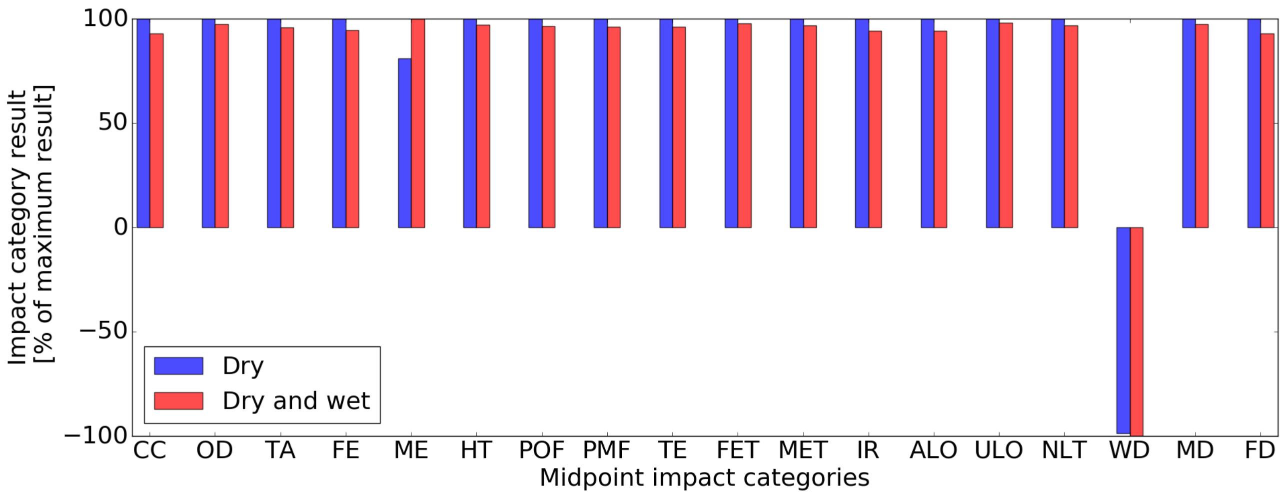
Up to this point, it became clear that classic LCA should be used to compare scenarios. In addition, different FUs are used in the literature which can lead to different results (see Subsection 1.4.4). Therefore, their influence on this specific case study will now be investigated using classic LCA. To achieve this, all midpoint impact categories will be used, because more information can be obtained in this way. For the final scenario analysis, only the above made selection will be used.

To analyse the influence of the FU, scenario 3. - only dry weather - and scenario 4. - dry and wet weather - will be used, because they show differences in dynamic behaviour of which the influence on the LCA outcomes can partially be predicted. For example, when considering the peaks in the influent flow rates during wet weather conditions (Figure C.1), it is certain that scenario 4. will cause more impact per time unit, since more water and pollutants need to be treated per time unit. Figure C.7 shows that this prediction is indeed true (except for WD due to the methodological choices in this thesis). It would however be more interesting to take the efficiency of the WWTP regarding its environmental impacts - environmental impacts caused per amount of pollutants or influent volume treated - into account during both operating conditions. The question then comes up what a good measure of this efficiency is. The answer probably is: an efficiency measure based on a variable that has much influence on the environmental impacts.

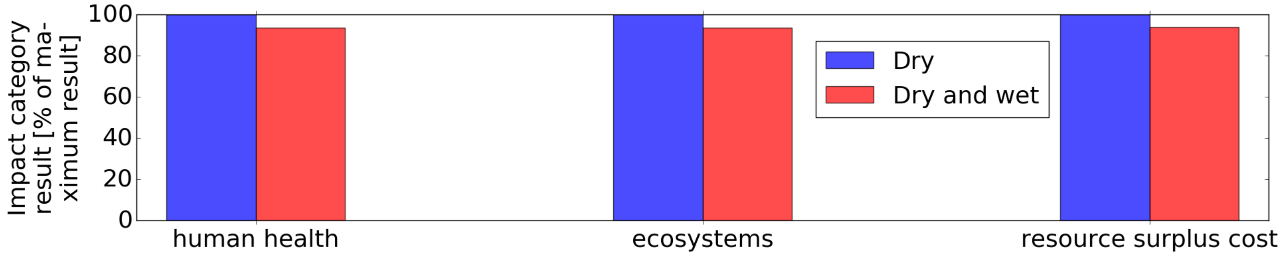
For instance, when looking at Figure 3.11 and 3.12, it can be seen that when using influent volume as FU, the dry weather scenario performs worse - except for ME, while dry weather is better for all impact categories when influent COD mass is used as FU (WD not taken into consideration). In the notebook, results for absolute impacts, total influent volume, and total influent COD are available. Total COD increases with a factor 1.94 from scenario 3. to 4., total influent volume with a factor 2.12. From scenario 3. to 4., all impacts increase with a factor of approximately 2, except ME which is multiplied with 2.63, which explains these results. Thus, by applying the FU influent volume, impacts - except for ME - become lower for scenario 4. than for scenario 3. This, however, is probably not correct. When more COD enters the plant, more CO_2 will be formed and hence more aeration is in addition needed. Also more sludge will be formed. When a larger amount of water enters the plant - i.e. pure water, not in terms of influent volume - none of this will happen. Thus, when using influent volume as FU, it might be that more volume is treated but that the pollutant load did not increase proportional to the increase in water volume. As a consequence, impacts will seem less because they are divided by a variable that has a higher value, but that is not very relevant for the environmental impacts. It is thus clear that using a variable that does not have much influence, can lead to misleading conclusions. The fact that volume of wastewater treated can be a bad choice as FU, is in accordance with conclusions of Corominas et al. (2013a). (In this thesis, influent water volume serves as approximation for volume of water treated). It might still be interesting to know how much impact is generated per volume of wastewater treated, but it is clearly important to understand the limitations related to this approach.

These conclusions can be used to criticise an interpretation of results provided by Rodriguez-Garcia et al. (2011), also mentioned in the review of Zang et al. (2015). They compared the FUs m^3 water treated and kg PO_4^{3-} removed when analysing, among others, WWTPs operated for organic matter removal (type 1) and WWTPs operated for organic matter and nutrient removal (type 2). Results show that climate change is lower for the former when m^3 water treated is the FU, but higher when kg PO_4^{3-} removed is the FU. They conclude that this better reflects the functionality when the focus is on P removal. However, for type 2 WWTPs, the removal efficiency of P was substantially higher and these results are thus probably caused by the fact that kg PO_4^{3-} removed is much higher for type 2 WWTPs (because when applying the FU, impacts are divided by it), while this variable is in fact not very relevant for the impacts caused by the type 1 WWTPs.

Next, it is probably true that to compare all scenarios in this thesis, the FUs kg COD in the influent (Figure 3.12), kg N in the influent (Figure C.9), and kg P in the influent (Figure C.8) all provide rather relevant measures for the service that is provided, namely removing them from the water until the effluent limit is met. It is interesting to compare them to the FU a day WWTP operation (Figure C.7). It can be seen that in all cases, the dry weather scenario is better. The difference however becomes smaller, when the former FUs are used - i.e. when LCIA results are scaled to a relevant measure for the functionality provided. All 3 result in very comparable LCIA results, which is caused by the fact that the ratio of any pair of the 3 FUs is almost the same between scenario 3. and 4. (calculable from Table 2.4). This all highlights the importance of choosing a relevant FU in WWTP LCA.



(a)



(b)

Figure 3.11: LCIA results for a classic LCA with the FU m^3 of influent. (a) Midpoint impact categories. (b) Endpoint impact categories. Compared scenarios: 3. dry weather conditions and 4. dry and wet weather conditions. See Table B.6 for impact category abbreviations (or the abbreviations section.)

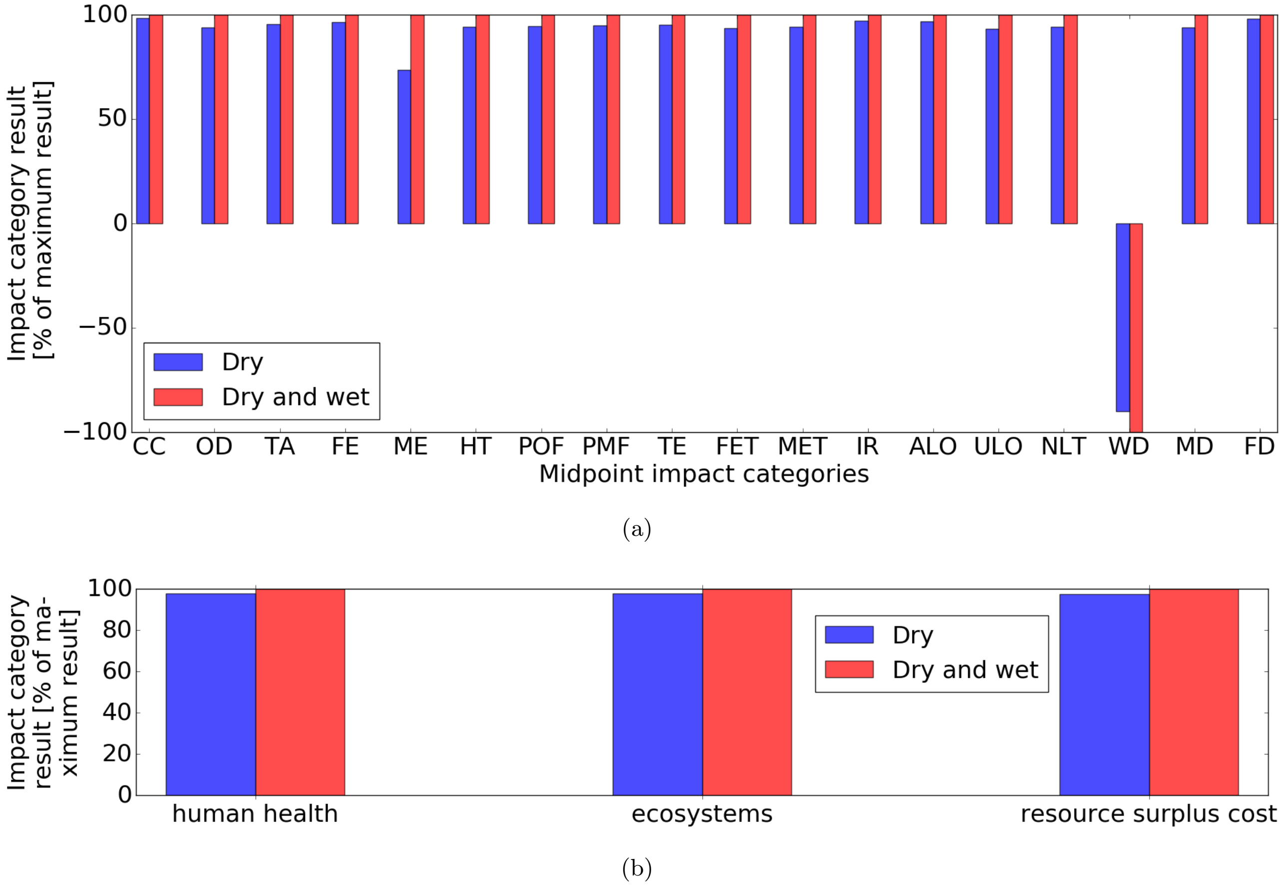


Figure 3.12: LCIA results for a classic LCA with the FU kg of COD in the influent. (a) Midpoint impact categories. (b) Endpoint impact categories. Compared scenarios: 3. dry weather conditions and 4. dry and wet weather conditions. See Table B.6 for impact category abbreviations (or the abbreviations section.)

3.7 Scenario analysis

Considering the time frame and length of this thesis, it will not be the intention of this section to provide an in-depth analysis from an LCA perspective. Normally, it is thoroughly analysed which scenarios seem or are better and what the causes are of these results. In addition, data quality of GHG emissions, sludge treatment, and $Al_2(SO_4)_3$ production is bad. Thus, the results of this analysis should be perceived as indications for further research instead of strong arguments for decision making. In this section, only overall conclusions will be presented briefly and some very relevant aspects regarding the coupling of dynamic WWTP models to (dynamic) LCA will be highlighted.
The intention of this, is to subject the above made hypotheses to a practical case study. The most

important aspects and resulting hypotheses of the above discussion are: Direct WWTP emissions contribute to a substantial effect to FE (which is trivial), and are thus worthwhile to decrease from a total environmental impact perspective. This was not the case in the category FET. In addition, impact peaks seemed to contribute to a substantial extent to the total FE result. A way of lowering the total FE result, is increasing Al dosing (chemical P removal). It was however hypothesized that this would lead to increased sludge production. Since results demonstrated that sludge treatment contributes to a substantial extent to the total impacts, it was in addition hypothesized that this would create a large environmental trade-off, which is to be avoided from the total environmental impacts perspective obtained through the LCA methodology. It was therefore proposed to add a feed-forward controller to only increase chemical dosing when peaks in influent PO_4^{3-} mass flow rates occur (Figure 2.6), thereby lowering the FE impact peaks but not the overall impacts. It was hypothesized that this still would be worthwhile, but that less trade-off would occur. In addition, the Eindhoven WWTP governing body, Waterschap the Dommel, considers increasing the TSS concentration in the ASTs. It was hypothesized that this would decrease sludge production but increase direct WWTP CO_2 emissions. Since it was determined that the midpoint category CC is the predominant contributor to the endpoints ecosystems (ES) and human health (HH), it would be interesting to investigate the effects of less wasted sludge but more CO_2 emissions, again from a total environmental impacts perspective.

Four scenarios will be involved in the scenario analysis. All 4 were performed with the influent data with both dry and wet weather conditions. Scenario 4. is the scenario with dry and wet weather conditions as it is used above, thus with nothing altered in the operational conditions. It will serve as the reference scenario. The other three scenarios are: 5. lowered upper setpoint of the effluent PO_4^{3-} controller (which increases overall PO_4^{3-} removal), 6. feed-forward controller to remediate peaks in effluent PO_4^{3-} emissions (Figure 2.6), and 7. increased TSS concentration in the ASTs. See Section 2.3 for a more elaborate description of these scenarios.

3.7.1 The functional unit (FU)

The FU a day WWTP operation will be chosen for the scenario analysis. Since all scenarios are run for the same time span, this is in fact equal to using no FU. Since in scenario 7. probably more COD will be removed than in the reference scenario, and in 5. and 6. more P will be removed than in the reference scenario, the FUs kg COD and kg P removed also seem suitable. However, all scenarios are subject to the same influent quality and involve one and the same WWTP (and thus also effluent limits). In addition, removing much more COD or P from the effluent might not be sensible. It would therefore be better to investigate what is needed to improve the water quality to a desirable level, as is for instance performed specifically for the Eindhoven case (Langeveld et al., 2013). LCA can subsequently be used to select scenarios that sufficiently achieve these results at the lowest possible absolute impacts. In this scenario analysis, a sensible criterion of sufficient functionality (i.e. pollutant removal) can be whether or not effluent limits are respected to a desirable extent.

3.7.2 The effluent phosphate controller

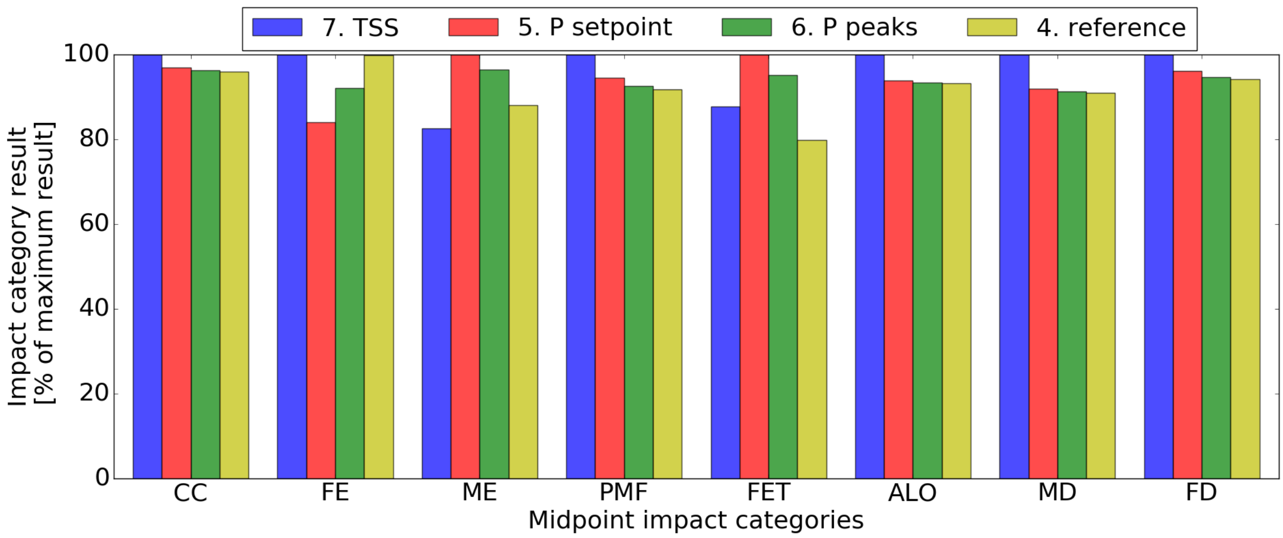
The following WWTP modelling result was relevant for the selection of the effluent PO_4^{3-} controller parameter settings: As evident from Figure C.3 (b) peaks of emitted PO_4^{3-} masses occurred in specific time intervals, such as the entire 2 first simulated days. In the latter time interval, the effluent limit of 1 mg L^{-1} TP was violated, but further in the simulation this occurred a second time (result not shown). This first violation will not be taken into account since it is caused by the fact that Al dosing has not started yet, as previously mentioned. The 2 newly introduced controller adaptations both resulted in the fact that the second violation no longer occurred (result not shown) and are therefore considered as scenarios that Waterschap the Dommel might want to investigate. However, the proposed feed-forward controller (Figure 2.6) is far from optimal and should be improved substantially if implementation were to be considered.

3.7.3 LCIA results

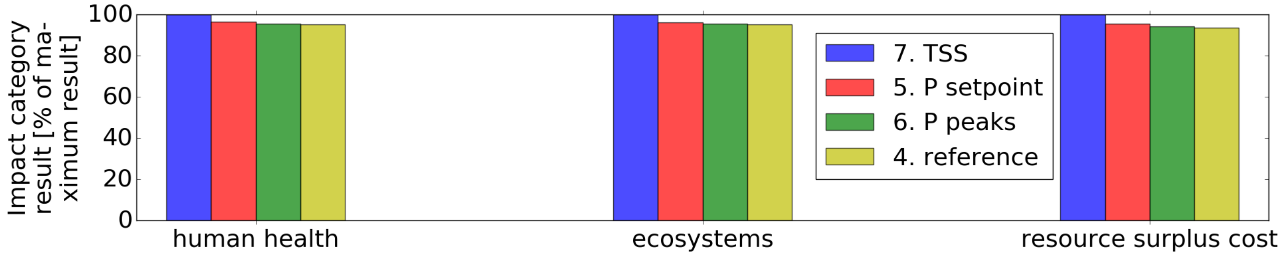
In Figure 3.13, all LCIA results - both mid- and endpoint - are shown. A short description of the 4 compared scenarios is given in Table 3.2.

Table 3.2: Short description of the 4 scenarios used in the scenario analysis. For an elaborate description, see Section 2.3. All 4 were performed with the influent data with both dry and wet weather conditions.

Scenario	Description
4.	No operational changes. Reference scenario.
5.	Lowered upper setpoint of effluent PO_4^{3-} controller. (Increased overall PO_4^{3-} removal.)
6.	Feed-forward controller to remediate peaks in effluent PO_4^{3-} emissions.
7.	Increased TSS concentration in the ASTs.



(a)



(b)

Figure 3.13: LCIA results for a classic LCA with the FU a day WWTP operation. (a) Midpoint impact categories. (b) Endpoint impact categories. Compared scenarios: 4. no operational changes: reference scenario, 5. lowered setpoint of the effluent PO_4^{3-} controller, 6. feed-forward controller to remediate peaks in effluent PO_4^{3-} emissions, and 7. increased TSS concentration in the ASTs. See abbreviations section or Table B.6 for impact category abbreviations.

Increased TSS concentration

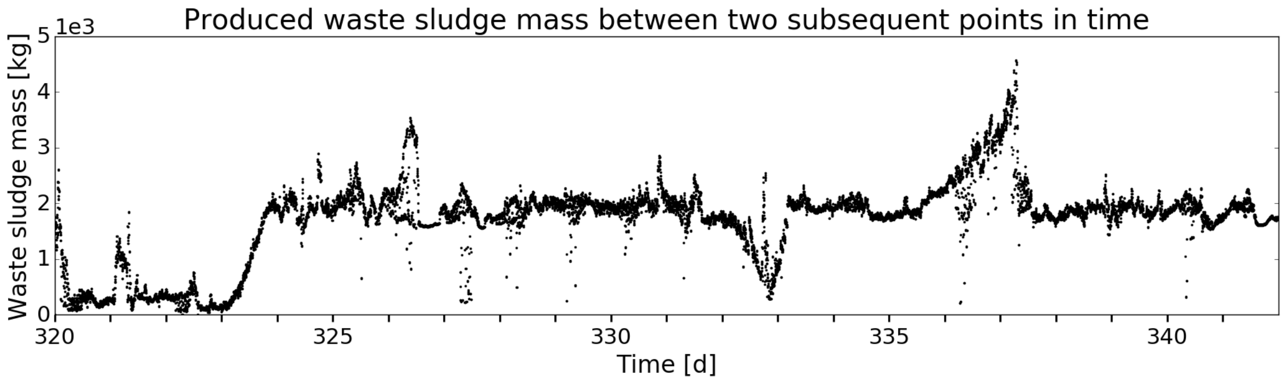
It can be seen that scenario 7. (increased TSS concentration in the ASTs) performs clearly worse than all other scenarios on 5 of the 8 considered midpoint categories and on all endpoint categories. The causes of these results are deducible from the LCI (Table 2.4): It can be seen that this scenario has the highest CO_2 production, as predicted. It also has the highest sludge production, the opposite of what was anticipated. Climate change (CC) is the main contributor to the endpoint category ecosystems (ES) and human health (HH), as previously determined. The “relevance of midpoints from their contributions to endpoints" analysis was only shown for the reference scenario. However, overall results for the other scenarios remained the same (result not shown). Previously, it was also determined that sludge treatment is an important contributor to mid- and endpoints in scenario 4. (reference scenario, Figure C.10). This is also true for scenario 7. (Figure C.13). This explains these results and substantiates the above conclusions that more sludge production (and GHGs) should be avoided, since sludge treatment contributes to a large extent to the environmental impacts (as do GHG emissions).

The cause of the additional sludge production can be seen in Figure 3.14. In comparison with scenario 4., there is much more sludge wasted in the first days in scenario 7. Total sludge production (thus not per day operation) was quantified for both scenarios from day 320 to 324.99 and from day 325 to 342: scenario 4. had a sludge production of 3.00e6 and 2.37e7 kg respectively, while in scenario 7. 5.36e6 and 2.44e7 kg were produced. Thus, for scenario 7., there is a bit more sludge wastage from day 325 to 342, but the greatest difference is indeed due to the first 5 days. The causes of this could be that in scenario 7. more $Al_2(SO_4)_3$ is dosed (Table 2.4). However, in scenario 5. and 6., even more $Al_2(SO_4)_3$ is dosed, but this did not result in more sludge production (which is unexpected). It seems therefore unlikely that only the Al dosing would be the cause of this. This is even more so, because the higher CO_2 production in scenario 7. proves that more COD is oxidized, which hence reduces sludge production. It can, in addition, not be excluded that the TSS concentration (sludge wastage) and effluent PO_4^{3-} concentration (Al dosing) controllers show a somewhat artificial start-up behaviour in the WWTP model. The fact that in both cases the Al dosing needs some time to start (Figures C.3 (b) and C.14 (a)) and that sludge wastage in scenario 7. switches from very low to more or less average a couple of times in the first 5 days (Figure 3.14) indicates this. Hence, a longer simulation time is required - for instance a whole year - in order to minimize the controller start-up behaviour on the results and to be certain which scenario produces considerably more sludge. Currently, however, it is very likely that no WWTP models with the level of detail as the one used in this thesis are capable of much longer simulations (De Mulder, 2017). This is very relevant for this thesis, since these results indicate that dynamic WWTP models still need to improve in order to get accurate LCA results.

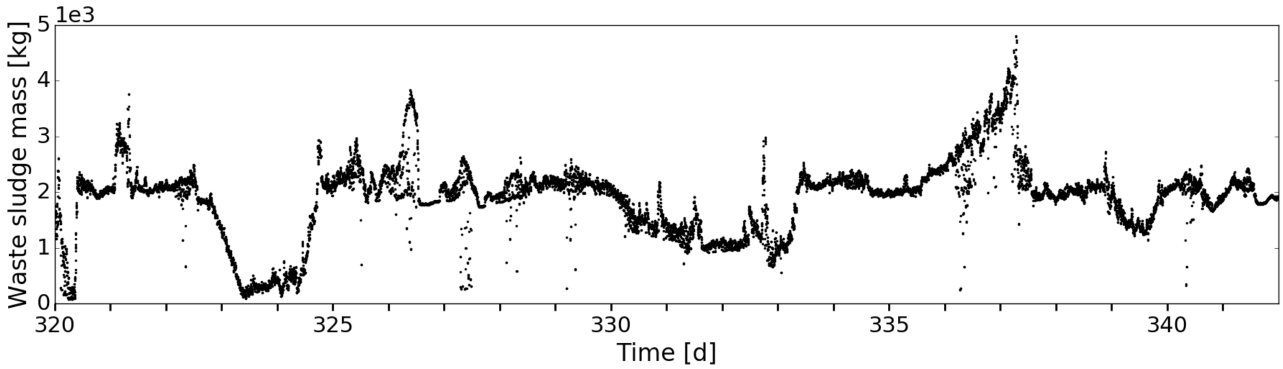
Since there is doubt about the credibility of the sludge production results, no conclusion about scenario 7. will be made. It might still be interesting to further investigate an increased TSS concentration in the ASTs. For instance, to determine if indeed substantially more sludge is produced due to these operational changes.

Phosphorus control scenarios

First, it can be seen that considerable improvements in FE are obtained in scenario 5. (lower setpoint) and 6. (peak control) in comparison with scenario 4. (reference scenario), respectively 16.3 and 7.5 %, which was the intention. (See Table 3.2 for short scenario description.)



(a)

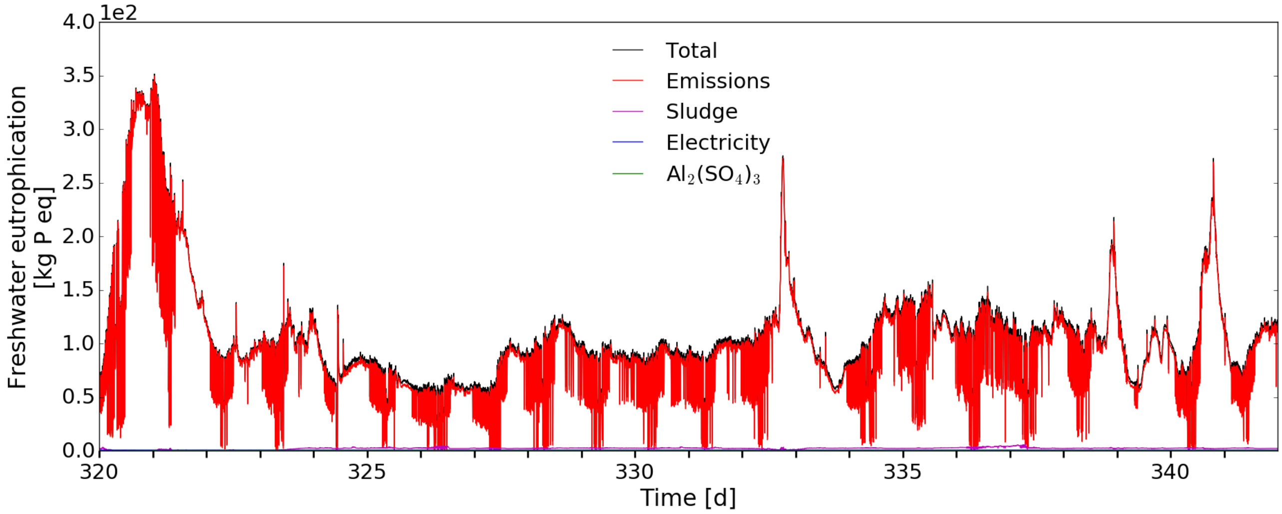


(b)

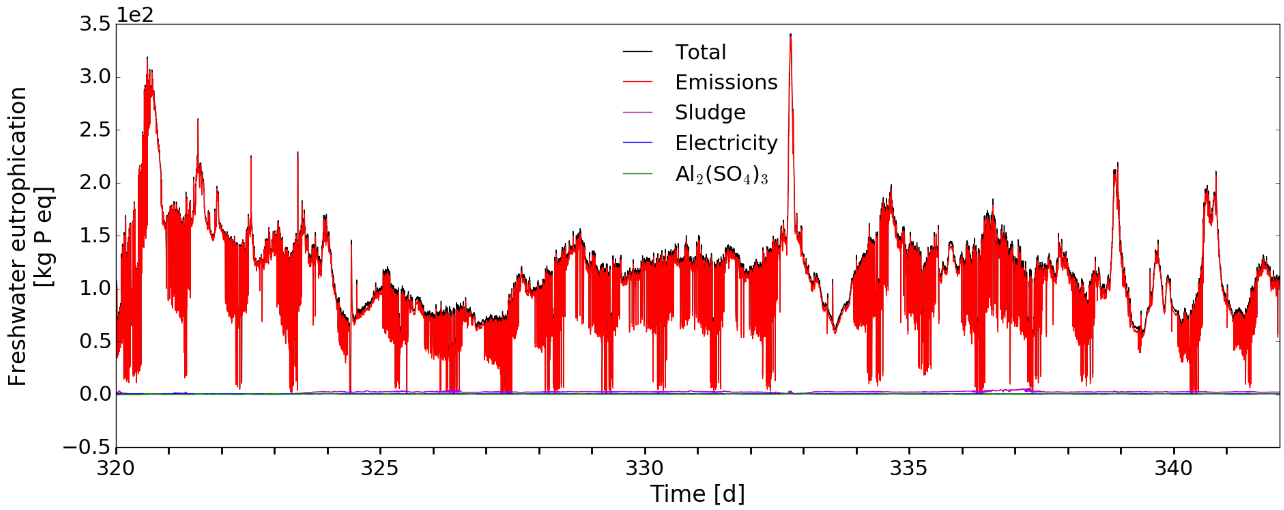
Figure 3.14: (a) Scenario 4.: dry and wet weather conditions (reference scenario). (b) Scenario 7.: increased TSS concentration in the biological tanks.

The dynamic FE LCIA results in Figure 3.15 and 3.7 will be used to analyse the consequences of the changes in the effluent PO_4^{3-} controller on the PO_4^{3-} emissions. (These results are very comparable to the results for the actual emitted PO_4^{3-} masses in Figure C.14 and C.3 (b).) First, it can be seen that the large peak during the first days is lowered much in scenario 6. This, however, is simply because the dosing normally would not have started yet. Hence, this cannot be called a success. In addition, as a consequence of the lowered peak, it can be seen that the mentioned rebound effect (Section 2.3) occurs around day 322 to 324. Next, overall emissions are lowered in scenario 5., i.e. the curve is shifted downwards. This was much clearer on the WWTP model results (not shown), but can be seen best around day 330 to 332. This seemed not to be the case in scenario 6., but as mentioned, the feed-forward controller is far from optimal. However, when FE impact peaks of scenario 4. (Figure 3.7) are compared to scenario 6., it can be seen that the impact peaks near day 333 and 341 are clearly lowered. This strongly indicates that the proposed feed-forward controller based on influent PO_4^{3-}

mass flow rate (Figure 2.6) is worthwhile to investigate further.
Besides, the contributions of the direct WWTP emissions to the FE results in Figure 3.15 were also converted into histograms (Figure 3.16) to demonstrate their usefulness for quantifying frequencies of impact peaks. It has to be repeated that peaks in scenario 6. were substantially lowered in the first days, which cannot be called a success. Still, from the 95th percentiles it is very clear that in 5 % of the time instants, impacts were higher in scenario 5. than 6. and even higher in the reference scenario (Figure 3.8).

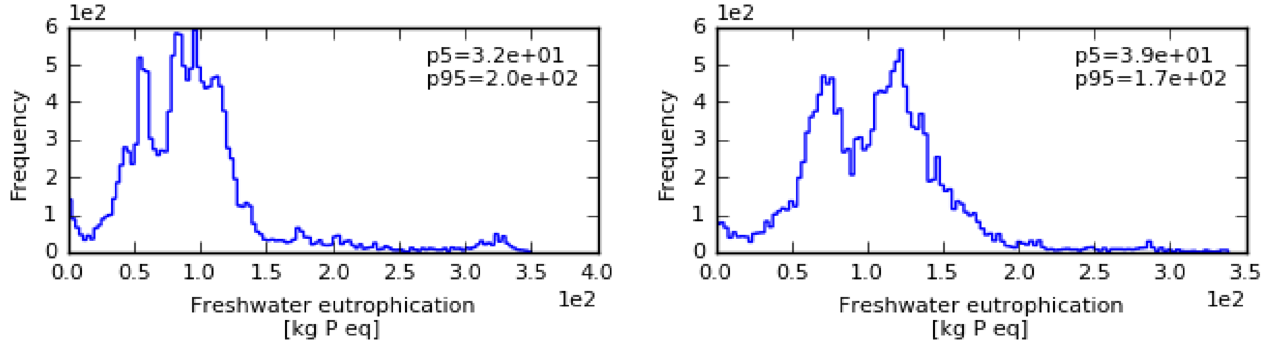


(a)



(b)

Figure 3.15: Time series of FE results. (a) Scenario 5.: lowered setpoint of the effluent PO_4^{3-} controller, (b) Scenario 6.: feed-forward controller to remediate peaks in effluent PO_4^{3-} emissions. FU: a day operation. For contribution analysis, total impacts are divided into 4 categories. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions.



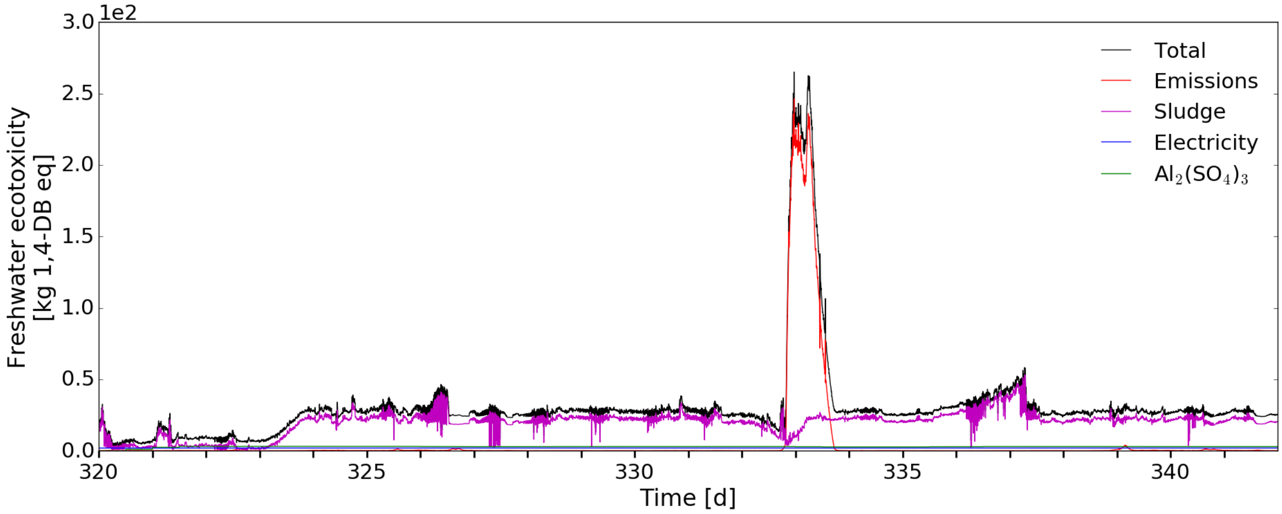
(a) (b)

Figure 3.16: Histograms obtained from the conversion of the time series, shown in Figure 3.15, of the contributions of direct WWTP emissions to the FE results. (a) Scenario 5.: lowered setpoint of the effluent PO_4^{3-} controller, (b) Scenario 6.: feed-forward controller to remediate peaks in effluent PO_4^{3-} emissions. FU: a day operation. p5 and p95 are the 5th and 95th percentiles respectively.

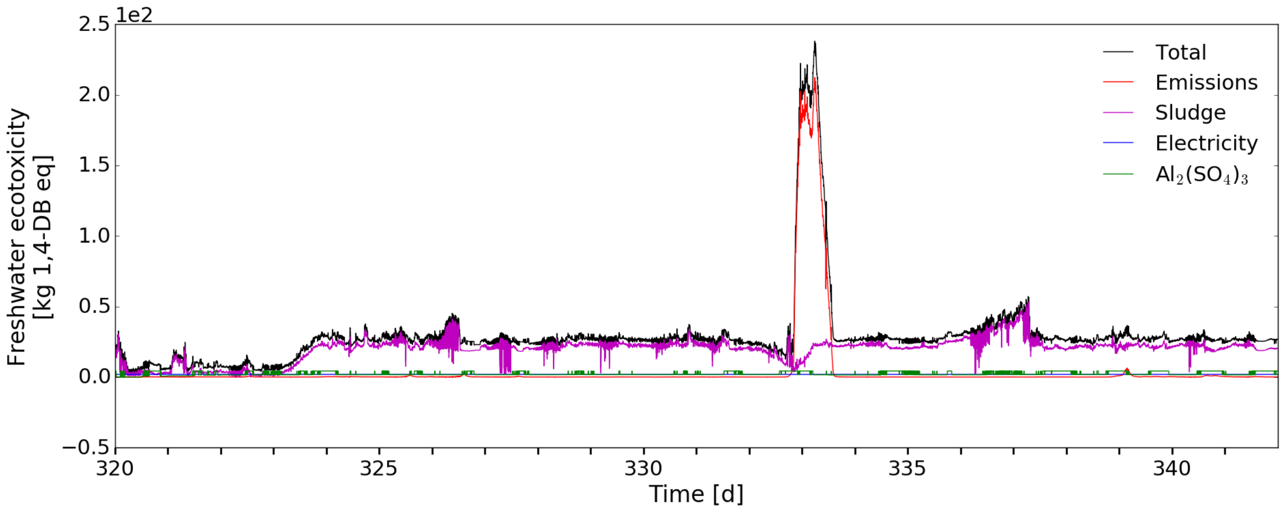
Next, it can be seen in Figure 3.13, that endpoint impacts are higher for scenario 6. (peak control) in comparison with the reference scenario and even higher for scenario 5. (lower setpoint), as anticipated. This, however, to a very low extent. The cause of the small extent of this increase can be found in the LCI (Table 2.4): Sludge production was the same for scenarios 4., 5., and 6. (In fact, the data in Table 2.4 are rounded substantially. Both in scenario 5. and 6., there was 0.06 % less sludge production than in the reference scenario.) This is not what was expected. It would be interesting to investigate the causes. This will, however, not be performed. In addition, CO_2 emissions are the same for the concerning scenarios and climate change (CC) was the main contributor to the endpoints ecosystems and human health, as previously determined. Moreover, in Table 2.4 can be seen that more $Al_2(SO_4)_3$ is dosed in scenario 6. and even more in scenario 5. From the contribution analysis of scenarios 4., 5., and 6. (Figures C.10, C.11, and C.12), however, it is clear that $Al_2(SO_4)_3$ production and transport only contributes to a small extent, which explains why only a small increase occurred.

In conclusion, the anticipated large trade-off did not occur because there is no increased sludge production. Still, it is shown that dynamic LCA is very valuable: It resulted in the conclusion that impact peaks in FE are worthwhile to remediate from a total impact perspective. This was not true for the impact peak in the category FET caused by direct WWTP emissions. The latter is interesting from the perspective of the Eindhoven WWTP management, but less so from a total impact perspective, due to the fact that the impact peak did not contribute to a large extent to the total midpoint result (Figure 3.2). It is also demonstrated that due to this approach, trade-offs can be avoided to some extent (although very modest in this case). It would, moreover, be interesting to combine this approach to a quantification of the amount of P removal that is needed to achieve a good ecological quality in the effluent receiving water, the Dommel. This can then be used as criterion, instead of applying the FU kg P removed and thereby thus implicitly assuming that more functionality (P removal) is better. This all, in addition, highlights the strength of coupling dynamic models to LCA. The ideas for scenario 6. were developed while analysing the results of this research. The results of applying scenario 6. were subsequently obtained in a very short time span after its creation and this at a very low cost: no operational changes were required at the Eindhoven WWTP and very few man-hours were required.

One remarkable LCIA result still needs to be clarified. It can be seen that both scenario 5. and 6. perform considerably worse in the impact categories ME and FET (Figure 3.13 (a)). The cause of this for FET can be seen in Figure 3.17. At day 333 a very large impact peak is caused by the direct WWTP emissions. In Figure C.1 (a) can be seen that a large peak in influent volumetric flow rate occurs at that time instant. It is thus very likely that the changes in the operational apsects caused by the enhanced Al dosing, result in a considerably worse performance during wet weather conditions. Results for ME point very strongly in the same direction (result not shown).
Two things can be concluded from this. Firstly, the impact peak in FET (due to emissions of acetic acid) at day 333, indicates that effluent limits are violated. This indeed happened: The Eindhoven NH_4-N effluent limit is 3 mg L^{-1}. In the reference scenario, it is violated for 18 hours, with a max. peak height of 12 mg L^{-1} NH_4-N. However, in scenarios 5. and 6., it is violated for 30 hours, with a max. peak height of 20 mg L^{-1}. The criterion "sufficiently meeting the effluent limits" is hence clearly not respected. Thus, the proposed scenarios - under their current form - should not be applied. The causes of the bad performance under rain weather conditions of scenario 5. and 6. could be investigated and remediated. This will however not be performed in this thesis. Secondly, it is very clear that in this case the impact peaks in FET are indeed important from a total impact perspective, since they are no longer negligible in the total result of this impact category (see also the changes this causes in the classic contribution analysis in Figures C.10 (a), C.11 (a), and C.12 (a)). This was of course not the intention, but it does - again - highlight the added value of dynamic LCA.



(a)



(b)

Figure 3.17: Time series of FET results. (a) Scenario 5.: lowered setpoint of the effluent PO_4^{3-} controller, (b) Scenario 6.: feed-forward controller to remediate peaks in effluent PO_4^{3-} mass flow rates. FU: a day operation. For contribution analysis, total impacts are divided into 4 categories. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions.

CHAPTER 4

Conclusion and future perspectives

4.1 Conclusion

In this thesis, a dynamic wastewater treatment plant (WWTP) model - of the Eindhoven WWTP - was coupled to life cycle assessment (LCA) and a dynamic LCA approach was developed, i.e. time series of LCA results were obtained. For this purpose Python™ scripts were developed that provide the possibility to perform both classic and dynamic LCA. They are available online for downloading: `https://github.com/TomLauriks/dynamic_WWTP_model_plus_LCA`. The ReCiPe life cycle impact assessment method was used and the scripts deliver results for all 18 ReCiPe midpoint and all 3 ReCiPe endpoint impact categories.

The resulting time series of dynamic LCA cannot directly be used to accurately determine differences between scenarios in specific impact categories, but average dynamic results could be compared. However, it was shown that a classic result - total impact per total value of the functional unit (FU) - and an average dynamic result - the arithmetic mean of the time series where each impact at a specific time instant is expressed per value of the FU in the respective time interval, are not necessarily equal for one and the same impact category and scenario. The possible extent of this difference was investigated. For the FU kg chemical oxygen demand (COD) in the influent, classic LCA results were compared to average dynamic results, for a specific scenario. This resulted in a difference of 40 % in the impact category fossil depletion. Since it is the function of the FU to scale the impacts to a comparable quantity, it seems that calculating the total impact divided by the value of the FU is more correct than calculating the arithmetic mean of an impact category time series. Thus, classic LCA should probably be used to compare scenarios.
In addition, in this thesis the FUs kg COD, kg total nitrogen (TN), and kg total phosphorus (TP) in the influent were used as approximation for amounts of pollutant removed. Applying kg TN as FU in

a dynamic LCA was performed. The thus obtained results indicate that pinpointing the exact time instant when an amount of pollutant is removed and relating it to the impacts caused by the processes achieving this removal might not be possible in the small time intervals in which the dynamic LCA results were calculated (2 minutes), due to the complex time related dynamics of a WWTP (model). Hence, other FUs than operating time might be irrelevant in dynamic LCA.
Due to these conclusions, classic LCA was used to compare scenarios and dynamic LCA was used to obtain more information.

To select relevant midpoint impact categories, the following approach was used: The extent to which midpoint categories contribute to endpoint categories was quantified. Midpoints of which the contribution was negligible, for instance 3 %, were not taken into account. For this purpose, dynamic LCA was used, which provides more information than classic LCA can, namely visualize impact peaks. If impact peaks would occur in a specific midpoint impact category, this could be an argument to certainly include it into the analysis.

The fact that information about impact peaks is available in dynamic LCA indeed proved to be a valuable addition to classic LCA. For instance, impact peaks in the impact category freshwater eutrophication (FE) were caused by direct WWTP emissions and substantially contributed to the total impact category score. In freshwater ecotoxicity (FET), direct WWTP emissions also caused an impact peak, but the latter clearly did not contribute substantially to the total FET result. It was thus clear that remediating impact peaks caused by direct WWTP emissions to improve the total impact category result was worthwhile in the category FE, but not in FET. The Eindhoven WWTP governing body, Waterschap the Dommel, could still choose to remediate the FET impact peak causes. However, dynamic LCA provided extra information from a broader perspective - as opposed to only considering effluent limits - that can be included into the decision making phase. In this thesis, it was decided to further investigate the effects of lowering the total impact in FE , i.e. lowering phosphorus (P) emissions.
A way of decreasing P emissions, for instance, is increasing overall chemical P removal, i.e. aluminium (Al) dosing in the case of the Eindhoven WWTP. It was hypothesized that this would create a large environmental trade-off, since results obtained through classic LCA indicated this. Therefore, a feed-forward controller was developed that only increases Al dosing if peaks in influent PO_4^{3-} mass flow rates are detected, as opposed to increasing the overall dosing. It was hypothesized that this still would be worthwhile, but that less trade-off would occur. In conclusion, the combination of classic and dynamic LCA assisted in identifying scenarios that could lead to efficient improvements of the current situation.

These hypotheses were subjected to a practical case study: The current situation - the reference scenario - was firstly compared to an increased overall Al dosing, and secondly to applying the proposed feed-forward controller. For the former, this resulted in 16.3 % improvement of FE and for the latter 7.5 %. The feed-forward controller indeed caused less trade-off, but the large anticipated trade-offs, did not occur. Still, it was shown that dynamic LCA can lead to developing efficient improvements and that LCA in general can lead to avoiding trade-offs.
In the scenario analysis, no functional unit (FU) was applied. It was argued that it would be more interesting to investigate the extent to which pollutant removal is needed to achieve a good ecological quality in the effluent receiving water. Through LCA, it can subsequently be investigated how to obtain this goal with minimum absolute environmental impacts. In this thesis, the criterion that the proposed operational changes should result in sufficiently respecting the effluent limits was used. The proposed scenarios, however, resulted in a considerably larger violation of effluent NH_4-N limits during rain weather conditions in comparison with the reference scenario. Hence, they should not be applied in their current form, but could still be worthwhile to investigate further.
LCA time series of FE results of the P removal scenarios were also converted into histograms, onto which 95th percentiles were also shown. This resulted in a clear representation of impact peak severities to be expected in 5 % of the time instants. This can provide additional information for decision making.

In addition, an increased total suspended solids (TSS) concentration in the activated sludge tanks (ASTs) was included into the scenario analysis, which resulted in an increased sludge production. This led to an overall environmental performance that was considerably worse than the other scenarios. Results, however, indicate that the cause of this might be the start-up behaviour of the modelled WWTP controllers and that longer simulations are needed to affirm whether or not these results seem logical. However, the WWTP model used in this thesis has a high level of detail, but is only able to simulate periods of up to 4 weeks with good confidence (3 weeks were used for the scenario analysis in this thesis). It is, in addition, very likely that no similar models exist that can reliably simulate much longer times spans. Hence, until considerably longer simulation times can be achieved, care should probably be taken when analysing LCA results obtained from highly detailed dynamic WWTP models.

Finally, it was concluded that if a FU for classic WWTP LCA is necessary, it should preferentially be an efficiency measure that has much influence on the environmental impacts. It was observed during rain weather conditions, that influent volume increased more than influent COD mass. Thus, during rain weather, influent pure water mass increased more than influent COD mass. Additional treatment of pure water will likely not result in the same environmental impacts increase as additional treatment of COD. Hence, using influent volume as FU in this case led to an additional downscaling of the impacts - that does not seem correct - in comparison with using influent COD mass as FU. Influent volume served in this thesis as approximation of treated water volume. The conclusion that treated water volume as FU might lead to misleading conclusions, is in line with findings in the literature.

4.2 Future perspectives

If a dynamic WWTP model is coupled to LCA, the step from classic to dynamic LCA is methodologically not very complicated: Instead of integrating over the whole simulation time span, the simulation time span has to be divided into smaller intervals and integration over every individual interval has to be performed. It is therefore probably worthwhile to always provide the functionality of dynamic LCA, when coupling dynamic (WWTP) models to LCA.

The most important limitation, was the fact that the Eindhoven model does not provide results for some data that are very important for the LCA results, for instance CH_4, N_2O, and CO_2 emissions. Quantification of CH_4 and N_2O emissions was obtained through emission factors and quantification of CO_2 emissions was performed through a mass balance in combination with a conversion factor, but this resulted in poor data quality. To improve the reliability of the LCA results, this data quality should be increased.
According to Foley et al. (2011), WWTP CH_4 emissions might originate from the sewer and already escape the system via the influent works. Hence, modelling these emissions might not be accurate and determining a site specific emission factor, for the Eindhoven WWTP, might be a good idea.
According to Ni and Yuan (2015) the fundamental mechanisms of N_2O production are still not fully understood. However, they state that mathematical modelling of N_2O emissions has reached a maturity that facilitates the estimation of site-specific N_2O emissions and it might thus be worthwhile to investigate the possibility of incorporating this into the Eindhoven model.
The applied mass balance to calculate oxidized COD mass seemed to result in trustworthy outcomes. However, still a conversion factor was necessary to convert oxidized COD into CO_2 emissions. Inclusion of the stoichiometry of the conversion of COD to CO_2 into the Eindhoven model, seems a worthwhile addition.
In addition, some processes that are present in reality at the Eindhoven WWTP, are not modelled in the WWTP model, for instance pumping energy in the primary sedimentation tanks and sludge thickening. If the Eindhoven WWTP governing body, Waterschap the Dommel, would be interested in further developing dynamic LCA, it might be a good idea to include the missing aspects into the model.

Finally, an important opportunity still remains in the application of dynamic LCA: It was mentioned that non-linearity is usually not considered in LCA (JRC-IES, 2011). If dynamic models (or time series of measurements) are coupled to LCA, the consequences of this can be investigated. For instance, in an EPA technical report on water quality for aquatic life in terms of ammonia (EPA, 2013), it can be found that acute biological effects as a consequence of ammonia toxicity do not seem to respond in a linear way to changes in ammonia concentrations in the lower concentration ranges. It would be interesting to investigate whether or not this has important consequences for LCA results.

Bibliography

(2013). Aquatic life ambient water quality criteria for ammonia - freshwater. Technical report, EPA.

Afman, M. R. and Korving, L. (2013). Milieuscore monoverbranding van zuiveringsslib. detailanalyse snb-monoverbranding, effect fosfaathergebruik. url: http://www.ce.nl/publicatie/milieuscore_monoverbranding_van_zuiveringsslib/1378. Technical report, CE Delft.

Ahn, J. H., Kim, S., Park, H., Rahm, B., Pagilla, K., and Chandran, K. (2010). N2O Emissions from Activated Sludge Processes, 2008-2009: Results of a National Monitoring Survey in the United States. *Environmental Science & Technology*, 44(12):4505–4511.

Alvarez-Gaitan, J. P., Short, M. D., Lundie, S., and Stuetz, R. (2016). Towards a comprehensive greenhouse gas emissions inventory for biosolids. *Water Research*, 96:299–307.

Amerlinck, Y. (2015). *Model refinements in view of improving wastewater treatment plant optimization: restoring the balance in sub model detail. Ghent University, Belgium.* PhD thesis. url: https://biblio.ugent.be/publication/6952234.

Ayyakkannu, K. and Chandramohan, D. (1971). Occurrence and distribution of phosphate solubilizing bacteria and phosphatase in marine sediments at Porto Novo. *Marine Biology*, 11:201–205.

Batstone, D. J., Keller, J., Angelidaki, I., Kalyuzhnyi, S. V., Pavlostathis, S. G., Rozzi, A., Sanders, W. T. M., Siegrist, H., and Vavilin, V. A. (2002a). The IWA Anaerobic Digestion Model No 1 (ADM1). *Water Science and Technology*, 45(10):65–73.

Batstone, D. J., Keller, J., Angelidaki, I., Kalyuzhnyi, S. V., Pavlostathis, S. G., Rozzi, A., Sanders, W. T. W., Siegrist, H., and Vavilin, V. A. (2002b). Anaerobic Digestion Model No. 1 (ADM1). Technical report, IWA Task Group on Modelling of Anaerobic Digestion Processes.

Benedetti, L., Langeveld, J., Van Nieuwenhuijzen, A. F., de Jonge, J., De Klein, J., Flameling, T., Nopens, I., Van Zanten, O., and Weijers, S. (2012). KALLISTO: cost effective and integrated optimization of the urban wastewater system Eindhoven. In *IWA World Water Congress, 8th, Papers*, page 3.

Bisinella de Faria, A. B., Spérandio, M., Ahmadi, A., and Tiruta-Barna, L. (2015). Evaluation of new alternatives in wastewater treatment plants based on dynamic modelling and life cycle assessment (DM-LCA). *Water Research*, 84:99–111.

Blom, B. (2013). Waterschap De Dommel. Beheren afvalwaterketen. Milieuprestatie 2013. Online, url: http://edepot.wur.nl/306675.

Boyle, W. C., Craven, A., Danley, W., and Rieth, M. (1994). Oxygen Transfer Studies at the Madison Metropolitan Sewerage District Facilities. Technical report, U.S. Environmental Protection Agency (EPA). EPA/600/R-94/096.

Corominas, L., Foley, J., Guest, J. S., Hospido A. Larsen, H. F., Morera, S., and Shaw, A. (2013a). Life cycle assessment applied to wastewater treatment: State of the art . *Water Research*, 47(15):5480–5492.

Corominas, L., Larsen, H. F., Flores-Alsina, X., and Vanrolleghem, P. A. (2013b). Including Life Cycle Assessment for decision-making in controlling wastewater nutrient removal systems. *Journal of Environmental Management*, 128:759–767.

de Haas, D. and Hartley, K. (2004). Greenhouse gas emission from BNR plants: do we have the right focus? Name of Conference: Sewage Management: Risk Assessment and Triple Bottom Line, Conference location: Cairns, Australia.

De Meester, S. (2017). Personal communication with professor De Meester from Ghent University, Department of Industrial Biological Sciences.

De Mulder, C. (2014). Impact of intrinsic and extrinsic parameters on the oxygen kinetic parameters of ammonia and nitrite oxidizing bacteria.

De Mulder, C. (2017). Personal communication with ir. Chaïm De Mulder, researcher at Ghent University, Faculty of Bioscience Engineering, Biomath.

De Mulder, C., Flameling, T., Langeveld, J., Amerlinck, Y., Weijers, S., and Nopens, I. (2017). Automating the raw data to model input process using flexible open source tools. In *Frontiers International Conference on Wastewater Treatment, Palermo, Italy.*

Elser, J. J., Bracken, M. E. S., Cleland, E. E., Gruner, D. S., Harpole, W. S., Hillebrand, H., Ngai, J. T., Seabloom, E. W., Shurin, J. B., and Smith, J. E. (2007). Global analysis of nitrogen and phosphorus limitation of primary producers in freshwater, marine and terrestrial ecosystems. *Ecology Letters*, 10(12):1135–1142.

Fang, L. L., Valverde-Perez, B., Damgaard, A., Plosz, B. G., and Rygaard, M. (2016). Life cycle assessment as development and decision support tool for wastewater resource recovery technology. *Water Research*, 88:538–549.

Flameling, T. (2016). Personal communication with Tony Flameling from Waterboard De Dommel.

Fleming Training Center (2016). Advanced Wastewater Treatment. Online, url: http://www.tennessee.gov/assets/entities/environment/attachments/study_3201.pdf.

Flores-Alsina, X., Gallego, A., Feijoo, G., and Rodriguez-Roda, I. (2010). Multiple-objective evaluation of wastewater treatment plant control alternatives. *Journal of Environmental Management*, 91(5):1193–1201.

Foley, J., de Haas, D., Hartley, K., and Lant, P. (2007). Life Cycle Assessment of Biological Nutrient Removal Wastewater Treatment Plants.

Foley, J., Yuan, Z., Keller, J., Senante, E., Chandran, K., Willis, J., Shah, A., van Loosdrecht, M., and van Voorthuizen, E. (2011). N2O and CH4 emission from wastewater collection and treatment systems. State of the Science Report. Technical report, GWRC.

Forster, P., Ramaswamy, V., Artaxo, P., Berntsen, T., Betts, R., Fahey, D. W., Haywood, J., Lean, J., Lowe, D. C., Myhre, G., Nganga, J., Prinn, R., Raga, G., Schulz, M., and Van Dorland, R. (2007). Changes in Atmospheric Constituents and in Radiative Forcing. Technical report, IPCC. In: Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change. [Solomon, S., D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Averyt, M.Tignor and H.L. Miller (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.

Gallego, A., Hospido, A., Moreira, M. T., and Feijoo, G. (2008). Environmental performance of wastewater treatment plants for small populations. *Resources Conservation and Recycling*, 52(6):931–940.

Gernaey, K. V., Jeppsson, U., Vanrollehem, P. A., and Copp, J. B. (2014). Benchmarking of Control Strategies for Wastewater Treatment Plants. Technical report, IWA Task Group on Benchmarking of Control Strategies for Wastewater Treatment Plants.

Goedkoop, M., Heijungs, R., Huijbregts, M., De Schryver, A., Struijs, J., and van Zelm, R. (2013). ReCiPe 2008. A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and endpoint level. First edition (version 1.08). Report I: Characterisation. Technical report, RIVM, CML, PRé Consultants, and Radboud Universiteit Nijmegen.

Goedkoop, M. and Spriensma, R. (2001). Eco-indicator 99, a damage oriented method for lifecycle impact assessment, methodology report. Third edition. Technical report, PRé Consultants.

Griffith, D. R., Barnes, R. T., and Raymond, P. A. (2009). Inputs of Fossil Carbon from Wastewater Treatment Plants to US Rivers and Oceans. *Environmental Science & Technology*, 43(15):5647–5651.

Guinée, J. B., Gorre, M., Heijungs, R., Huppes, G., Kleijn, R., de Koning, A., van Oers, L., Wegener Sleeswijk, A., Suh, S., Udo de Haes, H. A., de Bruijn, H., van Duin, R., and Huijbregts, M. A. J. (2002). *Handbook on life cycle assessment. Operational guide to the ISO standards. I: LCA in perspective. IIa: Guide. IIb: Operational annex. III: Scientific background.* Kluwer Academic Publishers.

Guo, J., Fu, X., Andrés Baquero, G., Sobhani, R., Nolasco, D. A., and Rosso, D. (2016). Trade-off between carbon emission and effluent quality of activated sludge processes under seasonal variations of wastewater temperature and mean cell retention time. *Science of the Total Environment*, 547:331–344.

Guo, L., Porro, J., Sharma, K. R., Amerlinck, Y., Benedetti, L., Nopens, I., Shaw, A., Van Hulle, S. W., Yuan, Z., and Vanrolleghem, P. A. (2012). Towards a benchmarking tool for minimizing wastewater utility greenhouse gas footprints. *Water Science & Technology*, 66(11):2483–2495.

Hadjimichael, A., Morera, S., Benedetti, L., Flameling, T., Corominas, L., Weijers, S., and Comas, J. (2016). Assessing urban wastewater system upgrades using integrated modeling, life cycle analysis and shadow pricing. *Environmental Science & Technology*, Just Accep.

Hauschild, M. Z., Goedkoop, M., Guinee, J., Heijungs, R., Huijbregts, M., Jolliet, O., Margni, M., De Schryver, A., Humbert, S., Laurent, A., Sala, S., and Pant, R. (2013). Identifying best existing practice for characterization modeling in life cycle impact assessment. *International Journal of Life Cycle Assessment*, 18(3):683–697.

Heinke, W. H., Tay, J. H., and Qazi, M. (1980). Effects of chemical addition on the performance of settling tanks. *Water Environment Federation.*

Henze, H., van Loosdrecht, M. C. M., and Ekama, G. (2008a). *Biological Wastewater Treatment: Principles, Modeling, and Design.* IWA Publishing.

Henze, M., Gujer, W., Mino, T., and van Loosdrecht, M. (2000). Activated sludge models ASM1, ASM2, ASM2d and ASM3. Edited by IWA task group on mathematical modelling for design and operation of biological wastewater treatment. Published by IWA Publishing in its Scientific and Technical Report series. Technical report, IWA.

Henze, M., van Loosdrecht, M. C. M., Ekama, G. A., and Brdjanovic, D., editors (2008b). *Biological Wastewater Treatment*. IWA Publishing.

Holmgren, K. E., Li, H., Verstraete, W., and Cornel, P. (2015). State of the Art Compendium Report on Resource Recovery from Water. Technical report, International Water Association.

IPCC (2006). 2006 IPCC Guidelines for National Greenhouse Gas Inventories. Volume 5: Waste. Chapter 6: Wastewater Treatment and Discharge. Online, url: http://www.ipcc-nggip.iges.or.jp/public/2006gl/pdf/5_Volume5/V5_6_Ch6_Wastewater.pdf. Technical report, IPCC.

IPCC (2007). Climate Change 2007: Synthesis Report. Synthesis Report. Technical report, IPCC.

ISO (2006a). International standard. ISO 14040. Second edition 2006-07-01. Environmental management - Life cycle assessment - Principles and framework. Technical report, ISO.

ISO (2006b). International standard. ISO 14044. First edition 2006-07-01. Environmental management - Life cycle assessment - Requirements and guidelines. Technical report, ISO.

JRC-IES (2010a). ILCD handbook. International Reference Life Cycle Data System. Framework and requirements for Life Cylce Impact Assessment models and indicators. First edition. Technical report, European Commission.

JRC-IES (2010b). ILCD handbook. International Reference Life Cycle Data System. General guide for Life Cycle Assessment - Detailed guidance. First edition. Technical report, European Commission.

JRC-IES (2011). ILCD handbook. International Reference Life Cycle Data System. Recommendations for Life Cycle Impact Assessement in the European context - based on existing environmental impact assessment models and factors. First edition. Technical report, European Commission.

Kampschreur, M. J. (2010). *Dynamics of nitric oxide and nitrous oxide emission during nitrogen conversion processes*. PhD thesis. url: http://repository.tudelft.nl/islandora/object/uuid:e48e4002-684f-4ede-95a7-47e33be018f5?collection=research.

Kim, D., Bowen, J. D., and Kinnear, D. (2015). Comprehensive Numerical Modeling of Greenhouse Gas Emissions from Water Resource Recovery Facilities. *Water Environment Research*, 87:1955–1969.

Langeveld, J. G., Benedetti, L., de Klein, J. J. M., Nopens, I., Amerlinck, Y., van Nieuwenhuijzen, A., Flameling, T., van Zanten, O., and Weijers, S. (2013). Impact-based integrated real-time control for improvement of the Dommel River water quality. *Urban Water Journal*.

Law, Y., Jacobsen, G. E., Smith, A. M., Yuan, Z. G., and Lant, P. (2013). Fossil organic carbon in wastewater and its fate in treatment plants. *Water Research*, 47:5270–5281.

Law, Y., Ye, L., Pan, Y., and Yuan, Z. (2012). Nitrous oxide emissions from wastewater treatment processes. *Philosophical Transactions of the Royal Society B: Biological Sciences*, 367:1265–1277.

Masoni, P. and Zamagni, A. (2011). Guidance Document for performing LCAs on Fuel Cells and H2 Technologies. Technical report, European Commission.

McCarty, P. L., Bae, J., and Kim, J. (2011). Domestic Wastewater Treatment as a Net Energy Producer–Can This be Achieved? *Environmental Science & Technology*, 45(17):7100–7106.

Meneses, M., Concepcion, H., and Vilanova, R. (2016). Joint Environmental and Economical Analysis of Wastewater Treatment Plants Control Strategies: A Benchmark Scenario Analysis. *Sustainability*, 8(4).

Meneses, M., Concepcion, H., Vrecko, D., and Vilanova, R. (2015). Life Cycle Assessment as an environmental evaluation tool for control strategies in wastewater treatment plants. *Journal of Cleaner Production*, 107:653–661.

Meneses-Jacome, A., Osorio-Molina, A., Parra-Saldivar, R., Gallego-Suarez, D., Velasquez-Arredondo, H. I., and Ruiz-Colorado, A. A. (2015). LCA applied to elucidate opportunities for biogas from wastewaters in Colombia . *Water Science and Technology*, 71(2):211–219.

Mouri, G., Takizawa, S., Fukushi, K., and Oki, T. (2013). Estimation of the effects of chemically-enhanced treatment of urban sewage system based on life-cycle management. *Sustainable Cities and Society*, 9:23–31.

Munoz, I., Gomez, M. J., Molina-Diaz, A., Huijbregts, M. A. J., Fernandez-Alba, A. R., and Garcia-Calvo, E. (2008). Ranking potential impacts of priority and emerging pollutants in urban wastewater through life cycle impact assessment. *Chemosphere*, 74(1):37–44.

Ni, B. J. and Yuan, Z. (2015). Recent advances in mathematical modeling of nitrous oxides emissions from wastewater treatment processes. *Water Research*.

Nopens, I. (2015). Modelling and control of Wastewater treatment plants. Course, Ghent University, Faculty of Bio-science Engineering, Academic year 2015-2016.

Nopens, I. (2017). Personal communication with professor Nopens from Ghent University, Faculty of Bioscience Engineering, Biomath.

Ontiveros, G. A. and Campanella, E. A. (2013). Environmental performance of biological nutrient removal processes from a life cycle perspective. *Bioresource Technology*, 150:506–512.

Pizzol, M., Christensen, P., Schmidt, J., and Thomsen, M. (2011). Impacts of "metals" on human health: a comparison between nine different methodologies for Life Cycle Impact Assessment (LCIA). *Journal of Cleaner Production*, 19(6-7):646–656.

PubChem (Visited at 14 may 2017). Aluminum phosphate. url: https://pubchem.ncbi.nlm.nih.gov/compound/Aluminum_phosphate.

Rahman, S. M., Eckelman, M. J., Onnis-Hayden, A., and Gu, A. Z. (2016). Life-Cycle Assessment of Advanced Nutrient Removal Technologies for Wastewater Treatment. *Environmental Science & Technology*, 50(6):3020–3030.

Redmon, D., C., B. W., and L., E. (1983). Oxygen Transfer Efficiency Measurements in Mixed Liquor Using Off-Gas Techniques. *Water Pollution Control Federation*, 55(11):1338–1347.

Remy, C. and Jekel, M. (2008). Sustainable wastewater management: life cycle assessment of conventional and source-separating urban sanitation systems. *Water Science & Technology*, 58(8):1555–1562.

Renou, S., Thomas, J. S., Aoustin, E., and Pons, M. N. (2008). Influence of impact assessment methods in wastewater treatment LCA. *Journal of Cleaner Production*, 16(10):1098–1105.

Rieger, L., Gillot, S., Langergraber, G., Ohtsuki, T., Shaw, A., Takcs, I., and Winkler, S. (2013). Guidelines for Using Activated Sludge Models. Scientific and Technical Report No. 22. Technical report, IWA Task Group on Good Modelling Practice.

Rodriguez-Garcia, G., Frison, N., Vazquez-Padin, J. R., Hospido, A., Garrido, J. M., Fatone, F., Bolzonella, D., Moreira, M. T., and Feijoo, G. (2014). Life cycle assessment of nutrient removal technologies for the treatment of anaerobic digestion supernatant and its integration in a wastewater treatment plant. *Science of the Total Environment*, 490:871–879.

Rodriguez-Garcia, G., Molinos-Senante, M., Hospido, A., Hernández-Sancho, F., Moreira, M., and Feijoo, G. (2011). Environmental and economic profile of six typologies of wastewater treatment plants. *Water Research*.

Rosso, D., Iranpour, R., and Stenstrom, M. K. (2005). Fifteen Years of Offgas Transfer Efficiency Measurements on Fine-Pore Aerators: Key Role of Sludge Age and Normalized Air Flux. *Water Environment Research*, 77:266–273. Water Environment Research.

Schaubroeck, T. and Dewulf, J. (2015). Clean Technology. Course, Ghent University, Faculty of Bioscience Engineering, academic year 2015-2016.

Semblante, G. U., Hai, F. I., Ngo, H. H., Guo, W. S., You, S. J., Price, W. E., and Nghiem, L. D. (2014). Sludge cycling between aerobic, anoxic and anaerobic regimes to reduce sludge production during wastewater treatment: Performance, mechanisms, and implications. *Bioresource Technology*, 155:395–409.

Sijstermans, L. (2016). Personal communication with Luc Sijstermans (Manager Process & Environmental issues N.V. Slibverwerking Noord-Brabant).

Steele, M. M., Anctil, A., and Ladner, D. a. (2014). Integrating algaculture into small wastewater treatment plants: process flow options and life cycle impacts. *Environmental science. Processes & impacts*, 16:1387–1399.

Takács, I., Patry, G. G., and Nolasco, D. (1991). A dynamic model of the clarification-thickening process. *Water Research*, 25(10):1263–1271.

Tay, J. H. (1982). Development of a settling model for primary settling tanks. *Water Research*.

Tchobanoglous, G., Burton, F. L., and Stensel, H. D. (2003). *Wastewater Engineering: Treatment and Reuse*. Fourth edition edition.

Telkamp, P., Reitsma, B. A. H., Marsman, H. J., and Blom, J. P. (2009). *Proceshandboek rwzi Eindhoven. Tweede druk.* Waterboard De Dommel. Process manual of the Eindhoven WWTP. Dutch.

Torfs, E. (2015). *Different settling regimes in secondary settling tanks: experimental process analysis, model development and calibration.* PhD thesis.

Tseng, L. D. Y., Robinson, A. K., Zhang, X. Y., Xu, X. M., Southon, J., Hamilton, A. J., Sobhani, R., Stenstrom, M. K., and Rosso, D. (2016). Identification of Preferential Paths of Fossil Carbon within Water Resource Recovery Facilities via Radiocarbon Analysis. *Environmental Science & Technology*, 50:12166–12178.

UNESCO (Visited at 22 October 2016). UNESCO. "Building peace in the minds of men and women". Water Scarcity and Quality. Online, url: http://en.unesco.org/themes/water-security/hydrology/water-scarcity-and-quality.

Van Loosdrecht, M. C. M. and Henze, M. (1999). Maintenance, endogeneous respiration, lysis, decay and predation. In *4th IAWQ Seminar on Modelling and Microbiology of Activated Sludge Processes*.

Verstraete, W. and Vlaeminck, S. E. (2011). ZeroWasteWater: short-cycling of wastewater resources for sustainable cities of the future. *International Journal of Sustainable Development and World Ecology*, 18(3):253–264.

VITO (2010a). Anaerobic Biological Wastewater Treatment. Online, visited at 31 Januari 2017, url: https://emis.vito.be/en/techniekfiche/anaerobic-biological-wastewater-treatment.

VITO (2010b). Biological nutrient removal. Online, visited at 22 October 2016, url: https://emis.vito.be/en/techniekfiche/biological-nutrient-removal.

VROM (2008). Protocol 8136 Afvalwater, t.b.v NIR 2008 uitgave maart 2008. Dutch.

Wang, X., Liu, J., Ren, N., and Duan, Z. (2012). Environmental profile of typical anaerobic/anoxic/oxic wastewater treatment systems meeting increasingly stringent treatment standards from a life cycle perspective . *Bioresource Technology*, 126:31–40.

Wentzel, M. C., Ubisi, M. F., Lakay, M. T., and Ekama, G. A. (2002). Incorporation of inorganic material in anoxic/aerobic and activated sludge system mixed liquor. *Water Research*, (36):5074–5082.

Zang, Y. W., Li, Y., Wang, C., Zhang, W. L., and Xiong, W. (2015). Towards more accurate life cycle assessment of biological wastewater treatment plants: a review. *Journal of Cleaner Production*, 107:676–692.

APPENDIX A
Additional information from the literature

A.1 Clear examples of the usefulness of life cycle assessment for wastewater treatment plants

In the following, 2 examples will be given of WWTP LCA studies with remarkable results.

In the study of Rahman et al. (2016) an LCA is performed to assess the environmental impact of advanced nutrient removal strategies. Some scenarios that apply primary and secondary wastewater treatment are compared to scenarios that, in addition to a primary and secondary treatment, also apply a tertiary treatment or multistage tertiary treatments. It is shown that by increasing nutrient removal from the wastewater, direct eutrophication potential caused by nutrients in the effluent decreases. However, indirect eutrophication potential - caused by nutrients emitted by energy and chemical usage - increases, because of increased chemicals and energy usage. In 2 scenarios applying multistage tertiary treatments, the total eutrophication potential is even bigger than in the scenarios applying a single tertiary treatment. (The uncertainty in the results of these multistage treatments is however very big). These results clearly demonstrate the usefulness, and maybe even the necessity, of applying LCA in decision making.

Conventional and source-separating urban sanitation systems were compared with regard to their ecological sustainability using LCA by Remy and Jekel (2008). These source separating systems are based on the separate collection and treatment of the different wastewater fractions, enabling the efficient recovery of nutrients and the reuse of treated wastewater. They were proposed as alternative to deal with some inherent disadvantages of the conventional urban sanitation system. The results indicate that source separation does not necessarily result in a system with less environmental impacts.

If the conventional system is energetically optimized and equipped with extended nutrient removal, its impact is comparable to the source-separating systems. However, source separation has the potential to offer ecological benefits depending on the system configuration. Especially the input of toxic heavy metals to agriculture with sewage sludge can be substantially lowered if separately collected urine and faeces are used as organic fertilizer.

APPENDIX B

Additional information about materials and methods

B.1 Some technical information on the Eindhoven WWTP

B.1.1 The activated sludge tanks

Some technical information of the Eindhoven WWTP ASTs can be found in Table B.1.

Table B.1: Some characteristics of the ASTs at the Eindhoven WWTP.

	Total	Per tank	Unit
Total volume		30,192	m^3
Volume anaerobic part		3,733	m^3
Volume anoxic part		9,525	m^3
Volume aerated part		16,933	m^3
Diameter (incl. outside wall)		75.7	m
Water height anaerobic part		7.5	m
Water height anoxic part		7.3	m
Water height aerated part		7	m
Dry weather average flow (DWA)	5,600		m^3/h
Rain weather average flow (RWA)	26,250		m^3/h
Anaerobic contact time at DWA		1	h
Biological sludge concentration		3.1	kg dm/m^3 [a]
Sludge concentration (biological + chemical fraction [b])		3.5	kg dm/m^3 [a]
Loading rate	0.064		kg BOD/kg dm/d^3 [a]
Maximum RAS ratio	0.432		times RWA
Min. flow rate RAS		1,416	m^3/h
Max. flow rate RAS		3,784	m^3/h
Max. flow rate recirculation A	1		times DWA
Max. flow rate recirculation B	8		times DWA

[a] dm: dry matter

[b] The chemical fraction of the sludge is formed due to the Al dosing.

B.2 Model of the wastewater treatment plant of Eindhoven

B.2.1 Overview of the whole plant model

An overview of the model as implemented in WEST, can be found in Figure B.1. As stated in Subsection 2.2.1, the model used in this thesis is an update of the model described by (Amerlinck, 2015). A version of Figure B.1 can also be found in (Amerlinck, 2015). The figure there is designated as Figure A.1. The figure in this thesis is different from the one in Amerlinck (2015). Some blocks are replaced or added, controllers with their data links are also shown here, and many of the blocks have other names. Therefore, in Table B.2 an overview of the blocks used in the model in this thesis

can be found.
Important differences between the model used in thesis and the model version of (Amerlinck, 2015) are: In this version, the controllers are also modelled. The model for the SST in this version is the Takács model (Takács et al., 1991). In this version, the underflow of the PST is also connected to a sludge disposal. In this way, mass of primary sludge and secondary sludge can be added together in this thesis (in the Python™ scripts) to simulate the behaviour of the real WWTP, since both are pumped to Mierlo through the same pipes (see Subsection 2.1.2).

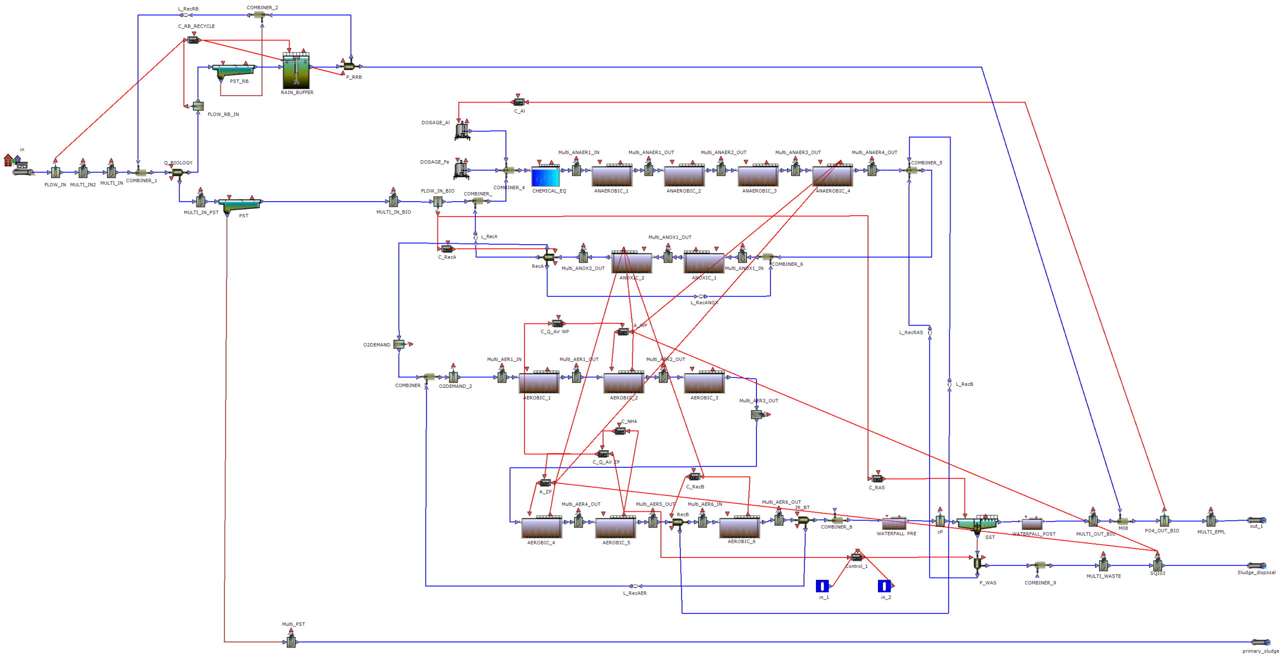


Figure B.1: Partial layout of the Eindhoven WWTP model - as it is used in this thesis, showing the most important components.

Table B.2: Overview of the blocks used in the model in this thesis (see also Figure B.1). Each block has an underlying model. The information in this table is partly based on Table A.1 in the document of Amerlinck (2015).

Name	WEST model name	Purpose of the model
in	Influent_in	Influent and fractionation model
FLOW_IN	Sensor_Flow	Measurement influent flow rate
MULTI_IN2	EffluentQualityIndex	Measurement water quality parameters influent
		Continued on next page

Table B.2 – continued from previous page

Name	WEST model name	Purpose of the model
MULTI_IN	MultiSensor	Measure and calculate variables not available as state variables
COMBINER_1	TwoCombiner	Combining influent and recycle from RBT
Q_BIOLOGY	AbsTwoSplitter	Split flow to biology and RBT
FLOW_RB_IN	Sensor_Flow	Measurement flow rate to RBT
PST_RB	PrimaryPointSettler	RBT model part 1 - removal suspended solids
RAIN_BUFFER	PumpedVolumeBuffer _Eindhoven	RBT model part 2 - storage, recycle, and overflow
P_RRB	AbsTwoSplitter	Recycle to influent pumps from RBT
C_RB_RECYCLE	raintank_Eindhoven	Flow rate control to influent pumps from RBT
COMBINER_2	TwoCombiner	Combining normal emptying and removed sludge
L_RecRB	DifferentialLoopBreaker	Model artefact
MULTI_IN_PST	MultiSensor	Measure and calculate variables not available as state variables
PST	Tay4	Sand trap and PST
MULTI_IN_BIO	MultiSensor	Measure quantities going into biology
COMBINER_3	TwoCombiner	Combining flow from PST and recirculation A
FLOW_IN_BIO	Sensor_Flow	Flow rate measurement
DOSAGE_Al	Alum	Al dosage
C_Al	OperatorDelayed	Control Al dose based on effluent PO_4^{3-} measurements
DOSAGE_Fe	IronHydroxide	Unused
COMBINER_4	ThreeCombiner	Combining main stream with dosed metal salts
CHEMICAL_EQ	MEChemical	Chemical PO_4^{3-} removal

Continued on next page

Table B.2 – continued from previous page

Name	WEST model name	Purpose of the model
Various blocks commencing with "Multi"	MultiSensor	Measurements
ANAEROBIC_1	FixVolumeASU	Anaerobic tank
ANAEROBIC_2	FixVolumeASU	Anaerobic tank
ANAEROBIC_3	FixVolumeASU	Anaerobic tank
ANAEROBIC_4	FixVolumeASU	Anaerobic tank
COMBINER_5	ThreeCombiner	Combining flow from anaerobic tank, RAS, and recirculation B to denitrification tank
COMBINER_6	TwoCombiner	Combining internal recirculation denitrification tank and flow from anaerobic tank
ANOXIC_1	FixVolumeASU	Denitrification tank
ANOXIC_2	FixVolumeASU	Denitrification tank
RecA	AbsThreeSplitter	Splitting flow from denitrification tank to recirculation A, internal recirculation denitrification tank, and aerated tanks
C_RecA	linear_Saturation	Control recirculation A
L_RecANOX	DifferentialLoopBreaker	Model artefact
L_RecA	DifferentialLoopBreaker	Model artefact
O2DEMAND	OD	Measurement O_2 demand in flow from denitrification tank to aerated tank
COMBINER_7	TwoCombiner	Combining flow from denitrification tank and internal recirculation aerated tank to aerated tank
O2DEMAND_2	OD	Measurement O2 demand in aerated tank
AEROBIC_1	FixVolumeASU	Aerated tank
AEROBIC_2	FixVolumeASU	Aerated tank (with winter aeration package)

Continued on next page

Table B.2 – continued from previous page

Name	WEST model name	Purpose of the model
A_WP	Irvine_Aeration_model _Carbon_foot_print	Winter aeration package
C_Q_Air WP	OnOffBand	Control airflow rate winter aeration package
AEROBIC_3	FixVolumeASU	Aerated tank
AEROBIC_4	FixVolumeASU	Aerated tank (with summer aeration package)
A_ZP	Irvine_Aeration_model _Carbon_foot_print	Summer aeration package
C_NH4	PID_AntiWindup _Saturation	Ammonium control
C_Q_Air ZP	PID_AntiWindup _Saturation	Control airflow rate summer aeration package
AEROBIC_5	FixVolumeASU	Aerated tank
RecB	AbsTwoSplitter	Combining recirculation B with flow from AEROBIC_5
C_RecB	PI_Saturation_recB_EHV	Control recirculation B
L_RecB	DifferentialLoopBreaker	Model artefact
AEROBIC_6	FixVolumeASU	Aerated tank
IR_BT	AbsTwoSplitter	Internal recirculation aerated tank
L_RecAER	DifferentialLoopBreaker	Model artefact
COMBINER_8	TwoCombiner	No function
WATERFALL_PRE	reaeration_tank	Model reaerating effect of cascade distribution system
cP	Sensor_COD	Measurement of COD
SST	Takacs	Secondary sedimentation tank
C_RAS	ConstantRatio_double	Control underflow rate of SST
WATERFALL_POST	reaeration_tank	Model reaerating effect of cascade distribution system

Continued on next page

Table B.2 – continued from previous page

Name	WEST model name	Purpose of the model
MULTI_OUT_BIO	MultiSensor	Measurement
M08	TwoCombiner	Combining effluent ASTs and overflow RBT
PO4_OUT_BIO	Sensor_PO4	PO_4^{3-} measurement in effluent
MULTI_EFFL	MultiSensor	Measurement
P_WAS	AbsTwoSplitter	Sludge wastage pump
Control_1	Operator	Control sludge wastage
SQI03	EffluentQualityIndex	Measurement water quality parameter in waste sludge
COMBINER_9	TwoCombiner	Combining primary and secondary waste sludge
MULTI_WASTE	MultiSensor	Measurement
L_RecRAS	DifferentialLoopBreaker	Model artefact
out_1	Effluent_out_1	Effluent discharge
Sludge_disposal	Effluent_sludge_disposal	Discharge of secondary sludge
primary_sludge	Effluent_out_2	Discharge of primary sludge

B.2.2 Biokinetic model

In Table B.3, a short description of all the state variables used in the biokinetic sub-model of the Eindhoven WWTP model can be found. This biokinetic model is based on ASM2d (Henze et al., 2000), but some minor adaptations were made (see Subsection 2.2.3). In Table B.4 the state variables are shown with their respective conversion factors, which illustrates their mass composition.

Table B.3: State variables of the Eindhoven biokinetic submodel. According to (Henze et al., 2000), variables denoted with S are soluble and only transported with water, variables denoted with X are particulate and are assumed to be associated with the activated sludge, and all components are assumed to be distributed homogeneously throughout the system.

State variable	Units	Description
S_A	[M(COD) L^{-3}]	Fermentation end products. Assumed to be acetate for stoichiometric computations.
S_{ALK}	[n(HCO_3^-) L^{-3}]	Alkalinity of the wastewater. Assumed to be HCO_3^- for stoichiometric computations.
S_F	[M(COD) L^{-3}]	Fermentable readily biodegradable organic substrates. Does not include fermentation products, since these are not fermentable.
S_I	[M(COD) L^{-3}]	Inert soluble organic material.
S_{N_2}	[M(N) L^{-3}]	N_2. Assumed to be the only nitrogenous product of denitrification.
S_{NH_4}	[M(N) L^{-3}]	NH_4^+ + NH_3. For electrical balance, all S_{NH_4} is assumed to be NH_4^+.
S_{NO_3}	[M(N) L^{-3}]	NO_3^- + NO_2^-. For stoichiomteric computations, assumed to be NO_3^- only.
S_{O_2}	[M(O_2) L^{-3}]	O_2
S_{PO_4}	[M(P) L^{-3}]	Inorganic soluble P, primarily ortho-phosphates. For the balance of electrical charges, it is assumed that 50% is $H_2PO_4^-$ and 50% HPO_4^{2-}, independently of pH.
X_{AUT}	[M(COD) L^{-3}]	Nitrifying organisms.
X_H	[M(COD) L^{-3}]	Heterotrophic organisms.
X_I	[M(COD) L^{-3}]	Inert particulate organic material.
X_{MeOH}	[M(TSS) L^{-3}]	Metal-hydroxides for P-precipitation. Assumed to be entirely $Fe(OH)_3$. Unused in the Eindhoven model.

Continued on next page

Table B.3 – continued from previous page

State variable	Units	Description
X_{MeP}	[M(TSS) L^{-3}]	Metal-phosphate, $MePO_4$, result of P-precipiation. Assumed to be entirely $FePO_4$. Unused in the Eindhoven model.
X_{PAO}	[M(COD) L^{-3}]	Phosphate-accumulating organisms (PAOs). The concentration X_{PAO} doesn't include the cell internal storage products X_{PP} and X_{PHA}, it only contains "true" biomass.
X_{PHA}	[M(COD) L^{-3}]	A cell internal storage product of PAOs. Primarily poly-hydroxy-alkanoates (PHA). Occurs only associated with X_{PAO} (but is not included therein). For stoichiometric computations assumed to be poly-β-hydroxy-butyrate $(C_4H_6O_2)_n$.
X_{PP}	[M(P) L^{-3}]	Poly-phosphate, a cell internal storage product of PAOs. Occurs only associated with X_{PAO} (but is not included therein). For stoichiometric computations, poly-phosphates are assumed to have following composition: $(K_{0.33}Mg_{0.33}PO_3)_n$.
X_S	[M(COD) L^{-3}]	Slowly biodegradable substrates. High molecular weight, colloidal and particulate organic substrates.
X_{TSS}	[M(TSS) L^{-3}]	Total suspended solids.
X_{Ii}	[M(TSS) L^{-3}]	Particulate inorganic inert material.

Table B.4: State variables of the Eindhoven model with their units and corresponding conversion factors $i_{c,i}$. These factors are normally intended to be used in the conservation of mass equations of ASM2d, but they also indicate the mass composition of the state variables. Missing values are equal to 0. The units of $i_{c,i}$ are [M_c M_i^{-1}], e.g. for i_{N,S_F} this becomes [M_N $M_{S_F}^{-1}$], hence its units are [g N (g COD)$^{-1}$]. In case only a value is shown, this value is retrieved from Henze et al. (2000). In case a value is assigned to a symbolic conversion factor, e.g. i_{N,S_F} = 0.03, this value is retrieved from the Eindhoven model.

		Index c, conservation for:			
Index i		COD g COD	N g N	P g P	Mass g TSS
State variable	Unit	$i_{COD,i}$	$i_{N,i}$	$i_{P,i}$	$i_{TSS,i}$
S_{O_2}	[g O_2]	-1			
S_F	[g COD]	1	i_{N,S_F}=0.03	i_{P,S_F}=0.01	
S_A	[g COD]	1			
S_{NH_4}	[g N]		1		
S_{NO_3}	[g N]	-64/14	1		
S_{PO_4}	[g P]			1	
S_I	[g COD]	1	i_{N,S_I}=0.033	i_{P,S_I}=0	
S_{ALK}	[mole HCO_3^-]				
S_{N_2}	[g N]	-24/14	1		
X_I	[g COD]	1	i_{N,X_I}=0.02	i_{P,X_I}=0.01	i_{TSS,X_I}=0.75
X_S	[g COD]	1	i_{N,X_S}=0.04	i_{P,X_S}=0.01	i_{TSS,X_S}=0.75
X_H	[g COD]	1	$i_{N,BM}$=0.07 [a]	$i_{P,BM}$=0.02	$i_{TSS,BM}$=0.9
X_{PAO}	[g COD]	1	$i_{N,BM}$=0.07	$i_{P,BM}$=0.02	$i_{TSS,BM}$=0.9
X_{PP}	[g P]			1	3.23
X_{PHA}	[g COD]	1			0.60
X_{AUT}	[g COD]	1	$i_{N,BM}$=0.07	$i_{P,BM}$=0.02	$i_{TSS,BM}$=0.9
X_{TSS}	[g TSS]				-1 [b]
X_{MeOH}	[g TSS]				1
X_{MeP}	[g TSS]			0.205	1
X_{Ii}	[g TSS]			Variable [c]	1

Continued on next page

Table B.4 – continued from previous page

Index i		Index c, conservation for: COD g COD	N g N	P g P	Mass g TSS
State variable	Unit	$i_{COD,i}$	$i_{N,i}$	$i_{P,i}$	$i_{TSS,i}$

[a] The index c = BM means biomass, which has g COD as unit.

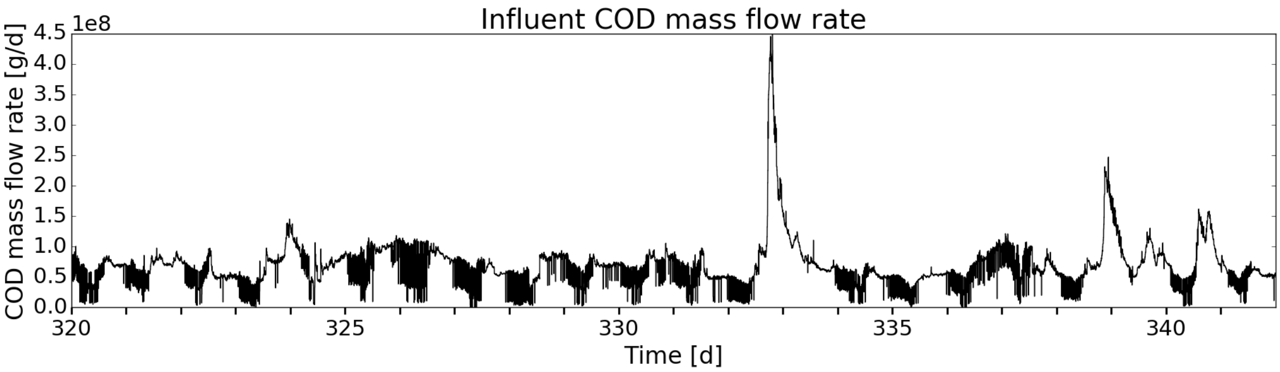
[b] TSS are counted twice, one time as the state variable X_{TSS} and a second time as the masses of the state variables that contribute to the TSS. Therefore, $i_{TSS,i}$ has to be negative to make the equation of the corresponding mass balance consistent.

[c] Precipitated P is added to X_{Ii} in the Eindhoven model (see Section 2.2.4). Therefore, its P content can vary due to the chemical P-removal.

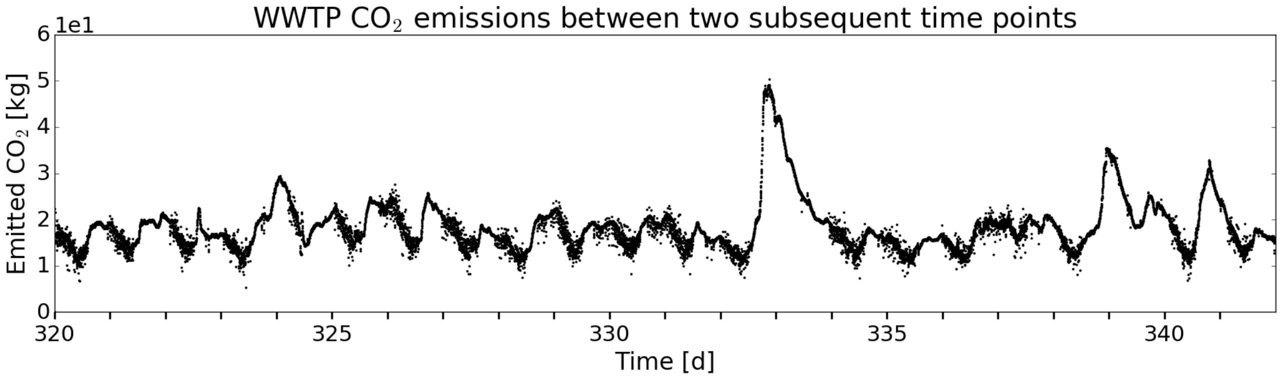
B.3 Life cycle inventory

B.3.1 Calculated CO_2 emissions

In Figure B.2 the influent COD mass flow rate is compared to the calculated WWTP CO_2 emissions as a result of COD oxidation in the ASTs, in order to get an idea of the correctness of the calculations (see Subsection 2.4.2). It is very clear that the trend of the CO_2 emissions follows the trend of the influent COD mass flow rate, which is indeed what is to be expected.



(a)



(b)

Figure B.2: Note that (a) shows the actual mass flow rate as a function of time and that every data point in (b) is the emitted CO_2 between the concerning and the previous point in time. The CO_2 emissions on this figure are only the emissions as a result of COD oxidation by the micro-organisms in the ASTs (both biogenic and fossil). In (a) a line is used instead of markers to plot the discrete points in time, to visualize the dynamic behaviour of the influent COD more clearly. Influent COD is plotted with markers in Figure C.1. These figures are valid for scenario 3. and 4. In case only dry weather is considered, the considered time span runs from day 320 to day 332. In case of dry and wet weather, from day 320 to 342.

B.4 Life cycle impact assessment

B.4.1 Characterization factors used in this thesis

The ReCiPe (http://www.lcia-recipe.net/) midpoint characterization factors used in this thesis can be found in Table B.5. Note the following abbreviation: acetic acid (AcOH). Clarification of midpoint impact category abbreviations and units can be found in Table B.6. The endpoint characterization factors used in this thesis can be found in Table B.7. The endpoint characterization factors were used to calculate LCIA results for 16 of the 18 midpoint categories. These 16 impact categories contribute to the 3 ReCiPe endpoint impact categories. Clarification of the abbreviations and units of the midpoint impact categories contributing to the endpoint categories can be found in Table B.8. To calculate the actual endpoint LCIA results, the results of the contributing midpoint categories were added together. Clarification of the abbreviations and units of the 3 endpoint impact categories can be found in Table B.9.

Abbreviations that might be not trivial to understand are explained in the mentioned tables. They will also be listed here, in order to make them appear in the abbreviations section at the beginning of this thesis. Non-trivial abbreviations: equivalent (eq), dichlorobenzene (DB), non methane volatile organic compounds (NMVOC), m^2·annum (m^2a), CC, OD, terrestrial acidification (TA), FE, ME, HT, POF, PMF, terrestrial ecotoxicity (TE), FET, marine ecotoxicity (MET), IR, ALO, ULO, NLT, WD, MD, FD, disability adjusted life years (DALY), climate change human health (CCHH), climate change ecosystems (CCES), HH, ES, and resource surplus cost (RSC).

Table B.5: ReCiPe midpoint characterization factors used in this thesis. The first column on the left contains the ReCiPe midpoint impact categories. Their abbreviations and units are clarified in Table B.6. The units of the characterized emissions can be found in Table 2.4. Characterization factors equal to zero, in fact do not exist. From this table also becomes clear to which categories the direct WWTP emissions do not contribute.

	CO_2	N_2O	fossil CH_4	biogenic CH_4	PO_4^{3-}	non-PO_4^{3-}-P	NO_3^-	non-NO_3^--N	AcOH	H_2O
CC	1	298	25	22.3	0	0	0	0	0	0
OD	0	0	0	0	0	0	0	0	0	0
TA	0	0	0	0	0	0	0	0	0	0
FE	0	0	0	0	0.33	1	0	0	0	0
ME	0	0	0	0	0	0	0.23	1	0	0
HT	0	0	0	0	0	0	0	0	0	0
POF	0	0	0.0101	0	0	0	0	0	0	0
PMF	0	0	0	0	0	0	0	0	0	0
TE	0	0	0	0	0	0	0	0	1.33e−4	0
FET	0	0	0	0	0	0	0	0	0.045	0
MET	0	0	0	0	0	0	0	0	1.33e−4	0
IR	0	0	0	0	0	0	0	0	0	0
ALO	0	0	0	0	0	0	0	0	0	0
ULO	0	0	0	0	0	0	0	0	0	0
NLT	0	0	0	0	0	0	0	0	0	0
WD	0	0	0	0	0	0	0	0	0	−0.001
MD	0	0	0	0	0	0	0	0	0	0
FD	0	0	0	0	0	0	0	0	0	0

Table B.6: ReCiPe midpoint impact categories, their units, and their abbreviations as used in this thesis. Less straightforward abbreviations used for the units: eq: equivalent, DB: dichlorobenzene, NMVOC: non methane volatile organic compounds, m^2a: m^2·annum.

Impact category	Abbreviation	Units
Climate change	CC	kg CO_2 eq
Ozone depletion	OD	kg CFC–11 eq
Terrestrial acidification	TA	kg SO_2 eq
Freshwater eutrophication	FE	kg P eq
Marine eutrophication	ME	kg N eq
Human toxicity	HT	kg 1,4–DB eq
Photochemical oxidant formation	POF	kg NMVOC
Particulate matter formation	PMF	kg PM10 eq
Terrestrial ecotoxicity	TE	kg 1,4–DB eq
Freshwater ecotoxicity	FET	kg 1,4–DB eq
Marine ecotoxicity	MET	kg 1,4–DB eq
Ionising radiation	IR	kBq U235 eq
Agricultural land occupation	ALO	m^2a
Urban land occupation	ULO	m^2a
Natural land transformation	NLT	m^2
Water depletion	WD	m^3
Metal depletion	MD	kg Fe eq
Fossil depletion	FD	kg oil eq

Table B.7: ReCiPe endpoint characterization factors used in this thesis. The first column on the left contains the ReCiPe midpoint impact categories that contribute to a specific endpoint category. Their abbreviations and units are clarified in Table B.8. The units of the characterized emissions can be found in Table 2.4. Characterization factors equal to zero, in fact do not exist. From this table also becomes clear to which categories the direct WWTP emissions do not contribute.

	CO_2	N_2O	fossil CH_4	biogenic CH_4	PO_4^{3-}	non-PO_4^{3-}-P	AcOH
CCHH	1.4e−6	4.17e-4	3.5e−5	3.12e−5	0	0	0
OD	0	0	0	0	0	0	0
HT	0	0	0	0	0	0	0
POF	0	0	3.94e−10	0	0	0	0
IR	0	0	0	0	0	0	0
PMF	0	0	0	0	0	0	0
CCES	7.93e−9	2.36e−6	1.98e−7	1.76e−7	0	0	0
TA	0	0	0	0	0	0	0
FE	0	0	0	0	1.47e−8	4.44e−8	0
TE	0	0	0	0	0	0	2e-11
FET	0	0	0	0	0	0	3.88e-11
MET	0	0	0	0	0	0	2.33e-14
ALO	0	0	0	0	0	0	0
ULO	0	0	0	0	0	0	0
NLT	0	0	0	0	0	0	0
MD	0	0	0	0	0	0	0
FD	0	0	0	0	0	0	0

Table B.8: ReCiPe midpoint impact categories contributing to the endpoint categories. Clarification of their units and their abbreviations as used in this thesis. DALY: disability adjusted life years.

Impact category	Abbrevation	Units
Climate change human health	CCHH	DALY
Ozone depletion	OD	DALY
Human toxicity	HT	DALY
Photochemical oxidant formation	POF	DALY
Particulate matter formation	PMF	DALY
Ionising radiation	IR	DALY
Climate change ecosystems	CCES	species.year
Terrestrial acidification	TA	species.year
Freshwater eutrophication	FE	species.year
Terrestrial ecotoxicity	TE	species.year
Freshwater ecotoxicity	FET	species.year
Marine ecotoxicity	MET	species.yr
Agricultural land occupation	ALO	species.year
Urban land occupation	ULO	species.year
Natural land transformation	NLT	species.year
Metal depletion	MD	$
Fossil depletion	FD	$

Table B.9: ReCiPe endpoint impact categories, their units, and their abbreviations as used in this thesis. DALY: disability adjusted life years.

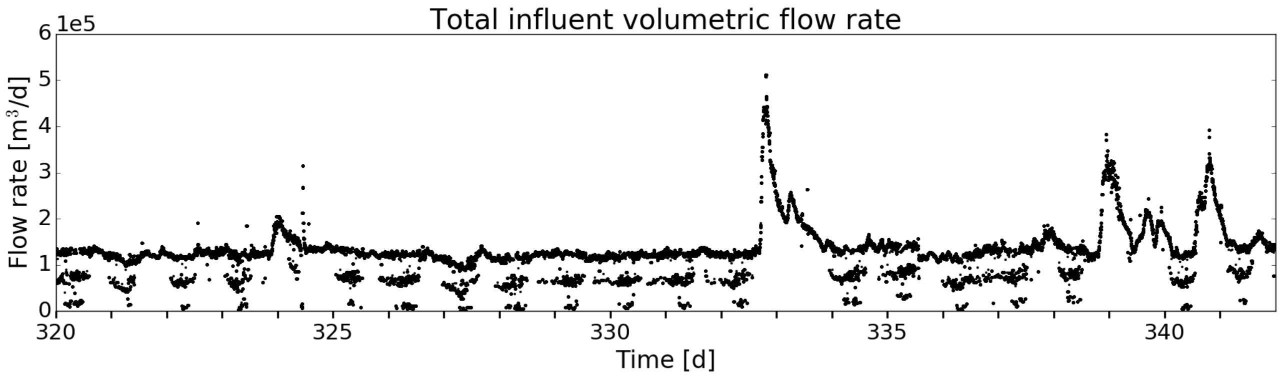
Impact category	Abbreviation	Units
Human health	HH	DALY
Ecosystems	ES	species.year
Resource surplus cost	RSC	$

APPENDIX C

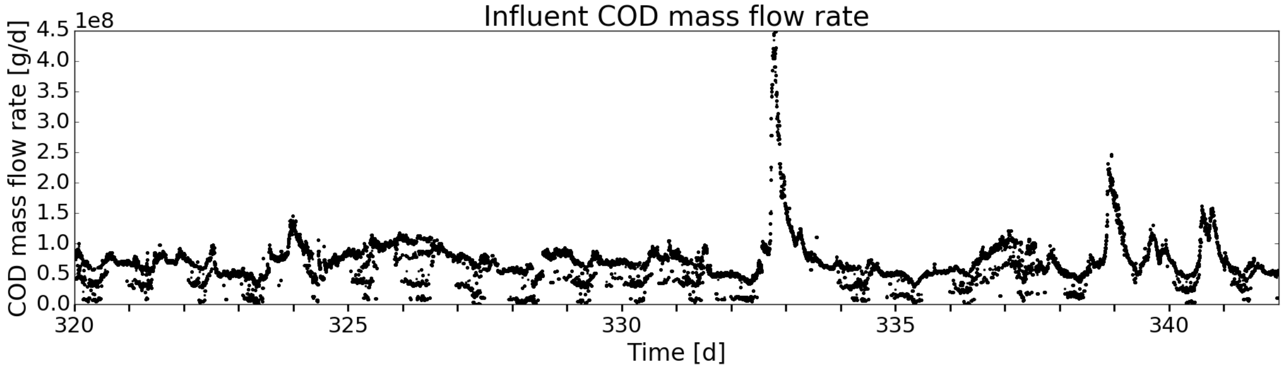
Additional information regarding results and discussion

C.1 Intermediate and WWTP model results for analysis of impact causes

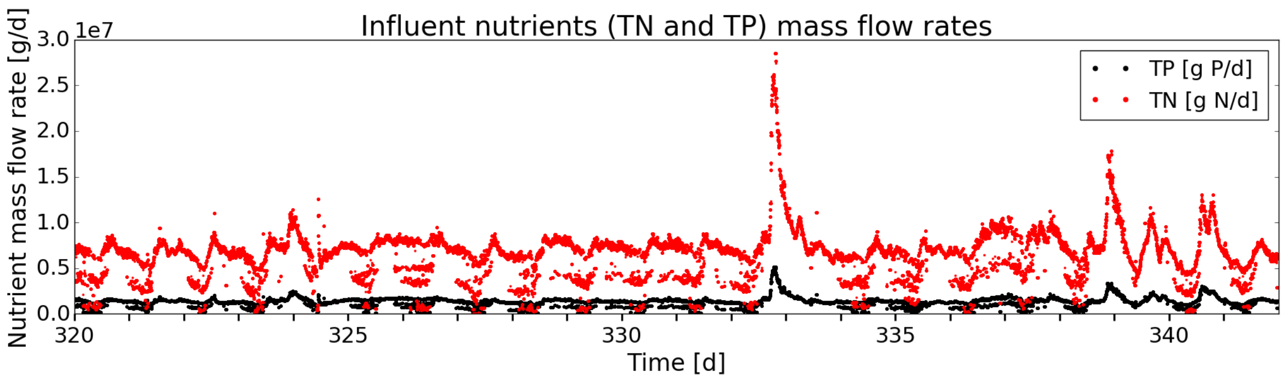
Plots of various variables are available in this appendix. The concerning variables are the WWTP model results listed in Table 2.2 and some intermediate results, i.e. emitted and consumed masses. In the latter case, each value is a result for the interval between the current and previous point in time. Results in this section are valid for scenario 4. (Section 2.3). These variables were used to search for the causes of the impacts as calculated by the LCIA. Note that scenario 3. is in fact also depicted, since scenario 3. uses the same influent data as scenario 4., but only runs to day 332, while scenario 4. continues until day 342. All other setting are the same in scenario 3. and 4. In Figure C.1, some influent flow rates are shown. The influent flow rates are in fact the same for all dynamic scenarios (scenario 3. to 7.). CO_2 emissions were already given in Figure B.2. In Figure C.3, some effluent nutrient emissions are shown, together with some influent nutrient mass flow rates and variables relevant for control actions taken by the controllers used for controlling nutrient emissions. In Figure C.2, water discharged through the effluent, some effluent emissions, and produced sludge mass are shown.



(a)

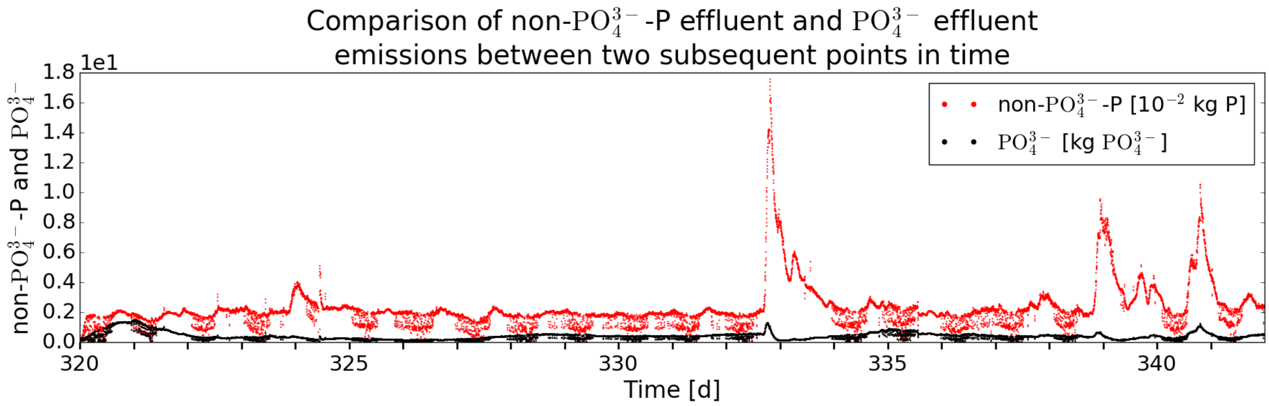


(b)

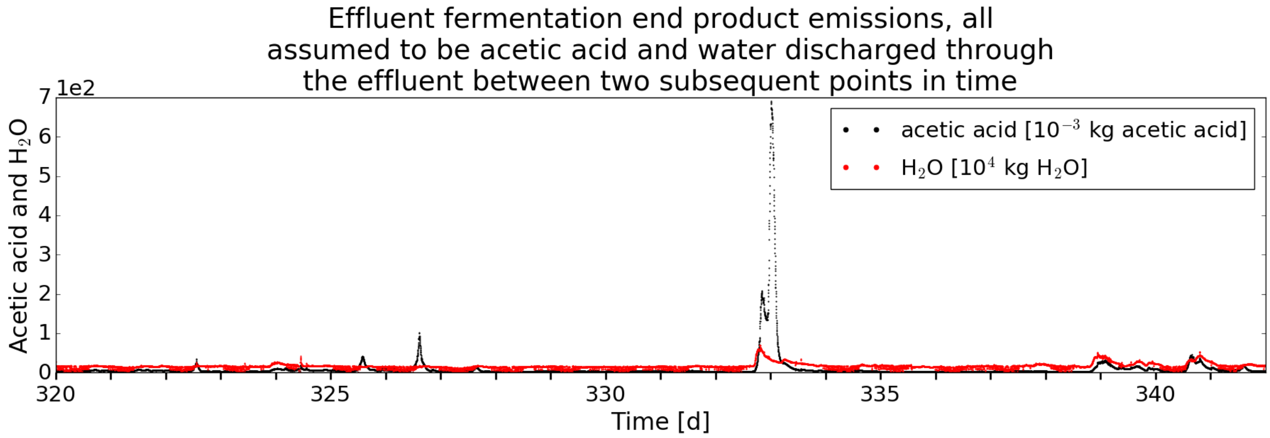


(c)

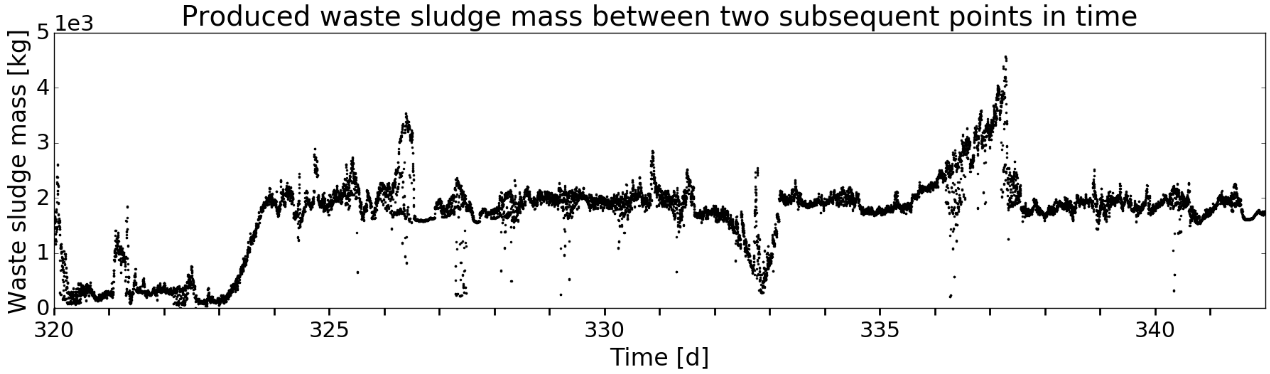
Figure C.1: Some flow rates in the influent. These figures are valid for all dynamic scenarios. However, in the case only dry weather is considered, the considered time span runs from day 320 to day 332. In case of dry and wet weather, from day 320 to 342.



(a)

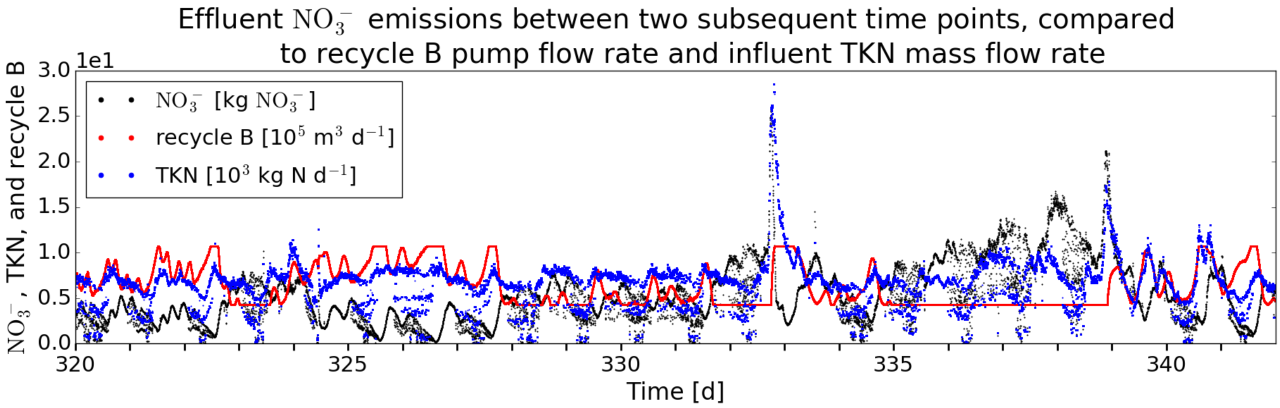


(b)

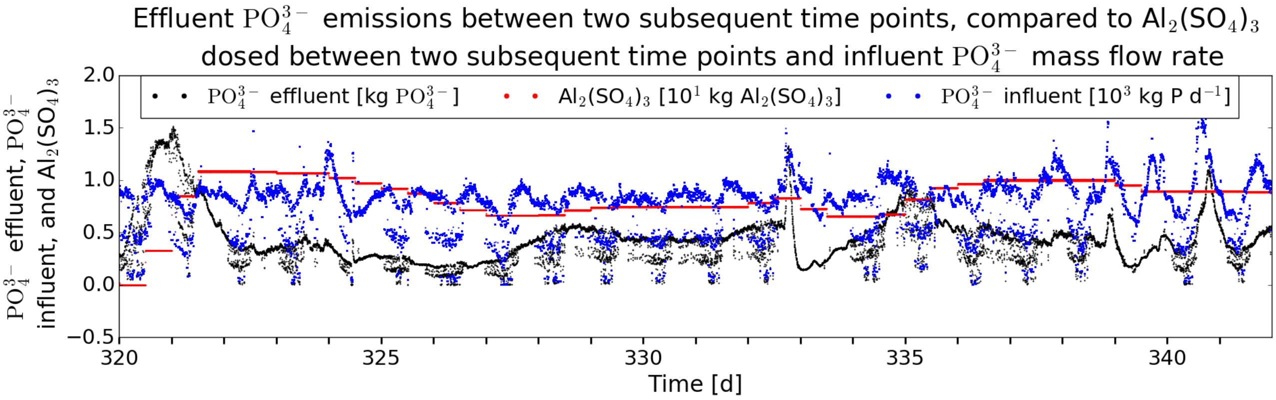


(c)

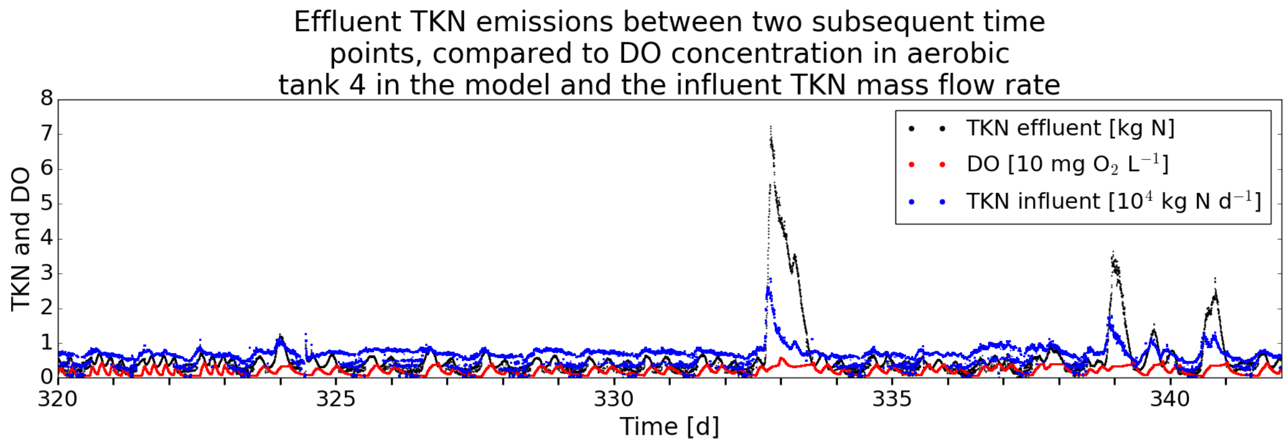
Figure C.2: Water discharged through the effluent, some effluent emissions, and produced sludge mass. These figures are valid for scenario 3. and 4. In case only dry weather is considered, the considered time span runs from day 320 to day 332. In case of dry and wet weather, from day 320 to 342.



(a)



(b)



(c)

Figure C.3: Plots of various effluent nutrient emissions. On each respective plot, these emissions are plotted together with a relevant influent nutrient mass flow rate and a variable that is relevant for the control actions taken to limit their emissions. These figures are valid for scenario 3. and 4. In case only dry weather is considered, the considered time span runs from day 320 to day 332. In case of dry and wet weather, from day 320 to 342.

C.2 Dynamic vs steady state: equality of influent substance amounts

In Table 2.4 the total amounts of some substances that went into the WWTP (model) through the influent divided by the simulation time can be seen (since the FU is a day WWTP operation). These amounts are exactly the same for the scenarios where dry or dry and wet weather conditions apply, respectively in the case of steady state and dynamic simulations. It will now be shown that this is always valid.

As example, consider the dry plus wet weather scenario. The influent data start at $t = 320$ days $= t_{start}$ and end at $t = 342$ days $= t_{end}$. The steady state simulation is executed with the average of the influent values. Consider for example the volumetric flow rate Q [L^3 T^{-1}]. The average of this value over the time interval $[t_{start}, t_{end}]$ is defined as:

$$Q_{avg} = \frac{\int_{t_{start}}^{t_{end}} Q dt}{t_{end} - t_{start}} \tag{C.1}$$

The steady state scenario is run for 250 days and only the last 21 days are used in the scenario analysis. The start and end of this 21 day time interval can be set equal to an arbitrary start and stop time, respectively t_1 and t_2. The total influent volume for the steady state case $V_{tot,SS}$ can be calculated by integrating the flow rate, in this case the average flow rate. It also has to be divided by the total time, in order to express it relative to the FU a day WWTP operation:

$$\frac{V_{tot,SS}}{t_2 - t_1} = \frac{\int_{t_1}^{t_2} Q_{avg} dt}{t_2 - t_1} = Q_{avg} \frac{\int_{t_1}^{t_2} dt}{t_2 - t_1} = Q_{avg} \frac{t_2 - t_1}{t_2 - t_1} = Q_{avg} \tag{C.2}$$

In case a dynamic simulation is performed, the simulation time span is equal to $[t_{start}, t_{end}]$. The total influent volume for the dynamic case can be calculated by integrating Q over the time interval $[t_{start}, t_{end}]$. To express this total volume per FU, it has to be divided by the total time span $[t_{start}, t_{end}]$. This is of course equal to equation C.1.

C.3 Classic vs average dynamic LCA results

By giving a counter example, it will now be proven that the average of the dynamic impact per FU doesn't have to be equal to the total impact per FU in the case of a classic LCA. For this proof the FU is 1 hour of WWTP operation. The deductions in this section will also lead to insights into the fact when both are or are not equal. An arithmetic average is calculated as follows:

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \tag{C.3}$$

where x_i are for instance observations, n is the total number of observations, and $\bar{x}$ is the arithmetic mean.
The average dynamic impact for a specific case can thus be calculated as follows:

$$\begin{aligned}
&\text{average dynamic impact} = \frac{\frac{I_1}{a} + \frac{I_2}{a} + \frac{I_2}{b} + \frac{I_3}{a}}{4} = \frac{\frac{bI_1}{ab} + \frac{bI_2}{ab} + \frac{aI_2}{ab} + \frac{bI_3}{ab}}{4} \\
&= \frac{bI_1 + (b+a)I_2 + bI_3}{4ab} = \frac{I_1 + (1 + a/b)I_2 + I_3}{4a}
\end{aligned} \tag{C.4}$$

where I stands for the absolute generated impact (thus not per FU) in a specific time interval and the subscripts refer to specific values. In this specific case, the FU is chosen as 1 hour of WWTP operation, thus a and b are hours of operation that generated the respective impacts. I_2 is used 2 times and a 3 times. The 4 summed instances in the example should nonetheless be viewed as observations at 4 different points in time. The same (symbolic) values were used for the sake of simplicity.
In case of a classic LCA, the total impact generated in the whole time span expressed per FU - i.e. divided by the total operating time - is calculated as follows:

$$\text{total impact in considered time span} = \frac{I_1 + I_2 + I_2 + I_3}{3a + b} = \frac{I_1 + 2I_2 + I_3}{3a + b} \tag{C.5}$$

It is easy to verify that both expressions are equal in the following cases:

$$\begin{aligned}
&2 = 1 + a/b \Leftrightarrow a/b = 1 \Leftrightarrow a = b, \text{ and} \\
&4a = 3a + b \Leftrightarrow a = b
\end{aligned} \tag{C.6}$$

If subsequently the following values are taken: $I_1 = 1$, $I_2 = 2$, $I_3 = 3$, $a = 1$, and $b = 2$, it can easily be verified that the equality does not hold. It is thus proven that in general the average dynamic impact doesn't have to be equal to the total impact if both are expressed relative to a specific FU.
In addition, if the value of the FU is the same for every observation (no matter which FU is chosen), the equality does hold in general:

$$\frac{\sum_i^n \frac{I_i}{a}}{n} = \frac{\sum_i^n I_i}{an} \tag{C.7}$$

Thus, results will probably be different in case a very varying FU is chosen. Note that in case the FU a day operation is chosen, this value is always the same in every considered time interval (except for the last time interval), which will thus probably lead to the same results. The extent of these influences is investigated in Section 3.3.

C.4 Selecting relevant midpoint impact categories

In Section 3.4, midpoint impact categories to be used in the subsequent analysis are selected. This was partially based on analysing the contributions of sub-processes of the product system on the total impacts (Figure B.6).

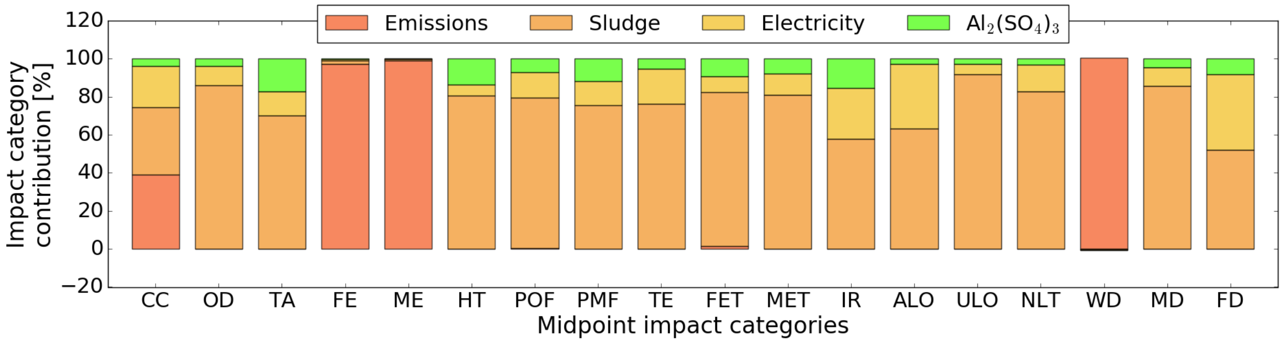


Figure C.4: Contribution analysis (classic LCA). Scenario: 4., FU: a day operation. For midpoint impact category abbreviations, see the abbreviations section or Table B.6. Emissions comprise effluent and GHG emissions, sludge comprises aspects related to sludge treatment, $Al_2(SO_4)_3$ comprises aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions.

C.5 Functional unit for dynamic LCA

In section 3.6.1, dynamic CC LCIA results of scenario 4. for the FU kg TN in the influent were plotted. However, the different contributions are not clearly visualized in the concerning plot. In Figures C.5 and C.6, all contributions (and the total results) are plotted separately.

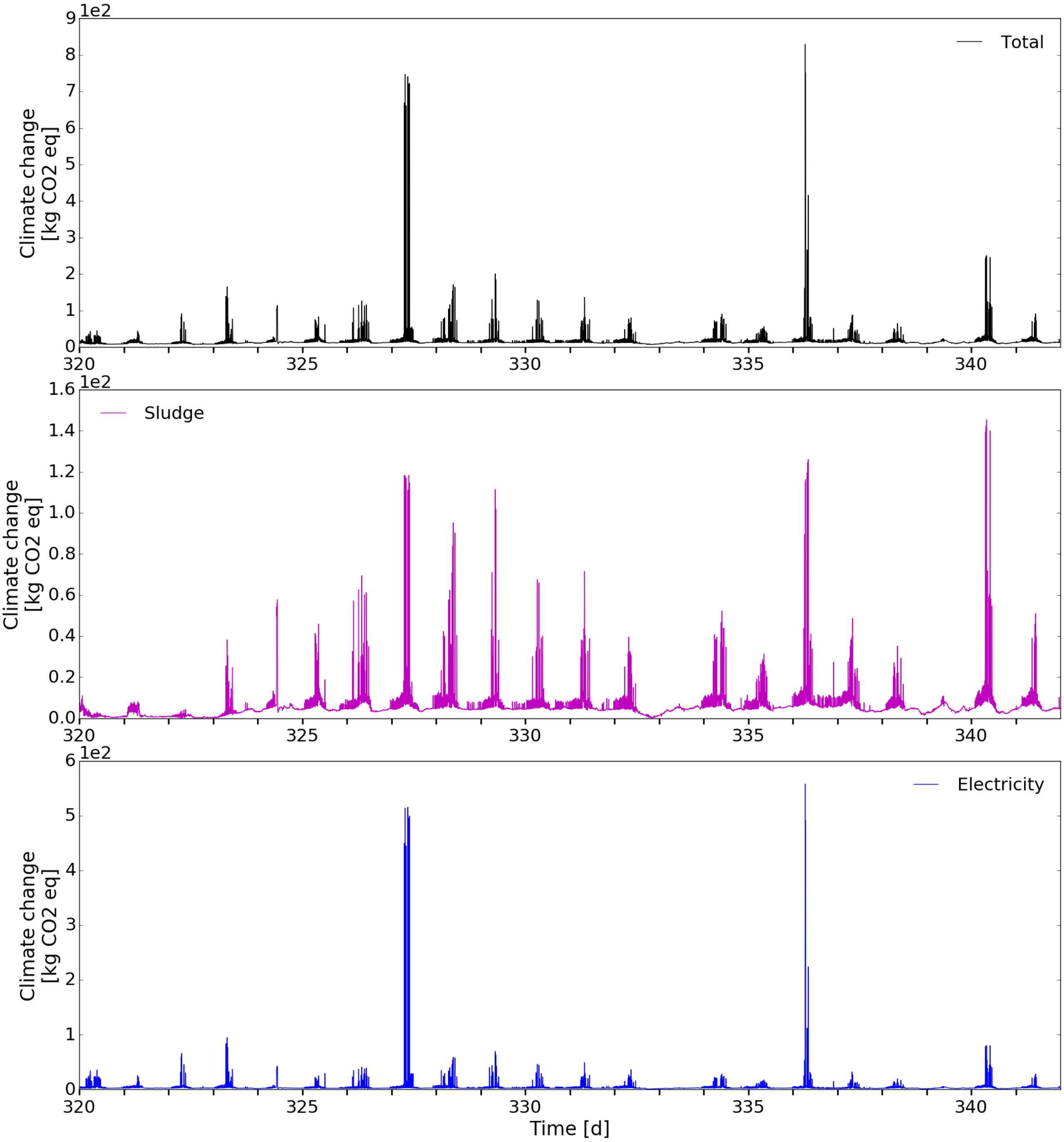


Figure C.5: Time series of midpoint impact category results for CC. Displayed scenario: 4., FU: kg N in the influent. For contribution analysis, total impacts are divided into 4 categories. Sludge comprises aspects related to sludge treatment. In Table 2.4 can be viewed what is included in the 4 subdivisions. The legends on the graph show whether the total result or a contribution is plotted.

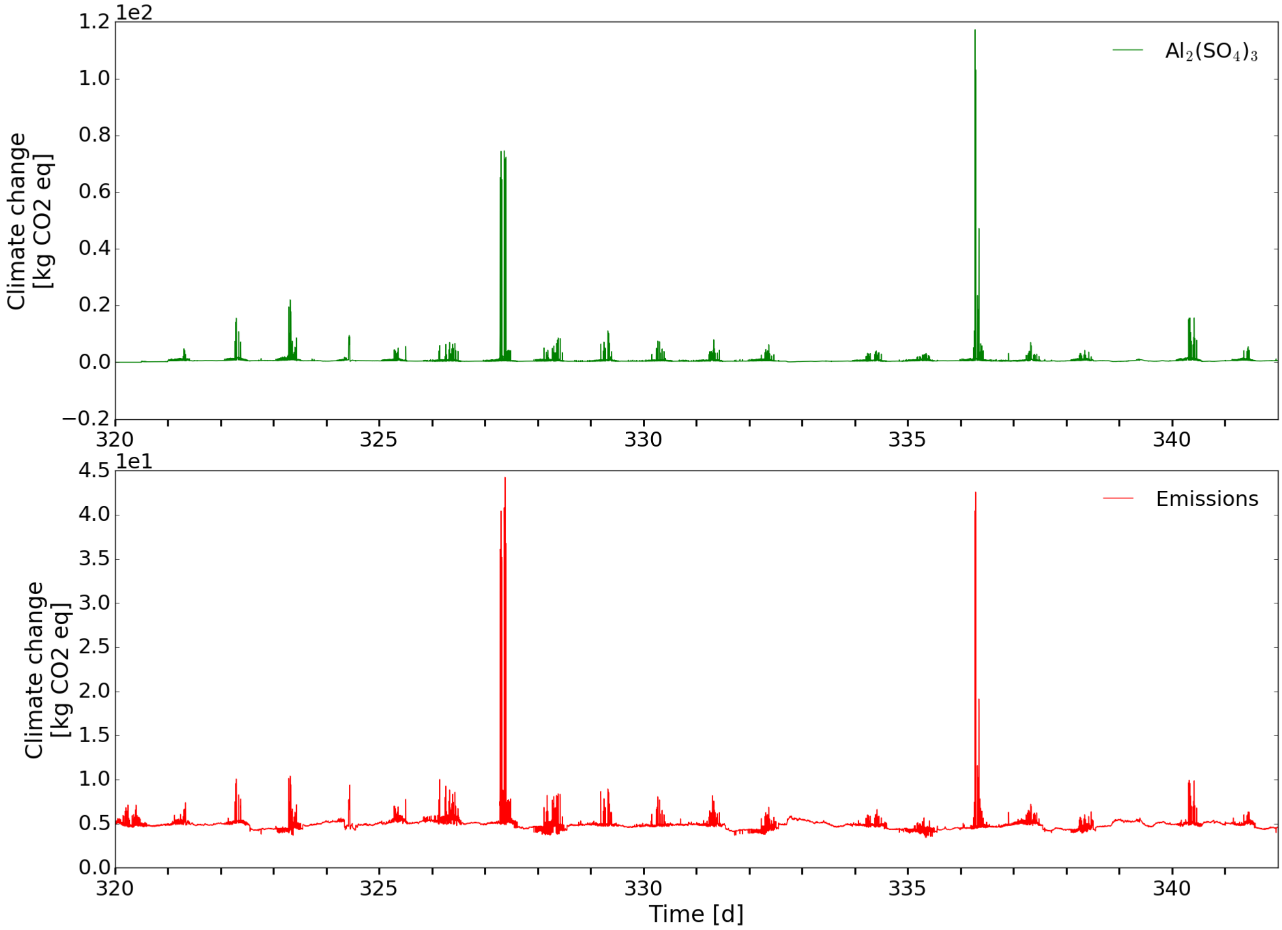


Figure C.6: Time series of midpoint impact category results for CC. Displayed scenario: 4., FU: kg N in the influent. For contribution analysis, total impacts are divided into 4 categories. Emissions comprise effluent and GHG emissions, $Al_2(SO_4)_3$ comprises aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions. The legends on the graph show which contribution to the total result is plotted.

It is in addition interesting to reflect upon the FUs not yet provided in the notebook: kg COD or kg nutrients removed. They are, probably, the most interesting ones, since it was observed at the Eindhoven WWTP - thus for the same effluent limits - that removal percentages are different during dry and wet weather conditions (De Mulder, 2017). However, how to define them in a dynamic context is, not very straightforward. In the classic case a good approximation is the total mass that went into the WWTP in the considered time span, minus the mass that went out through the effluent. Mass can accumulate in the WWTP and the mentioned methodology is therefore an approximation, but on larger time intervals the approximation will be very good. However, in many of the reactors or units in the Eindhoven model (Figure 2.5), concentrations can change and thus mass can indeed accumulate. When looking at the time intervals used for the dynamic LCA in this thesis, 2 minutes, mass removed = mass in - mass effluent can no longer be applied. The question on how to quantify “removed” then comes into play.

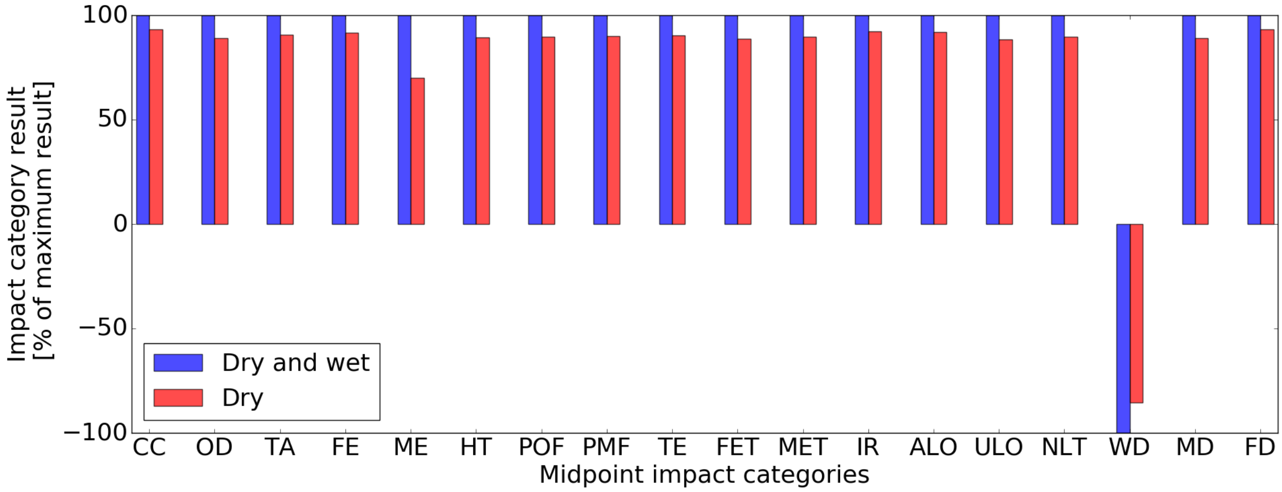
First, P cannot leave the system any other way then via sludge or effluent discharge. It is hence probably the most sensible way to say that P is removed, when it is discharged via sludge discharge (whether or not in the solid phase). This, however, will cause the following problem: the first days, there is almost no sludge production (Figure C.2 (c)). Thus, when applying this definition, it will seem as if there is no P removal in that time interval. In reality, however, WWTP processes - not related to sludge treatment - are of course removing P and causing environmental impacts as a consequence. In this thesis, kg P in the influent serves as an approximation for P that is treated, since the Eindhoven WWTP is well maintained and monitored (Blom, 2013; Benedetti et al., 2012) and thus lives up to treatment standards. When looking at the influent COD mass flow rate and the biological response, CO_2 production (Figure B.2), the dynamics correspond much better than when comparing sludge production and influent pollutant loads (Figure C.2 (c) and C.1). Thus, certain impacts as a consequence of P treatment will probably coincide to a large extent with influent P mass dynamics. However, impacts of sludge treatment now no longer coincide with the dynamics of the used FU, thus the problem remains.

Next, COD is probably easier. It can leave the system through its oxidation to CO_2, which is not a state variable. Oxidized COD simply disappears from the system. Hence, COD is removed when it is oxidized to CO_2, which was indeed calculated (Figure B.2). In addition, COD is also removed when it is discharged via the sludge. If both were taken into account as removal of COD, probably impacts of COD oxidation and sludge treatment are scaled more or less at the right time instants. This is not yet provided in the notebook and could be done in the future.

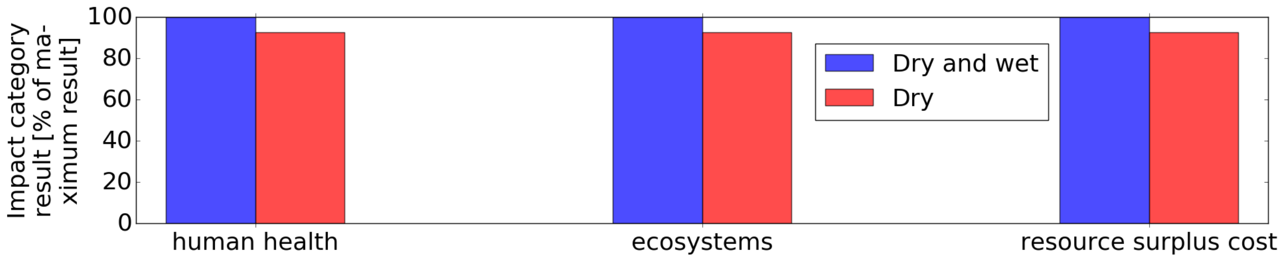
The same goes for N removal. NH_4^+ can be converted into NO_3^- and further into N_2. To quantify the mass of N_2 formed in a specific time interval, a mass balance over the reactors where this can occur is required, analogously to the COD mass balance (not yet provided). Alternatively, one of the sub-models of the Eindhoven model could be changed such that the nitrification rate in each AST would be an accessible result (which at the moment, is not the case.) This would be a quantification of the amount of N removed by denitrification. In addition, N is also removed via sludge discharge. However, still problems remain: for conversion of NH_4^+ to NO_3^-, aeration is needed. However, after this conversion, N is not removed. It is removed during nitrification, but the aeration was needed to make this possible. It thus seems that the exact time instants when impacts occur might be hard to link to the provided functionality of pollutant removal, due to the complex time related dynamics of a WWTP (model).

C.6 Influence of the functional unit

Some additional results used in the reasoning in Section 3.6.2 are given here. All the figures show classic LCIA results of scenario 3. and 4., this for the FU a day WWTP operation (Figure C.7), kg P in the influent (Figure C.8), and kg N in the influent (Figure C.9).



(a)

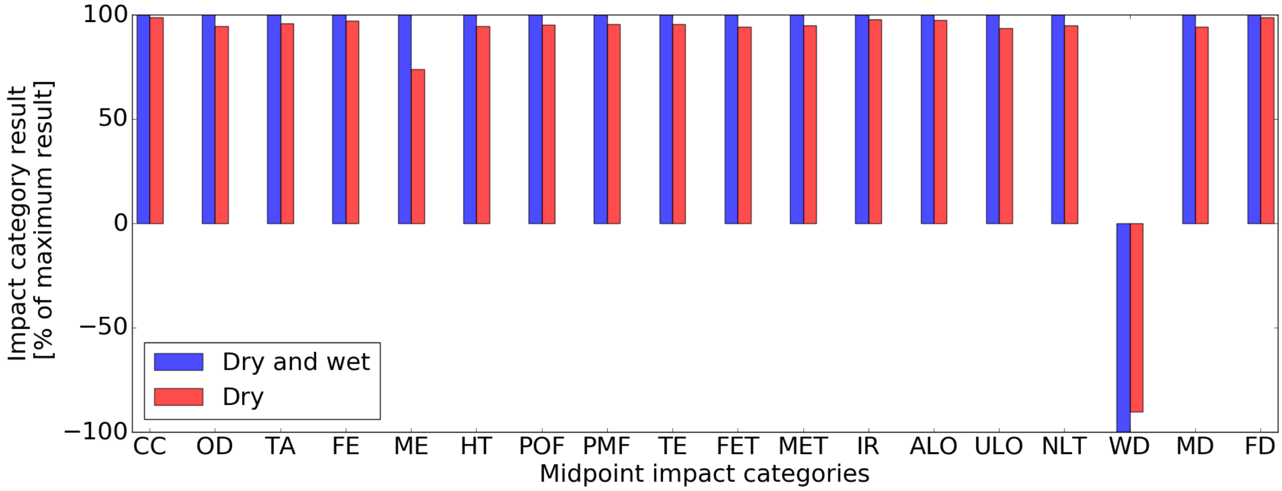


(b)

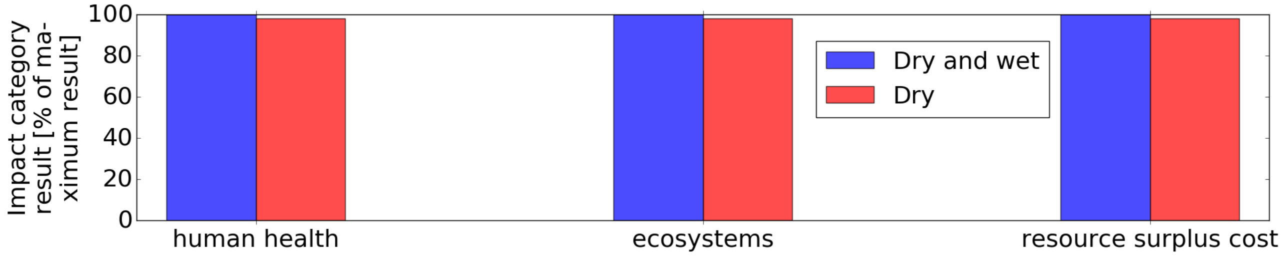
Figure C.7: LCIA results for a classic LCA with the FU a day WWTP operation. (a) Midpoint impact categories. (b) Endpoint impact categories. Compared scenarios: 3. dry weather conditions and 4. dry and wet weather conditions. See Table B.6 for impact category abbreviations (or the abbreviations section.)

C.7 Scenario analysis

Some additional figures used in the scenario comparison are available in this section: Figure C.10: contribution analysis for scenario 4.: dry and wet weather conditions (reference scenario), Figure C.11:



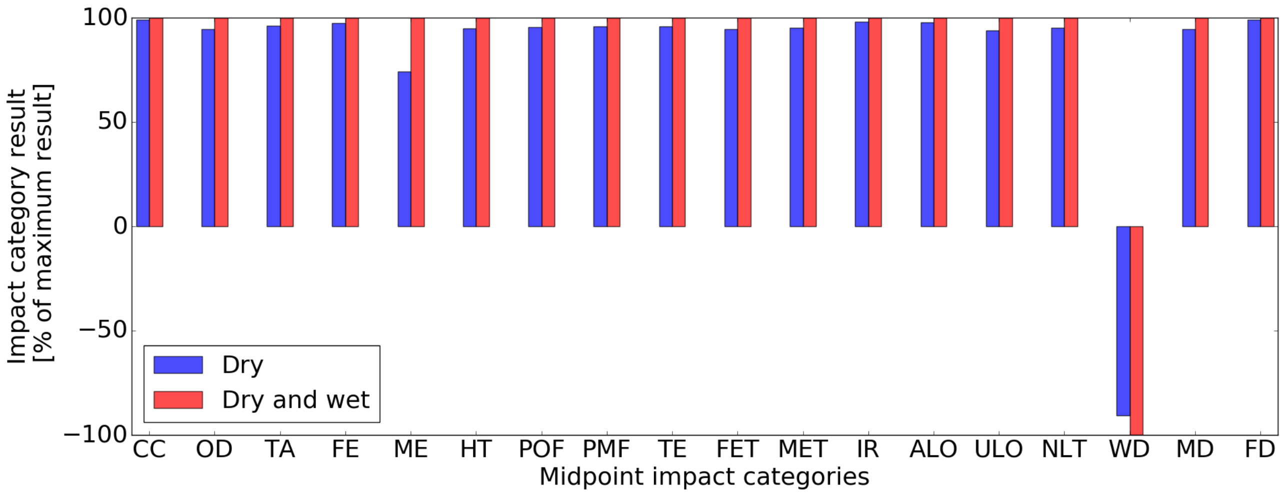
(a)



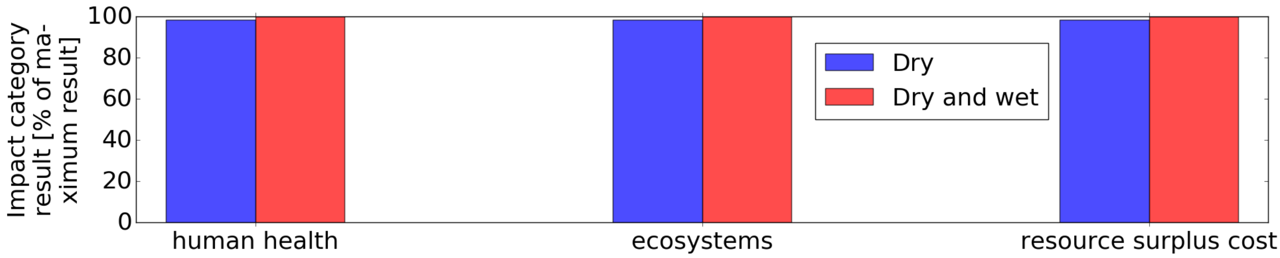
(b)

Figure C.8: LCIA results for a classic LCA with the FU 1 kg P in the influent. (a) Midpoint impact categories. (b) Endpoint impact categories. Compared scenarios: 3. dry weather conditions and 4. dry and wet weather conditions. See Table B.6 for impact category abbreviations (or the abbreviations section.)

contribution analysis for scenario 5.: lowered setpoint of the effluent PO_4^{3-} controller, Figure C.12: contribution analysis for scenario 6.: feed-forward controller to remediate peaks in effluent PO_4^{3-} mass flow rates, Figure C.13: contribution analysis for scenario 7.: increased TSS concentration in the ASTs, and Figure C.14: effluent PO_4^{3-} emissions and control action to limit these emissions for scenario 5., 6., and 7.

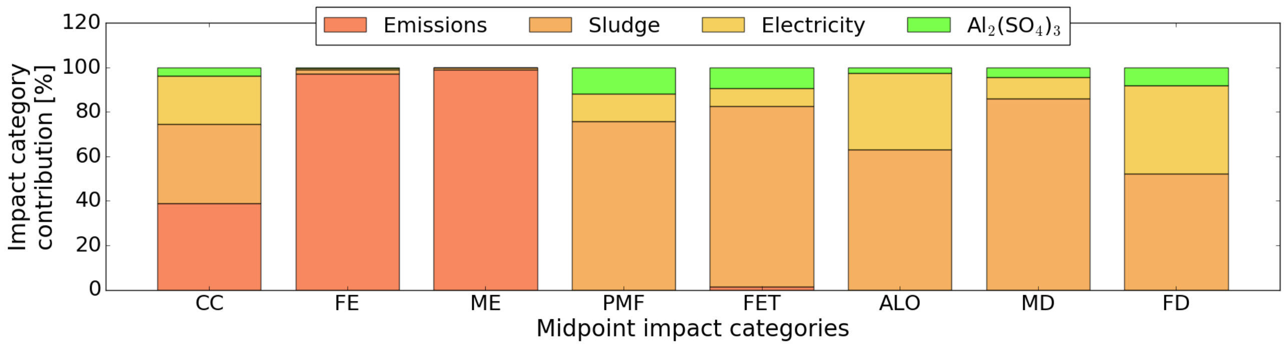


(a)

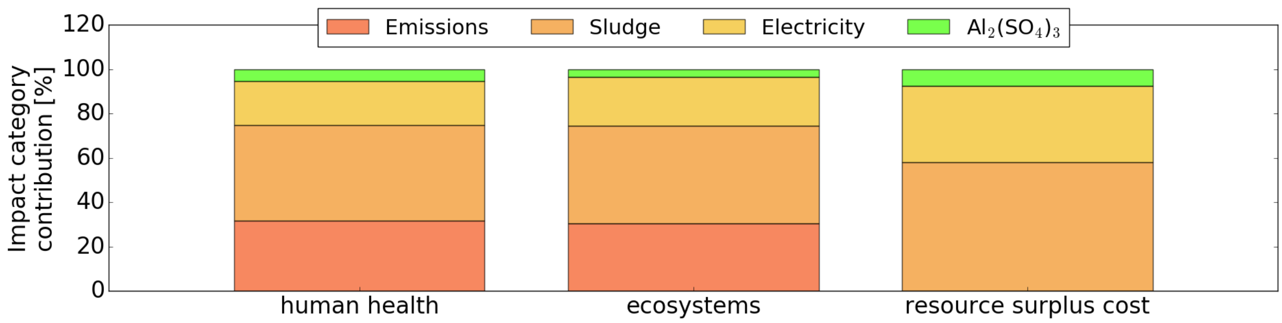


(b)

Figure C.9: LCIA results for a classic LCA with the FU 1 kg N in the influent. (a) Midpoint impact categories. (b) Endpoint impact categories. Compared scenarios: 3. dry weather conditions and 4. dry and wet weather conditions. See Table B.6 for impact category abbreviations (or the abbreviations section.)



(a)



(b)

Figure C.10: Contribution analysis of the LCIA results for a classic LCA with the FU a day WWTP operation. Scenario 4.: dry and wet weather conditions (reference scenario). (a) Midpoint impact categories. (b) Endpoint impact categories. See abbreviations section or Table B.6 for impact category abbreviations. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions.

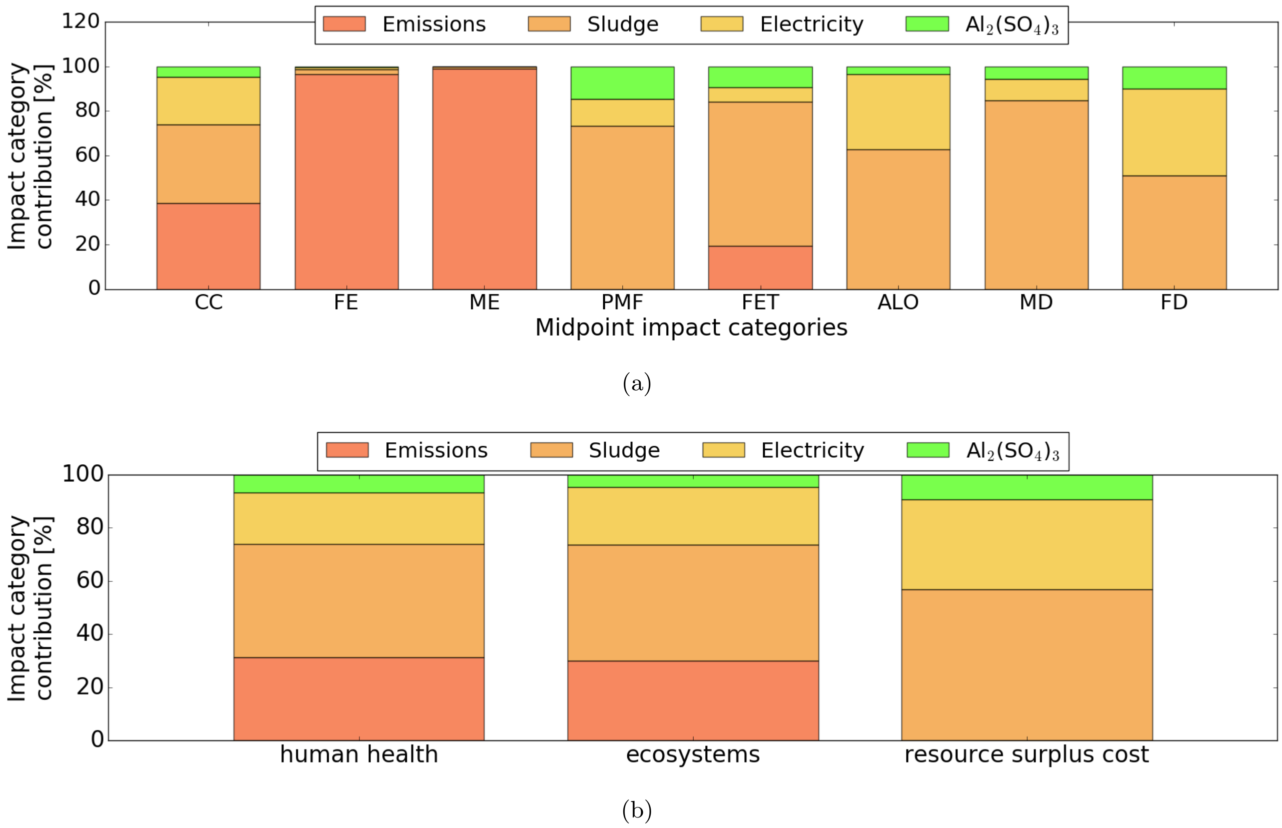
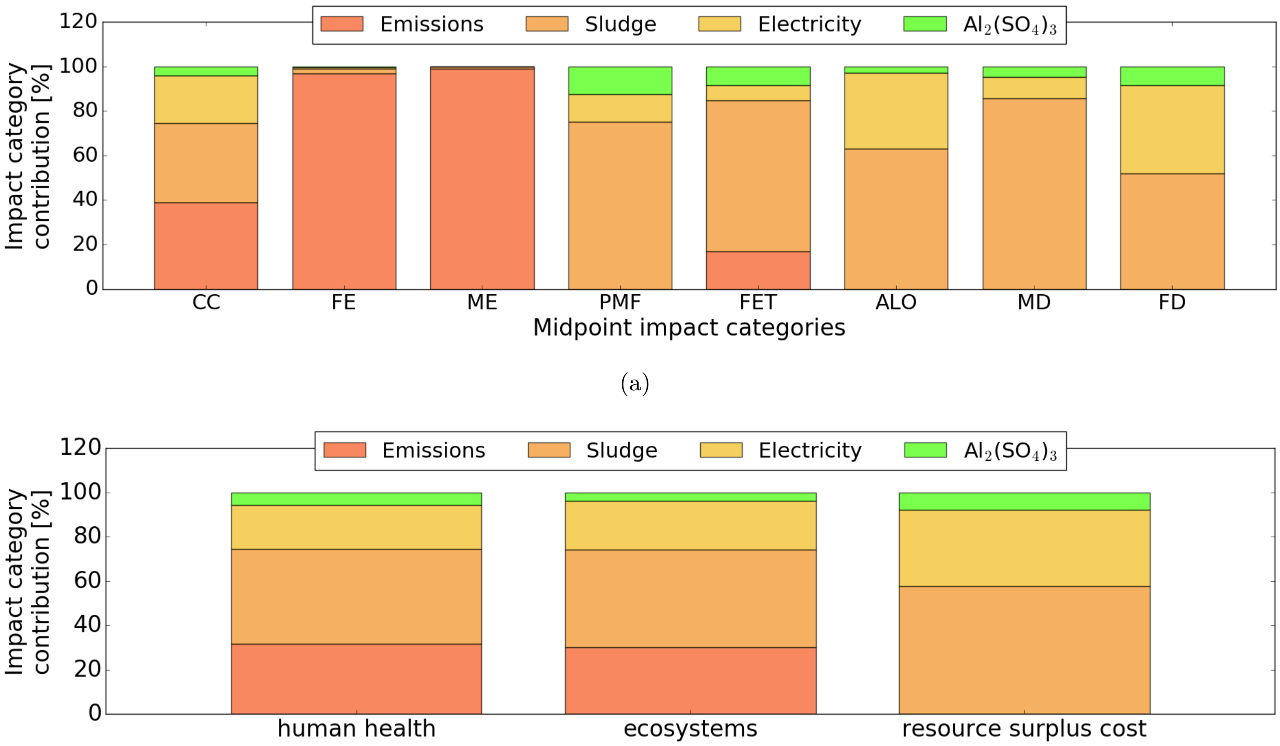


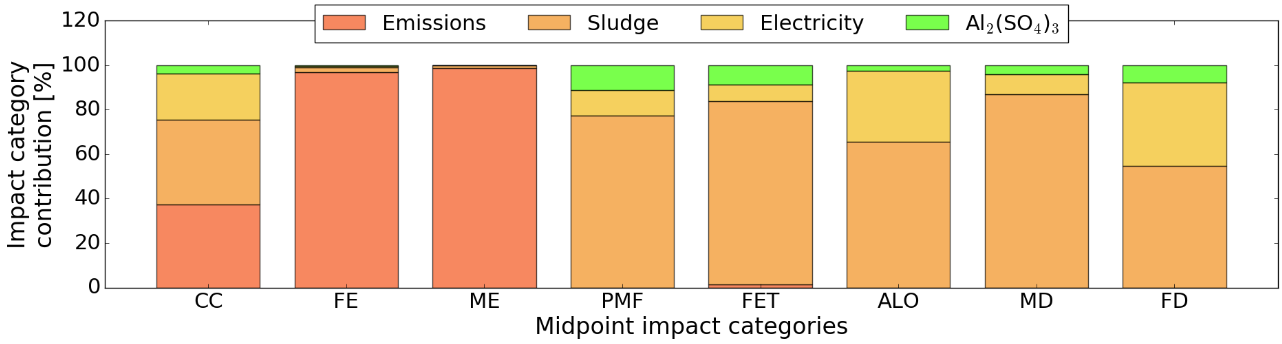
Figure C.11: Contribution analysis of the LCIA results for a classic LCA with the FU a day WWTP operation. Scenario 5.: lowered setpoint of the effluent PO_4^{3-} controller. (a) Midpoint impact categories. (b) Endpoint impact categories. See abbreviations section or Table B.6 for impact category abbreviations. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions.



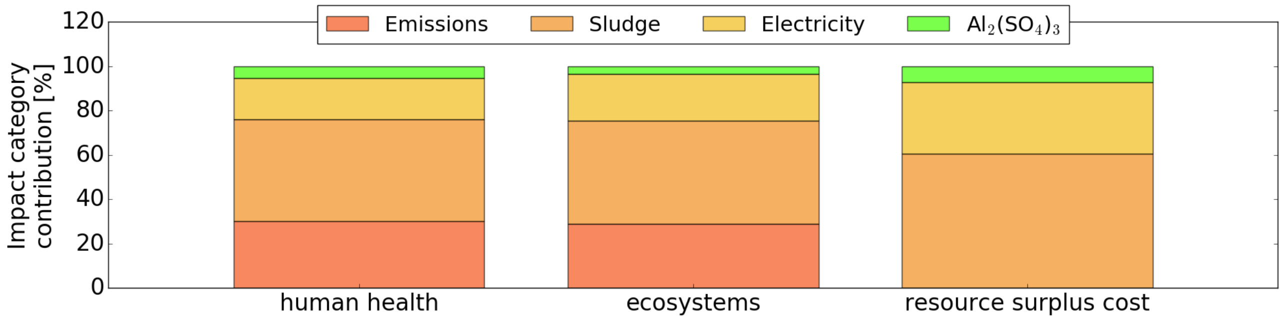
(a)

(b)

Figure C.12: Contribution analysis of the LCIA results for a classic LCA with the FU a day WWTP operation. Scenario 6.: feed-forward controller to remediate peaks in effluent PO_4^{3-} mass flow rates. (a) Midpoint impact categories. (b) Endpoint impact categories. See abbreviations section or Table B.6 for impact category abbreviations. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions.

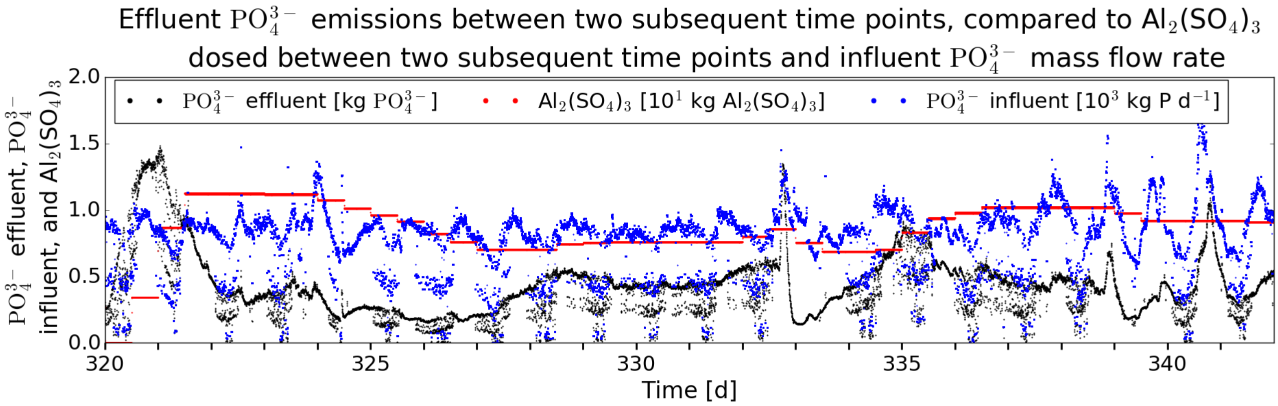


(a)

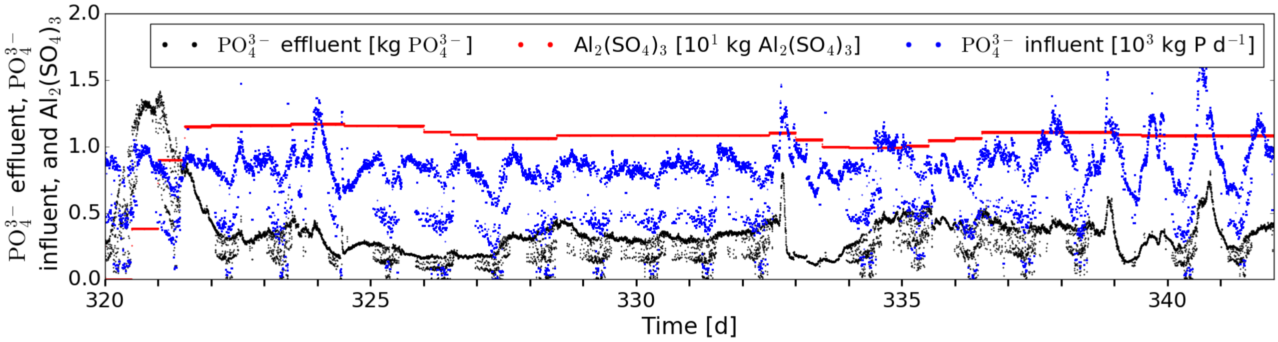


(b)

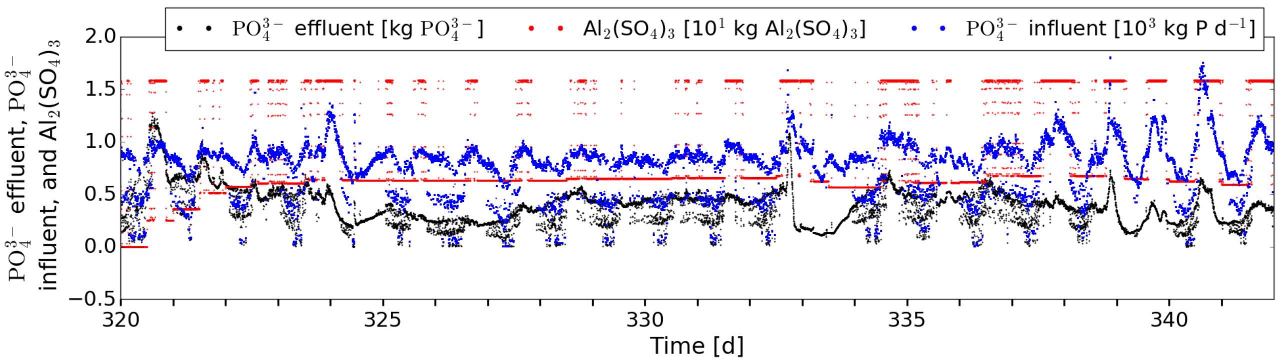
Figure C.13: Contribution analysis of the LCIA results for a classic LCA with the FU a day WWTP operation. Scenario 7.: increased TSS concentration in the biological reactors. (a) Midpoint impact categories. (b) Endpoint impact categories. See abbreviations section or Table B.6 for impact category abbreviations. Emissions include effluent and GHG emissions, sludge includes aspects related to sludge treatment, $Al_2(SO_4)_3$ includes aspects related to its production and transport. In Table 2.4 can be viewed what is included in the 4 subdivisions.



(a)



(b)



(c)

Figure C.14: (a) Scenario 7.: increased TSS concentration in the biological tanks, (b) Scenario 5.: lowered setpoint of the effluent PO_4^{3-} controller, and (c) Scenario 6.: feed-forward controller to remediate peaks in effluent PO_4^{3-} mass flow rates.