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Master Thesis

Modelling the effect of salt from road runoff on nitrification at Freistadt Wastewater Treatment Plant

Submitted by

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Affidavit

I hereby declare that I have authored this master thesis independently, and that I have not used any assistance other than that which is permitted. The work contained herein is my own except where explicitly stated otherwise. All ideas taken in wording or in basic content from unpublished sources or from published literature are duly identified and cited, and the precise references included.

I further declare that this master thesis has not been submitted, in whole or in part, in the same or a similar form, to any other educational institution as part of the requirements for an academic degree.

I hereby confirm that I am familiar with the standards of Scientific Integrity and with the guidelines of Good Scientific Practice, and that this work fully complies with these standards and guidelines.

Vienna, 01.08.2022 Nikola JOVANOVIC *(manu propria)*

Preface and Acknowledgements

At this point, I would like to thank all the people who contributed to the successful completion of this master thesis.

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Abstract

In this master thesis, the impact of road salt on nitrification in an activated sludge plant was numerically simulated. Simulations were run in the SIMBA# modelling software using the Freistadt wastewater treatment plant (WWTP) as a case study. Firstly, the literature review of road salt impacts on wastewater treatment plants was examined. The findings from the literature showed that salt can have both positive and negative impacts on WWTP and that these effects are influenced mostly by the amount of salt concentration. Secondly, a model describing the impact of salt on nitrification was developed. Consequently, the salt model was implemented in SIMBA# and calibrated and validated, respectively. For the Freistadt WWTP, four scenarios have been simulated. The first scenario was 24 hour salt dosing with 0.5, 1.0, 1.5, and 2.0 g NaCl/l. The second scenario was dosed with the same concentration, but with a longer exposure time of 48 hours. Third scenario was the decrease in the influent water temperature to 6, 5, and 4 °C. The last scenario was the increase in influent water quantities to 5 000, 6 000 and 7 000 m³/day. Results showed that the impact of salt on nitrification depends mostly on the amount of salt concentration and salt dosing exposure time. The nitrification rate and effluent NH_4-N concentrations improved, when the sodium chloride dosings were less than 1.0 g/l. When the threshold of 1.0 g NaCl/l was exceeded, inhibition started to occur. Prolonged salt dosing times amplified the positive and negative effects of the salt dosing. The impact of lower influent water temperature was negligible. Increased quantities of influent water improved the removal rates of NH_4-N.

Kurzfassung

In dieser Masterarbeit wurde der Einfluss von Streusalz auf die Nitrifikation in einer Belebtschlammanlage numerisch simuliert. Die Simulationen wurden mit der Modellierungssoftware SIMBA# durchgeführt, wobei die Kläranlage Freistadt als Fallbeispiel diente. Zunächst wurde die Literaturübersicht über die Auswirkungen von Streusalz auf Kläranlagen untersucht. Die Erkenntnisse aus der Literatur zeigten, dass Salz sowohl positive als auch negative Auswirkungen auf Kläranlagen haben kann und dass diese Auswirkungen hauptsächlich von der Salzkonzentration beeinflusst werden. Zweitens wurde ein Modell entwickelt, das die Auswirkungen von Salz auf die Nitrifikation beschreibt. Anschließend wurde das Salzmodell in SIMBA# implementiert und kalibriert bzw. validiert. Für die Kläranlage Freistadt wurden vier Szenarien simuliert. Das erste Szenario war eine 24-stündige Salzdosierung mit 0,5; 1,0; 1,5 und 2,0 g NaCl/l. Das zweite Szenario war eine Dosierung mit der gleichen Konzentration, aber mit einer längeren Expositionszeit von 48 Stunden. Im dritten Szenario wurde die Temperatur des einfließenden Wassers auf 6, 5 und 4 °C gesenkt. Das letzte Szenario war die Erhöhung der Zulaufwassermenge auf 5 000, 6 000 und 7 000 m³/Tag. Die Ergebnisse zeigten, dass die Auswirkungen des Salzes auf die Nitrifikation hauptsächlich von der Höhe der Salzkonzentration und der Dauer der Salzdosierung abhängen. Die Nitrifikationsrate und die NH_4-N-Konzentration im Abwasser verbesserten sich, wenn die Natriumchlorid-Dosierung unter 1,0 g/l lag. Wurde der Schwellenwert von 1,0 g NaCl/l überschritten, setzte eine Hemmung ein. Längere Salzdosierungszeiten verstärkten die positiven und negativen Auswirkungen der Salzdosierung. Die Auswirkungen einer niedrigeren Zulaufwassertemperatur waren vernachlässigbar. Höhere Zulaufwassermengen verbesserten die Entfernungsraten von NH_4-N.

1. Introduction

In Austria, there is a mix of Alpine and Continental climates. Because of this climate, during the winter months of December, January and February, salt is being dispersed on roads to prevent the formation of ice and salt. The salt lowers the freezing temperature of the water and thus prevents possible vehicle accidents. This has a positive effect on road safety, but it creates problems for the wastewater treatment processes. When the air temperature rises, or during rain events, the salt that is dispersed on roads, ends up in the sewer system and consequently in the wastewater treatment plant. Flesch (2020) states that wastewater treatment plant operators reported that during these events, when there is an increase in inflow chloride concentration, there are possible operational impairments. These impairments are the break-up of sludge flocs, decreased removal efficiencies, problems with sludge settling, increased effluent concentrations, etc.

The topic of the impact that road salt has on wastewater treatment plants is not widely researched. Thus, the exact consequences that lower salt (NaCl) concentration has on wastewater treatment plants are unknown. The road salt concentrations in the influent of wastewater treatment plants are usually up to 2-3 g NaCl/l (Flesch, 2020). These salt concentrations are much lower than concentrations that occur in coastal areas due to the infiltration of sea and ocean water into the sewer systems.

This work is based on the example of the Freistadt wastewater treatment plant (WWTP). The Freistadt WWTP is located in upper Austria and has a capacity of 30 000 PE (Matzinger, 2017). According to wastewater treatment plant personnel, the facility is on the edge of capacity. In the vicinity of the city of Freistadt, a new highway is planned to be built. Since the wastewater treatment plant is on the edge of its capacity, there are concerns what impacts this additional salt may have on the plant. Unfortunately, there was no available data on the chloride measurements at Freistadt WWTP, thus this work is focused more on the identification of possible impacts that different road salt concentrations have on nitrification at activated sludge wastewater treatment plants. These impacts are then numerically simulated in the WWTP software SIMBA#.

2. Objectives and Scope

2.1 Objectives

The main objectives of this thesis are:

1) Literature review of road salt impacts on wastewater treatment plants
2) Development of a numerical model for salt impact on nitrification
3) Implementation of the developed model in SIMBA# and examination of the impact of salt on the WWTP performance using different scenarios

Literature review of road salt impacts on wastewater treatment plants

The main goal of the literature review is to find out the possible impacts that certain sodium-chloride concentrations have on wastewater treatment plants. This research should be done for the salt concentrations up to 3 g NaCl/l. Special attention should be put on the impact of salt on nitrification.

Development of a numerical model for salt impact on nitrification

After the literature review, the impacts of salt on the WWTP should be known and the work on the numerical model for nitrification rate can be done. Based on the literature review, a set of equations need to be computed, that describe the nitrification rate based on salt concentration.

Modelling in SIMBA# - implementation of the developed model in SIMBA# and examination of the impact of salt on the WWTP performance using different scenarios

When the equations that describe the nitrification rate based on salt concentration are created, the first step is implementation of these equations in SIMBA# software. Secondly, based on the literature review, the work on scenario creation needs to be done. Scenarios should include parameters that influence the removal efficiencies, e.g.:

- Different salt concentrations
- Different salt exposure times
- Decrease of water temperatures
- Change in influent quantities

2.2 Structure of the Master thesis

In chapter 3, the fundamentals that were needed to write this thesis were analysed. Firstly, some of the wastewater treatment simulation basics were described, such as preconditions needed for the computation of a good model -its limits, use cases, etc. Secondly, the difference between static and dynamic simulation was discussed and a brief description of the history of activated sludge modelling was mentioned. In the next chapter, different activated sludge models were explained. Furthermore, the steps in GMP unified protocol were described, since its steps were followed in this thesis as a modelling guide. After a description of the GMP unified protocol, the basic data of the Freistadt wastewater treatment plant was provided. The conclusion of chapter 3 was done with a literature review of road salt impacts on WWTP. This chapter provides insight into the effects of salt on oxygen uptake rates, removal efficiencies, sludge settling, etc. Chapter 4, materials and methods, describes the formulation of the numerical model. Also, it provides a description of SIMBA# software and gives a general overview of the implementation of numerical model and scenarios in SIMBA#. The last chapter in chapter 4 describes how were the steps in GMP Unified protocol followed in this thesis. Subsequently, chapter 5 describes in detail the development of the numerical model and its implementation into SIMBA#. It also shows the steps of calibration, validation and implementation of scenarios. Lastly, it displays modelled results and interpretations of these results. Chapters 6 and 7 provide the final conclusions and summary of the entire work done in this thesis.

3. Fundamentals

3.1 Basics of simulations in wastewater treatment

Wastewater treatment plants are complex systems with lots of parameters influencing their operation. A tool that can be used to predict the behavior of these parameters is simulators. Simulators can describe the state of real-world systems and their processes with mathematical equations using numerical models. There are many advantages to this:

- Experiments on wastewater treatment plants can be very expensive
- Better planning and less cost in the operational phase
- Avoidance of endangering microorganisms
- Processes can be inspected and adapted without long time delay

The first step in building a model is calibration. To appropriately calibrate the model, sufficient and accurate data is needed. Before the data sets are inserted into the model, they should be checked for errors and plausibility (Rieger et al.,2013).

In addition, Rieger et al. (2013) state that modelling can be used for the following purposes (Figure 1):

- Prognostic – Describes the future events
- Diagnostic – Describes the involved processes and mechanisms
- Educational – Describes the exchange of knowledge between experts and beginners, but also for training of wastewater treatment personnel

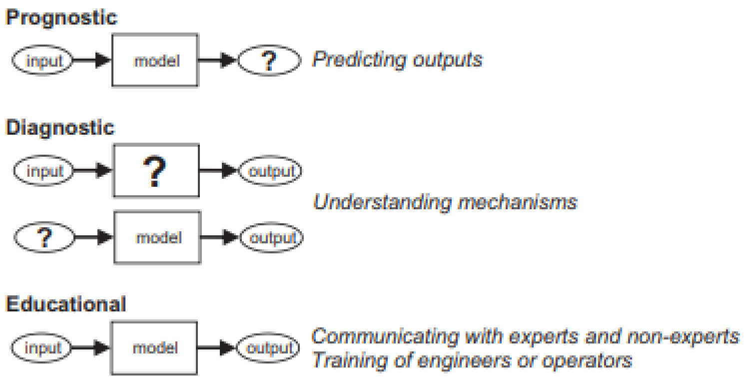

Figure 1. Purposes of modelling (Rieger et al., 2013, p. 5)

When modelling, it is important to keep the model as simple as possible, but complex enough to fulfill the intended modelling purpose.

3.2 Dynamic vs. static simulation

Static design and expansion of wastewater treatment plants in Austria are regulated by DWA-A 131 (2016). Static simulation is used for designing the parts of the wastewater treatment plant, such as the volume of the activated sludge tank and the amount of recirculation. The first step in the static design of wastewater treatment plants is to determine the required purification and set the inflow data. With the inflow data and selected process method (single-stage, two-stage), sludge volume index and sludge age are calculated. Based on SVI and SRT the following parameters are determined: return sludge volume, system volume and air quantity (Alex et al., 2015). Static calculations can be done in an Excel file and don't require any additional (specialized) software.

Unlike static simulation, the inflow parameters (Water quantity, COD, Nitrogen, Phosphorus) for dynamic simulations are not constant over time. This allows much more detailed representation and control of a system state. With the help of dynamic simulations, the following models of wastewater treatment plant can be created (Langergraber, 2020):

- Input model
- Biokinetic model
- Clarifier model
- Hydraulic and transport model
- Pump model
- Sensor model
- Controller model
- Aeration model
- Output model

Although the dynamic simulation has a lot of advantages, there are also some negatives. Dynamic simulations are often time-consuming, they need special software and an experienced modeller.

3.3 History of activated sludge modelling

According to Rieger et al. (2013), the development of the Activated Sludge System started in 1912, when Penfold and Norris made a connection between bacterial growth and substrate concentration. In the year 1914, Ardern and Lockett invented the "Activated Sludge Process". Further development of activated sludge kinetics was done by Monod in 1942, where the bacterial growth was represented using a mathematical equation. Garrett and Sawyer in 1952 defined the behavior of mixed bacterial cultures also with Monod kinetics. Further improvement of kinetics models was done by Herbert in 1958, by introducing the concept of endogenous respiration. Through the late '50s and '60s, McKinney and Eckenfelder described the stoichiometry of sludge oxidation and they developed a mathematical representation of the kinetics of activated sludge in completely mixed reactors. The rapid expansion of the use of models happened in the mid-80s with the development of computer power. A graphical representation of the history of activated sludge models is shown in Figure 2.

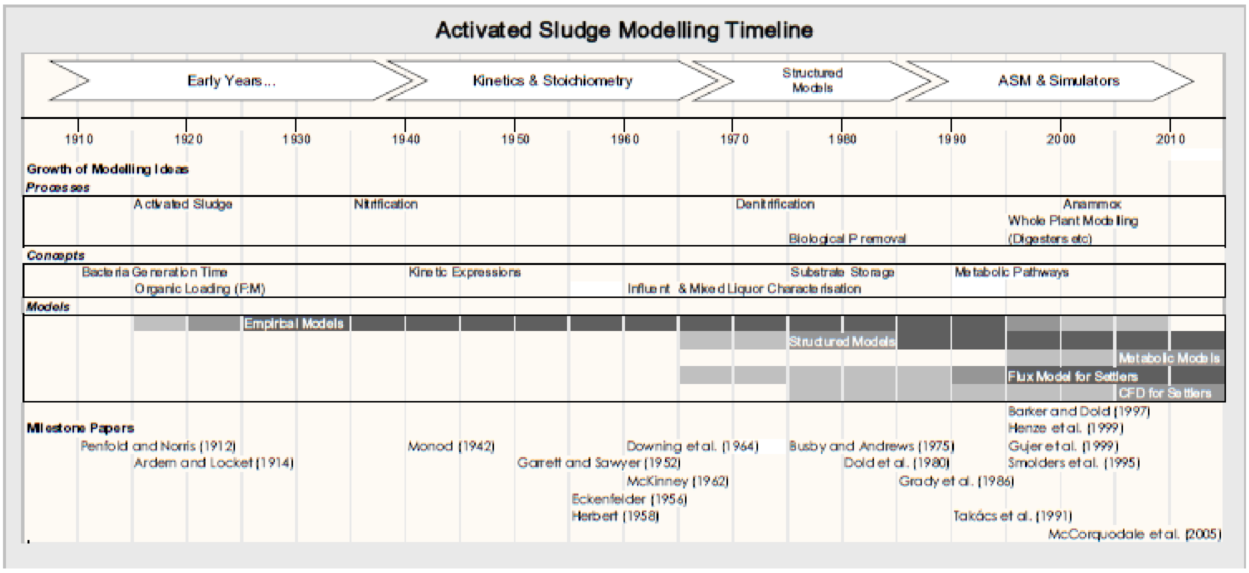

Figure 2. History of activated sludge models (Rieger et al.,2013)

3.4 Activated Sludge Models

3.4.1 Activated Sludge Model 1 – ASM1

International Water Association (IWA) in 1982 set up a task group "Mathematical Modelling for Design and Operation of Biological Wastewater Treatment" to define an activated sludge system that includes nitrification, denitrification and carbon removal. The results of the task group were finalized in IAWPRC Activated Sludge Model No.1 [ASM1] (Henze et al., 1987).

As mentioned before, ASM1 is capable of simulating the processes of nitrification, denitrification, and carbon degradation, but ASM1 can't simulate phosphorous removal. For this type of process simulation ASM2d, Barker & Dold, or ASM3+P would be better suited.

Activated Sludge Model No.1 consists of 13 components and 8 processes (Langergraber, 2020).

Components of ASM1 are (Langergraber, 2020):

1) SI – Soluble inert organic matter
2) SS – Soluble biodegradable organic matter
3) XS – Slowly biodegradable particulate organic matter
4) XI – Non-degradable particulate matter
5) XBH – Heterotrophic biomass
6) XBA – Autotrophic biomass
7) XP – particulate products of decay processes
8) SO - Soluble oxygen
9) SNO – Soluble nitrate and nitrite nitrogen
10) SNH – Soluble ammonia nitrogen (NH_4-N)
11) SND – Soluble organic nitrogen
12) XND – Particulate organic nitrogen
13) SALK – Alkalinity

13 Components of ASM1 can be divided into COD fractions (SI, SS, XS, XBH, XI, XBA, XP, SO), Nitrogen fractions (SND, XND, SNH, and SNO,) and water alkalinity (Salk). The notation “S” stands for soluble substances and “X” for particulate substances. A better, graphical representation of components of ASM1 is in Figure 3.

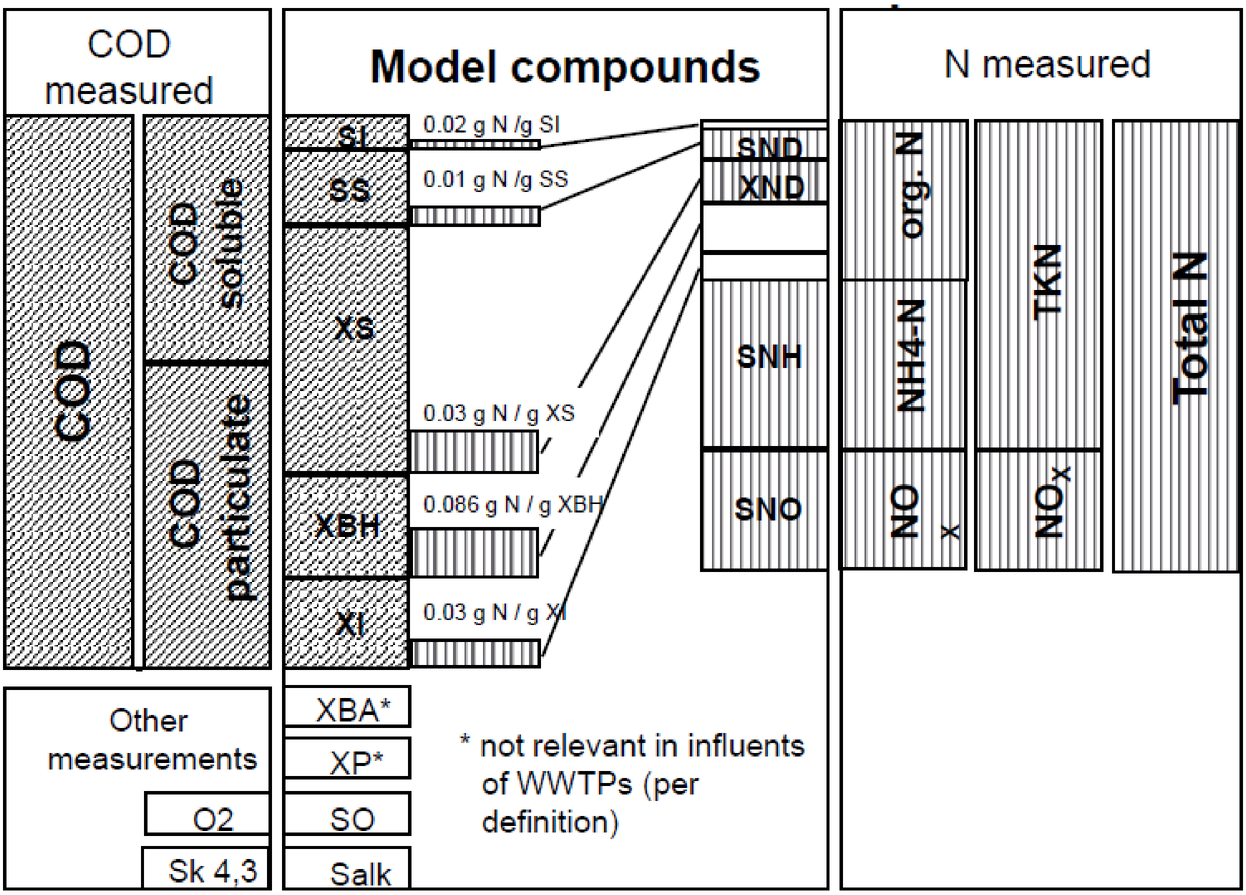

Figure 3. Components of ASM1 (Langergraber, 2020)

ASM1 can simulate the following processes (Langergraber, 2020):

- Heterotrophic growth under aerobic conditions
- Heterotrophic growth under anoxic conditions
- Death of heterotrophic organisms
- Autotrophic growth under aerobic conditions
- Death of autotrophic organisms
- Hydrolysis of dead biomass
- Hydrolysis of particulate organic nitrogen compounds
- Ammonification of the dissolved organic nitrogen compounds

For a better depiction of Stoichiometry and Kinetic reactions of ASM1, the Gujer matrix was compiled (Henze et al., 1987). Gujer matrix for ASM1 can be seen in Figure 4.

j	Component i → / Process ↓	1 S_I	2 S_S	3 X_I	4 X_S	5 $X_{B,H}$	6 $X_{B,A}$	7 X_P	8 S_O	9 S_{NO}	10 S_{NH}	11 S_{ND}	12 X_{ND}	13 S_{ALK}	Process Rate, ρ_j $[ML^{-3}T^{-1}]$
1	Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)X_{B,H}$
2	Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14\cdot 2.86Y_H}-i_{XB}/14$	$\hat{\mu}_H\left(\frac{S_S}{K_S+S_S}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\times\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{B,H}$
3	Aerobic growth of autotrophs						1		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\hat{\mu}_A\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A}$
4	'Decay' of heterotrophs				$1-f_P$	-1		f_P					$i_{XB}-f_P i_{XP}$		$b_H X_{B,H}$
5	'Decay' of autotrophs				$1-f_P$		-1	f_P					$i_{XB}-f_P i_{XP}$		$b_A X_{B,A}$
6	Ammonification of soluble organic nitrogen										1	-1		$\frac{1}{14}$	$k_a S_{ND} X_{B,H}$
7	'Hydrolysis' of entrapped organics		1		-1										$k_h\frac{X_S/X_{B,H}}{K_X+(X_S/X_{B,H})}\left[\left(\frac{S_O}{K_{O,H}+S_O}\right)+\eta_h\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{B,H}$
8	'Hydrolysis' of entrapped organic nitrogen											1	-1		$\rho_7(X_{ND}/X_S)$
	Observed Conversion Rates $[ML^{-3}T^{-1}]$	$r_i=\sum_j \nu_{ij}\rho_j$													
	Stoichiometric Parameters: Heterotrophic yield: Y_H; Autotrophic yield: Y_A; Fraction of biomass yielding particulate products: f_P; Mass N/Mass COD in biomass: i_{XB}; Mass N/Mass COD in products from biomass: i_{XP}	Soluble inert organic matter $[M(COD)L^{-3}]$	Readily biodegradable substrate $[M(COD)L^{-3}]$	Particulate inert organic matter $[M(COD)L^{-3}]$	Slowly biodegradable substrate $[M(COD)L^{-3}]$	Active heterotrophic biomass $[M(COD)L^{-3}]$	Active autotrophic biomass $[M(COD)L^{-3}]$	Particulate products arising from biomass decay $[M(COD)L^{-3}]$	Oxygen (negative COD) $[M(-COD)L^{-3}]$	Nitrate and nitrite nitrogen $[M(N)L^{-3}]$	$NH_4^+ + NH_3$ nitrogen $[M(N)L^{-3}]$	Soluble biodegradable organic nitrogen $[M(N)L^{-3}]$	Particulate biodegradable organic nitrogen $[M(N)L^{-3}]$	Alkalinity – Molar units	Kinetic Parameters: Heterotrophic growth and decay: $\hat{\mu}_H$, K_S, $K_{O,H}$, K_{NO}, b_H; Autotrophic growth and decay: $\hat{\mu}_A$, K_{NH}, $K_{O,A}$, b_A; Correction factor for anoxic growth of heterotrophs: η_g; Ammonification: k_a; Hydrolysis: k_h, K_X; Correction factor for anoxic hydrolysis: η_h

Figure 4. Gujer matrix for ASM1 (Henze et al., 1987, p.7)

3.4.2 Activated Sludge Model 2 – ASM2 and ASM2D

After the completion of Activated Sludge Model No.1 [ASM1] (Henze et al., 1987), further work was carried out in broadening the ASM1. Since ASM1 is not able to simulate phosphorus removal, Activated Sludge Model No.2 [ASM2] was created (Henze et al., 1999). To enable the simulation of phosphorus removal, further biological parameters were added to ASM2. The biomass concentration X_{BM} in ASM2 has an internal cell structure, which was the prerequisite for the inclusion of phosphorus removal. Furthermore, for the inclusion of chemical phosphorus precipitation, 2 chemical processes were added (Henze et al., 2000).

Henze et al., 1987 stated that ASM2d slightly widens the scope of ASM2. The improvement is in the inclusion of phosphorus accumulating organisms (PAOs), as their internal cell, organic storage is used for denitrification.

Even though ASM2 made improvements over the ASM1 and thus incorporated more processes and parameters for simulation, this complexity can lead to longer computing times and more computer power.

3.4.3 Activated Sludge Model 3 – ASM3

With the development of computer power, the limiting factors for model development also slowly vanished. This is obvious in the example of ASM1. Since in the mid-1980s, computers didn’t have very high computation power, the single process of lysis was implemented to describe all decay processes. Since then, technology has drastically improved. This led to the evolution of ASM and the creation of ASM3 (Henze et al., 2000).

ASM3 introduced the separation of heterotroph and nitrifier conversion processes (Figure 5.) and thus solved the inelegant implementation of decay processes in ASM1 and led to a better, more realistic, representation of reality (Henze et al., 2000).

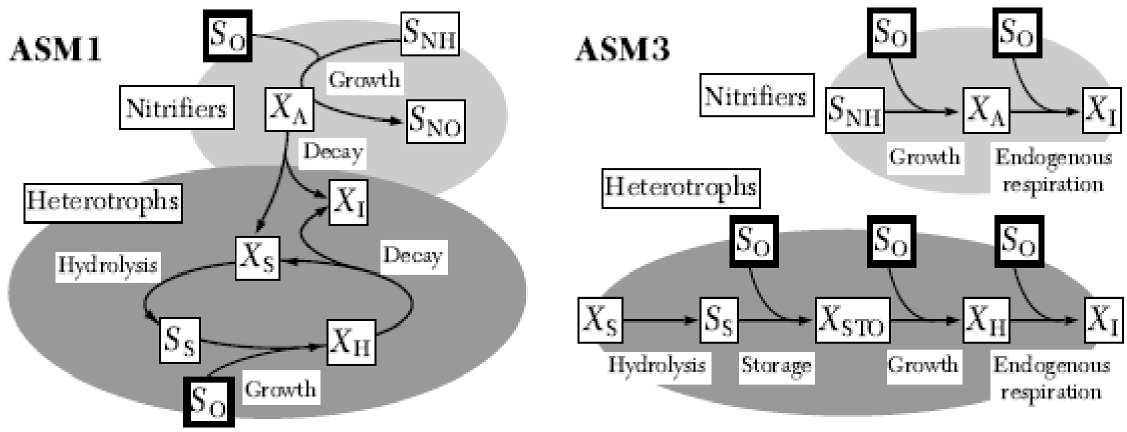

Figure 5. Flow of COD in ASM1 and ASM3 (Henze et al., 2000, p.105)

ASM3 consists of 13 components and 12 processes, represented in Figure 6. (Langergraber, 2020). Components of ASM3 are divided into soluble compounds S, and particulate compounds X (Henze et al., 2000).

Soluble compounds S are: Dissolved oxygen S_{O2}, Inert soluble organic material S_I, Readily biodegradable organic substrates (COD) S_S, Ammonium plus ammonia nitrogen S_{NH4}, Dinitrogen S_{N2}, Nitrate plus nitrite nitrogen $S_{NOX,}$ and Alkalinity of the wastewater S_{ALK}.

Particulate compounds X are: Inert particulate organic material X_I, Slowly biodegradable substrates X_S, Heterotrophic organisms X_H, Cell internal storage product of heterotrophic organisms X_{STO}, Nitrifying organisms $X_{A,}$ and Suspended solids X_{SS}.

ASM3 was used in the modelling software (SIMBA#) on this thesis, specifically ASM3h. Even though ASM3 has a lot of advantages, some factors limit its use. Henze et al. (2000) state that this model was created for domestic wastewater systems with no significant industrial impact. Furthermore, it is limited to aerobic and anoxic processes. ASM3 is designed for use for inflow water temperatures in the range of 8-23 °C and outside of this range, there is a possibility of inaccurate results. Also, the pH value should be between 6.5 and 7.5.

j ↓	Compound i →		1	2	3	4	5	6	7	8	9	10	11	12	13
	Process		S_{O_2}	S_I	S_S	S_{NH_4}	S_{N_2}	S_{NOX}	S_{ALK}	X_I	X_S	X_H	X_{STO}	X_A	X_{SS}
	Expressed as →		O_2	COD	COD	N	N	N	Mole	COD	COD	COD	COD	COD	SS
1	Hydrolysis			f_{S_I}	x_1	y_1			z_1		-1				$-i_{X_S}$
Heterotrophic organisms, aerobic and denitrifying activity															
2	Aerobic storage of S_S		x_2		-1	y_2			z_2				Y_{STO,O_2}		t_2
3	Anoxic storage of S_S				-1	y_3	$-x_3$	x_3	z_3				$Y_{STO,NOX}$		t_3
4	Aerobic growth of X_H		x_4			y_4			z_4			1	$-1/Y_{H,O_2}$		t_4
5	Anoxic growth (denitrific.)					y_4	$-x_5$	x_5	z_5			1	$-1/Y_{H,NOX}$		t_5
6	Aerobic endog. respiration		x_6			y_6			z_6	f_I		-1			t_6
7	Anoxic endog. respiration					y_7	$-x_7$	x_7	z_7	f_I		-1			t_7
8	Aerobic respiration of X_{STO}		x_8										-1		t_8
9	Anoxic respiration of X_{STO}						$-x_9$	x_9	z_9				-1		t_9
Autotrophic organisms, nitrifying activity															
10	Aerobic growth of X_A		x_{10}			y_{10}		$1/Y_A$	z_{10}					1	t_{10}
11	Aerobic endog. respiration		x_{11}			y_{11}			z_{11}	f_I				-1	t_{11}
12	Anoxic endog. respiration					y_{12}	$-x_{12}$	x_{12}	z_{12}	f_I				-1	t_{12}
Composition matrix $\iota_{k,I}$															
k	*Conservatives*														
1	ThOD	g ThOD	-1	1	1		-1.71	-4.57		1	1	1	1	1	
2	Nitrogen	g N		i_{N,S_I}	i_{N,S_S}	1	1	1		i_{N,X_I}	i_{N,X_S}	$i_{N,BM}$		$i_{N,BM}$	
3	Ionic charge	Mole +				1/14		$-1/14$	-1						
	Observables														
4	SS	g SS								i_{SS,X_I}	i_{SS,X_S}	$i_{SS,BM}$	0.60	$i_{SS,BM}$	

j	Process	Process rate equation ρ_j, all $\rho_j \geq 0$.
1	Hydrolysis	$k_H \cdot \frac{X_S/X_H}{K_X + X_S/X_H} \cdot X_H$
Heterotrophic organisms, aerobic and denitrifying activity		
2	Aerobic storage of S_S	$k_{STO} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_S}{K_S + S_S} \cdot X_H$
3	Anoxic storage of S_S	$k_{STO} \cdot \eta_{NOX} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NOX}}{K_{NOX} + S_{NOX}} \cdot \frac{S_S}{K_S + S_S} \cdot X_H$
4	Aerobic growth	$\mu_H \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{STO}/X_H}{K_{STO} + X_{STO}/X_H} \cdot X_H$
5	Anoxic growth (denitrification)	$\mu_H \cdot \eta_{NOX} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NOX}}{K_{NOX} + S_{NOX}} \cdot \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{STO}/X_H}{K_{STO} + X_{STO}/X_H} \cdot X_H$
6	Aerobic endogenous respiration	$b_{H,O_2} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot X_H$
7	Anoxic endogenous respiration	$b_{H,NOX} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NOX}}{K_{NOX} + S_{NOX}} \cdot X_H$
8	Aerobic respiration of X_{STO}	$b_{STO,O_2} \cdot \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \cdot X_{STO}$
9	Anoxic respiration of X_{STO}	$b_{STO,NOX} \cdot \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \cdot \frac{S_{NOX}}{K_{NOX} + S_{NOX}} \cdot X_{STO}$
Autotrophic organisms, nitrifying activity		
10	Aerobic growth of X_A, nitrification	$\mu_A \cdot \frac{S_{O_2}}{K_{A,O_2} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{A,NH_4} + S_{NH_4}} \cdot \frac{S_{ALK}}{K_{A,ALK} + S_{ALK}} \cdot X_A$
11	Aerobic endogenous respiration	$b_{A,O_2} \cdot \frac{S_{O_2}}{K_{A,O_2} + S_{O_2}} \cdot X_A$
12	Anoxic endogenous respiration	$b_{A,NOX} \cdot \frac{K_{A,O_2}}{K_{A,O_2} + S_{O_2}} \cdot \frac{S_{NOX}}{K_{A,NOX} + S_{NOX}} \cdot X_A$

Figure 6. Stoichiometric matrix with kinetic rate expressions for ASM3

(Henze et al., 2000, p. 111)

3.5 GMP Unified Protocol

3.5.1 Introduction

The use of mathematical models has been welcomed by many engineers around the world for training, optimization, research, and design of activated sludge systems. These models are a valuable tool only if the results are comparable to "real world" outcomes. For this to be true, it is useful to have a unified approach to modelling and documentation, which can simplify the relation and assessment of models. This type of standardization would lead to improvements in use, accuracy, and knowledge of modellers and models.

In 2009, the IWA task group on good modelling practice (GMP) tried to provide guidance for the biggest recognized problems that prevent widespread use of activated sludge models in practice, which are: Cost and time, Model structure, Model application, and Modelling procedure. The result was compiled in IWA Scientific and Technical Report (STR) – Guidelines for Using Activated Sludge Models (Rieger et al., 2013).

3.5.2 Overview

Rieger et al. (2013) stated that GMP Unified Protocol is a guideline for modellers and stakeholders. It is represented in a graphical form (Figure 7.) with a 5-stage "step by step" guide. The 5 stages of GMP Unified Protocol are:

1) Project Definition
2) Data Collection and Reconciliation
3) Plant Model Set-Up
4) Calibration and Validation
5) Simulation and Result Interpretation

As it can be seen from Figure 7. the protocol was separated into 5 distinct stages. At the end of each stage, there is a question loop that serves as a reminder for a modeller and a stakeholder. This reminder is put in place to provide control and optimization in each part of the project. It can also be regarded as a "Reach of consensus".

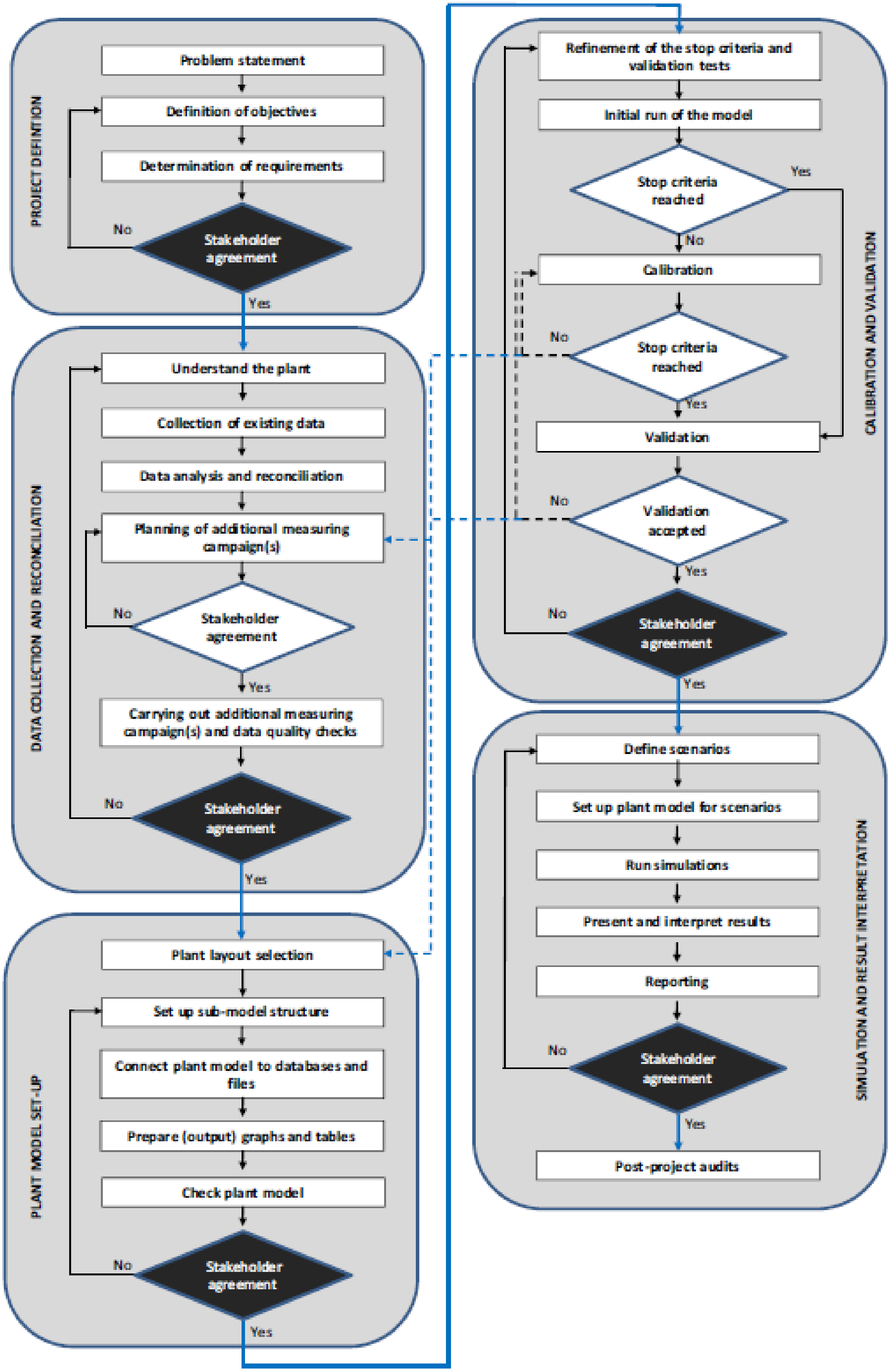

Figure 7 GMP Unified Protocol (Rieger et al. 2013, p. 27)

3.5.3 Stages of GMP Unified Protocol

Project definition

Rieger et al. (2013) state that the block "Project definition" is made from the following steps: problem statement, definition of objectives and determination of requirements. Project definition is one of the most important steps in the GMP Unified Protocol. In this step, a clear set of objectives should be set. This allows the establishment of a good design plan and ensures that time and money are spent as productively as possible.

Problem statement - In every modelling project, it is paramount to specify the exact reason why is this system being modelled. To what question should the model offer the answer. This question should be explicit and accurate, but also easily understandable to all involved parties.

Definition of objectives - When the problem has been clearly defined, it needs to be broken up into smaller chunks (objectives). For a clear object definition, a different set of factors need to be taken into an account: model boundaries, level of complexity, stop criteria, stakeholder responsibilities, and known constraints.

Determination of requirements - When all the objectives have been specified, the establishment of exact procedures and requirements needed for implementation of these objectives should be placed. The following processes should be taken into an account: setting up individual tasks, data requirements, necessary workforce, time frame, deliverables, and budget.

When the problem statement, the definition of objectives, and determination of requirements are in place, the final step is consultation and negotiation with a stakeholder. Only with approval from a stakeholder should the work on Data collection and reconciliation be proceeded.

Data collection and reconciliation

According to Rieger et al. (2013), data collection and reconciliation is the most time-consuming part of the project. This is because to have an accurate and usable model, appropriate work must be done in generating high-quality data sets. The verification of this data set is then in turn.

Understand the plant - To better understand the ins and outs of a WWTP, a visit to the plant is essential. Talking with WWTP personnel can give valuable insight into the operation of a plant. With their help and piping and instrumentation diagram - treatments steps, loadings, the connection between tanks, the flow of internal recirculation, etc. can be acquired. Also, they can provide insight into the operational modes for different temperatures and loadings. The majority of available data in WWTP are taken from automatic samplers. Thus, their position and operation (volume, flow, or time) must also be noted.

Collection of existing data - After consultation with WWTP personnel, all available data that is collected in WWTP can be obtained. Rieger et al. (2013), give the following division of data types: input data (flow rate, influent concentration, WW characterization…), physical data (number of tanks, their volume, flow scheme...), operational settings (controllers, flow rates, flow splits…), performance data (MLSS, SRT, effluent concentration, WAS concentration…), and additional info (connected industries, sewer system…).

Data analysis and reconciliation – Before inserting the acquired data into the model, it is paramount to execute the necessary "quality control" of the existing data. Skipping this step may result in the inaccurate output of the model results. Rieger et al. (2013) state that it can be distinguished between systematic, random, and outlier errors. "*Systematic errors can be characterized as offsets (or shifts), signal drifts (change of signal over time), or calibration curve errors (linear or non-linear). Random errors can be split into random errors related to the instrument and the measuring principle (which are typically not reducible) and random errors related for example, to environmental conditions, sensor installation, measuring frequency, or signal transmission. Outliers are gross errors and are typically removed based on statistical analysis*" (Rieger et al., 2013, p. 44).

Furthermore, Rieger et al., (2013) define 4 steps in the data reconciliation procedure:

1) Fault Detection
2) Fault Isolation
3) Fault Identification
4) Data reconciliation

Planning of additional measuring campaigns – When the necessary analysis of existing data has been completed, it´s possible that some required data is missing or there are errors in it. In this case, additional measuring campaigns are to be planned. Since measuring campaigns are often very costly and time-consuming, it is necessary to obtain the stakeholder agreement before their implementation.

Carrying out additional measuring campaigns and data quality checks – After additional measuring campaigns have been completed, it is necessary to control them for errors, as done in the previous step. If all the final data and stakeholder agreements have been collected, it is possible to proceed to the next block – "Plant model set-up".

Plant model set-up

Plant layout selection – The plant layout selection depends on the expected goal of the model. This goal dictates how detailed the model (sub-models) should be. Also, according to Rieger et al., (2013), model boundaries, subsystems, and their interactions are to be considered when setting the layout of the model.

Set up the sub-model structure – When setting up the sub-model structure, the following steps need to be defined: modelled layout, model selection, model set-up, and connections between sub-models. These steps are usually done in simulation software (e.g. SIMBA#). Simulation software allows an intuitive representation of model parts and their connection. This is done by a simple – "Drag and drop" function of pre-existing modules inside the software. Depending on the structure of the model, the modeller can also choose which reactor model is best suited.

Connect plant model to databases and files - After the completion of the model structure, input data can be inserted. For dynamic simulations, time series of concentrations and flows are needed.

Prepare (output) graphs and tables – After a certain number of simulation runs, it is necessary to compare the output simulation values and measured data. In Simulation software, calculated output values are represented as tables or graphs. A graph with a side-by-side comparison of modeled and measured data can be a good visual indicator of the accuracy of a model.

Check plant model – As mentioned in a previous step, simulation software provides modellers with a good comparison of modeled and measured values. When running a dynamic simulation, real-world WWTP is appropriately implemented in a model if, when running initial simulations, no error messages appear. For the cost and deadline of the project, it is necessary to also take into account the duration of simulation runs. If the simulation times are too long, project deadlines and budgets may be breached. Thus, stakeholder agreement should also be acquired at this step.

Calibration and validation

Mathematical equations are used to describe the real processes of WWTP (Rieger et al., 2013). To transpose the real processes into the numerical model, some simplifications must be made. This results in a model that is not fully compatible with the real-world WWTP, so it is necessary to improve it by process of calibration and validation. The process of calibration consists of tweaking different model parameters. For the first runs of the model, it is advisable to run the model in a modeling software with default values of model parameters. Each change of model parameters would show in a model (e.g., change in nitrogen removal). In this way measured and modeled data can be compared and adjust the accuracy of the model. Model parameters can be operational, physical, stoichiometric, and kinetic (Rieger et al., 2013). Since this is an iterative process, it is often time-consuming and requires the experience of a modeler. The calibration process is finished when an acceptable difference between measured and modeled data is reached. This is called "Stop criteria" and then the process of validation follows. The process of validation consists of running different tests to ensure the fulfillment of modeling objectives.

Refinement of the stop criteria and validation test – For the process of model calibration it is necessary to define when there is no more need for the change of model parameters – the "Stop criteria". Rieger et al., (2013) state that stop criteria can be limited with a maximum number of model runs, minimum or maximum values of parameters, minimum values for the objective functions, etc. After calibration, special data sets (that were not used in the calibration step) can be used to validate the model.

The initial run of the model – As mentioned before, to ensure representable results in models, data sets are divided into data sets for calibration and data sets for validation. After running the model for the first time with calibration data sets as an input, starts the iterative process of model calibration.

Calibration – It is very unlikely that the first model run will reach stop criteria. Depending on the difference between the measured objective function and simulated modeled result, the modeller is provided with valuable information on which "wheel" to turn. If pre-collected measurements on model parameters are available, they can improve the accuracy and calibration of the model. Also, specific data on the type of wastewater coming to the WWTP (e.g. from certain industries), different experimental results from the literature, etc. can influence modellers to adjust certain modelling parameters (Rieger et al., 2013).

Validation – When “Stop criteria” is reached, the calibration process is finished. To ensure the model’s accuracy, specific data sets can be used to validate the model. These data sets can also include (depending on the modeling objective) the specific cases of high loading of WWTP, winter conditions with lower water temperatures, etc. If the model passes the check also with these specific data sets, validation is accepted.

Simulation and result interpretation

Simulation and results interpretation is the last block of Unified Protocol. It answers all the objectives set in the first block “Project Definition” and advocates for any of the objectives that it didn’t meet (Rieger et al., 2013). If the block “Project Definition” is well defined, it will show the exact scope and number of scenarios that need to be executed in the “Simulation and result interpretation” block.

Define scenarios – Rieger et al., (2013) state that the number and scope of scenarios need to resolve all the objectives that are defined in the project definition. The time of the simulation computation depends on the following factors (Rieger et al., 2013):

1) Steady-state vs dynamic
2) Input data
3) Control parameters
4) Simulation time constraints
5) Output management

Set up plant models for scenarios – Set up of plant models for scenarios depends on the data requirements for steady-state and/or dynamic simulation and possible adjustment of plant model layout. For the fulfillment of the project objective, it is often necessary to adjust the layout for one (or more) of the following reasons: plant expansion, plant upgrade, plant optimization, maintenance and construction impacts, or extreme event assessment (Rieger et al., 2013).

Run simulations – When running simulations, the job of the modeller is to set the model and interpret the output results. When output results are non-intuitive, certain steps need to be made to ensure the rectification of the mistakes. These can be changing from steady-state simulation to dynamic, control of the input data, initial conditions, etc.

Present and interpret results – Modern software like SIMBA# allows for an intuitive representation of the output results in the form of tables and charts that can be exported for further processing. This processing of output data allows the modeller to interpret and present the results and objectives. It also allows the modeller to spot inconsistencies and errors in results. This type of representation also allows easy comparison between scenarios, which makes interpretation easier.

Reporting – This is the final step of the GMP unified protocol. After the final stakeholder agreement, all the technical documentation should be compiled in a way that follows the blocks of the GMP unified protocol. Technical documentation should contain all input data, plant model parameters, output data, and any other data that would allow replication of the model at a later date. This should be done because of control, further optimization of WWTP in the future, and education of inexperienced modellers.

3.6 Freistadt wastewater treatment plant

Since the visit to the Freistadt WWTP was not possible, the data about the plant was taken from the thesis of Matzinger (2017). The Freistadt WWTP collects wastewater from the city of Freistadt and four more municipalities: Lasberg, Rainbach, Grünbach, and Waldburg. The WWTP is located in Upper Austria on the outskirts of the city of Freistadt. It has a capacity of 30 000 population equivalent. This capacity was reached through WWTP expansion in 2007 and 2008. At the end of 2021, there was an additional expansion to the capacity of 38 000 population equivalent.

The collected wastewater from 5 municipalities is fed to the WWTP through a channel flow regulator, with a maximum flow of 175 l/s. Any wastewater excess to the WWTP is fed to the relief rain reservoir. After a rain event, this excess water is pumped to the WWTP via 2 submersible pumps.

Freistadt wastewater treatment plant is comprised of the following cleaning stages:

- Mechanical cleaning
- Biological cleaning
- Sludge stabilization

The layout of the plant is shown in Figure 8. The first stage at Freistadt WWTP is mechanical cleaning. Mechanical cleaning is the process of removing pollution and waste through a screen system, sand trap, and primary clarifiers.

As the influent wastewater reaches the treatment plant via a channel, the large incoming waste fractions are removed from the wastewater with a screen system. The screen system removes all waste larger than 3 mm which is automatically transported with a conveyor system. In the case of failure or maintenance purposes, there is a bypass channel with an additional screen. After the screen system, the wastewater reaches the sand trap. The sand trap has a circular water motion, which allows the separation of water and heavier particles through centrifugal force. Through this, sand and other heavier particles end up in the center of a sand trap, from where they are removed. Because of redundancy reasons, there is also a bypass channel for the sand trap. Furthermore, in the sand trap there are inflow, temperature, and pH measurement devices and samplers. In the channel after the sand trap, venturi with an echo sounder records the inflow quantities of wastewater. The final stage of mechanical cleaning is primary clarification. In the primary clarification step, water from the venturi channel is drastically slowed down in a large tank. This slowing-down of water allows particles in wastewater to settle on the bottom of the tank, from which it can be then removed. In Freistadt WWTP, primary clarification consists of two primary clarifier tanks. Both tanks have a volume of 200 m^3 and a surface of 100 m^2. Removing of primary sludge is done with a bridge scraper and sludge is transported to static thickener with a help of two submersible pumps. Also, because of elevation difference, wastewater is transported from primary clarification to activated sludge tanks with four centrifugal pumps.

The biological stage consists of four activated sludge tanks and three secondary clarifiers. The first two aerated activated sludge tanks (1 and 2) have a volume of 1 050 m^3. Also, they have aeration zones and denitrification zones. The first two aerated tanks can be operated in parallel or in series. The last two aerated activated sludge tanks (3 and 4) have a volume of 1 500 m^3. All aerated tanks have an oxygen probe for O_2 control, and tanks 3 and 4 also have an ammonium probe, which allows aeration control based on NH_4 concentration. Aeration tanks 3 and 4 are designed in a way that enables recirculation to aeration tanks 1 or 2. Furthermore, there is an option of recirculating wastewater from tank 2 to tank 1. The wastewater flows further from aerated activated sludge tanks to secondary clarification. In Freistadt WWTP there are three horizontal longitudinal tanks. All three tanks have a volume of 1015 m^3. Secondary clarifiers enable sludge particles to settle on the bottom of the tank, where they are pushed to the two hoppers in the bottom with a chain scraper. From the hoppers, sludge is recirculated via a return sludge pump station. There are 3 centrifugal pumps, for each of the 3 secondary clarifiers. Furthermore, the return sludge pumping station contains flow quantities measurement device for return sludge quantities control. Excess sludge is removed in the return pumping station with a help of three valves. Cleaned water, that is separated from the particles, is drained from a secondary clarifier via 4 perforated drainage pipes. The water effluent is collected in the drainage channel, which also contains flow quantities and water quality sampling measurements.

Sludge stabilization is an anaerobic process that takes place in an anaerobic digestion tower. Sludge is fed to the anaerobic digestion tower from the sludge dewatering process and static thickener. The process of digestion creates gas and stabilized sludge. Stabilized sludge is transported from the digestor and dewatered, and then is ready for agricultural use as a fertilizer.

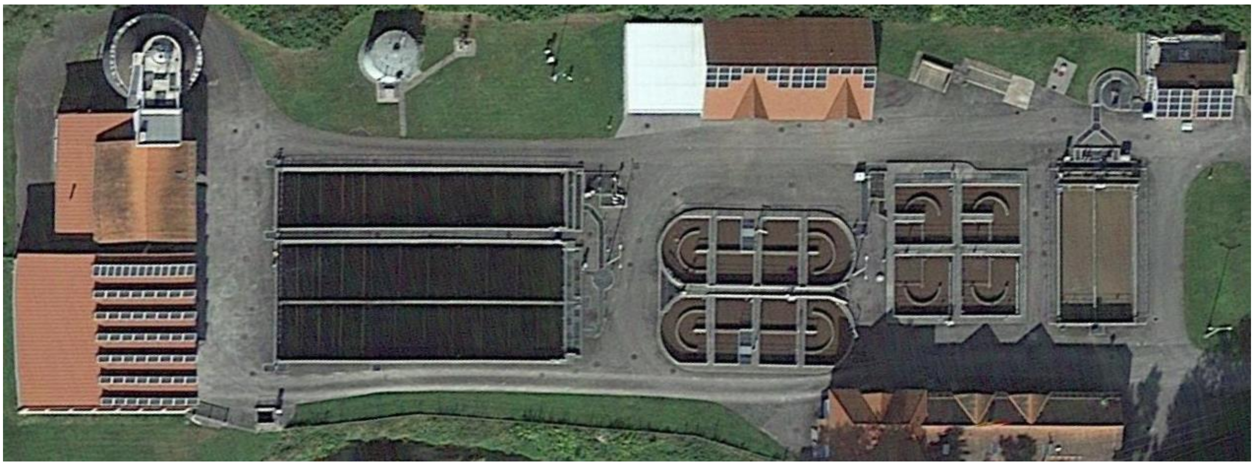

Figure 8. Freistadt wastewater treatment plant (Google Earth, 2008)

3.7 Road salt impacts on WWTP

3.7.1 Basics

The available literature on the impact of road salt is very scarce. The existing literature is mostly focused on the higher concentrations of salt (>10 g NaCl/l), which occur in coastal areas, and not on the lower – shock-like loads that come from street surface runoff. These concentrations are usually around 1-3 g NaCl/l (Flesch 2020).

Autotrophic and heterotrophic bacteria respond differently to the type of salt loading and salt concentration. There are two main types of salt loading: shock-like and continuous. Pernetti & Di Palma (2005) have done experiments with shock-like and continuous salt loading. After the shock-like loading, there was a respiration inhibition between 4% and 84%. Since respiration data is a good indicator of carbon removal efficiencies, it can be used for its prediction. Also, when the experiments were done with continuous salt loading, it was determined that after continuous loading activated sludge can quickly adapt to higher salt concentrations. The difference between respiration inhibition with shock-like and continuous loading is shown in Figure 9.

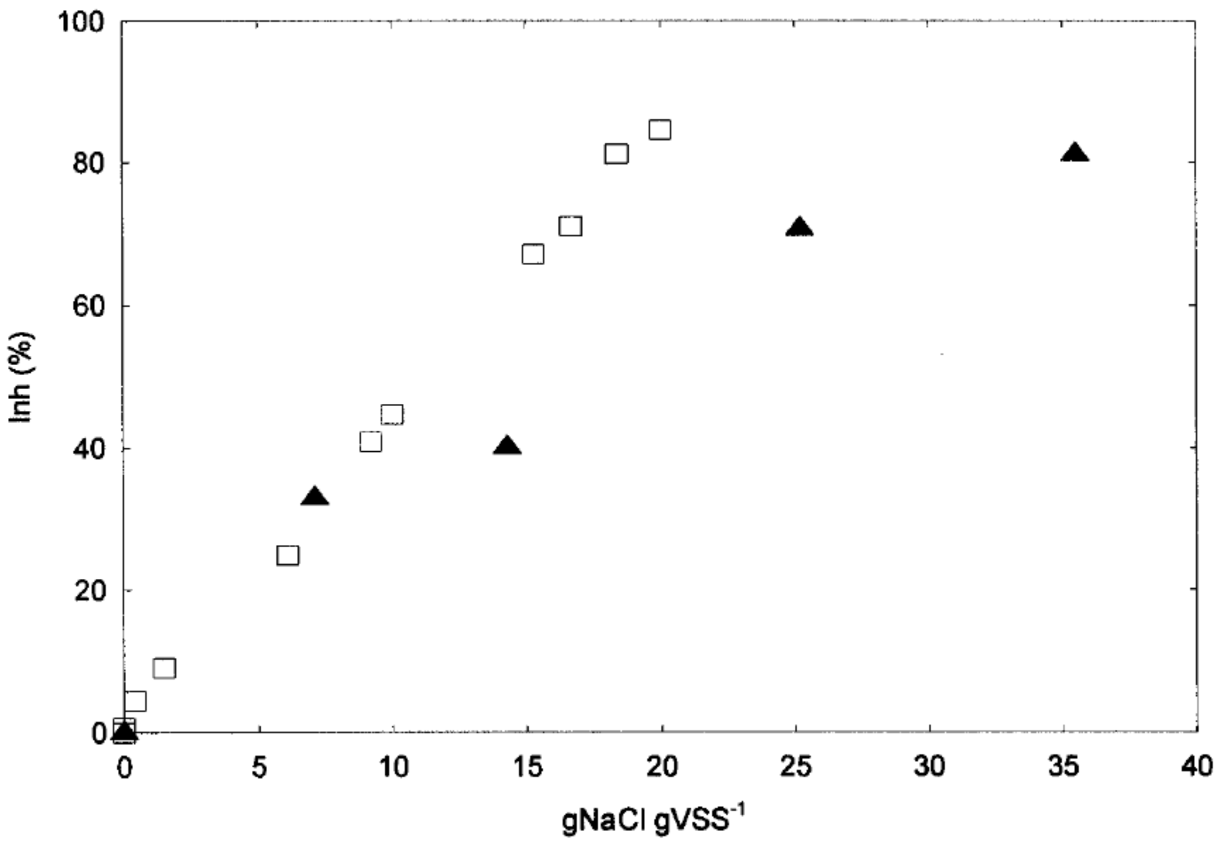

Figure 9. Respiration inhibition of activated sludge with shock-like (square) and continuous loading (triangle) (Pernetti & Di Palma, 2005)

Tauber et al. (2021) and Flesch (2020) did an experiment on a small-scale WWTP. Dosing of the wastewater with various concentrations of salt and monitoring of different oxygen uptake rates and effluent quality was done. In total 5 test phases on an experimental WWTP were done. Along with an experimental WWTP, they examined the data from 3 wastewater treatment plants in Austria.

Tauber et al. (2021) and Flesch (2020) showed that autotrophic and heterotrophic oxygen uptake rates are dependent on salt concentration and period of exposure. There were no adverse effects on autotrophic and heterotrophic bacteria when the salt concentration was below 1 g NaCl/l. Furthermore, in 75% of the tests, there was a positive increase in autotrophic and heterotrophic oxygen uptake rates. This was also shown at a full-scale WWTP. With the salt concentration of 0.7 g NaCl/l, there was an increase in almost all specific oxygen uptake rates (Figure 10).

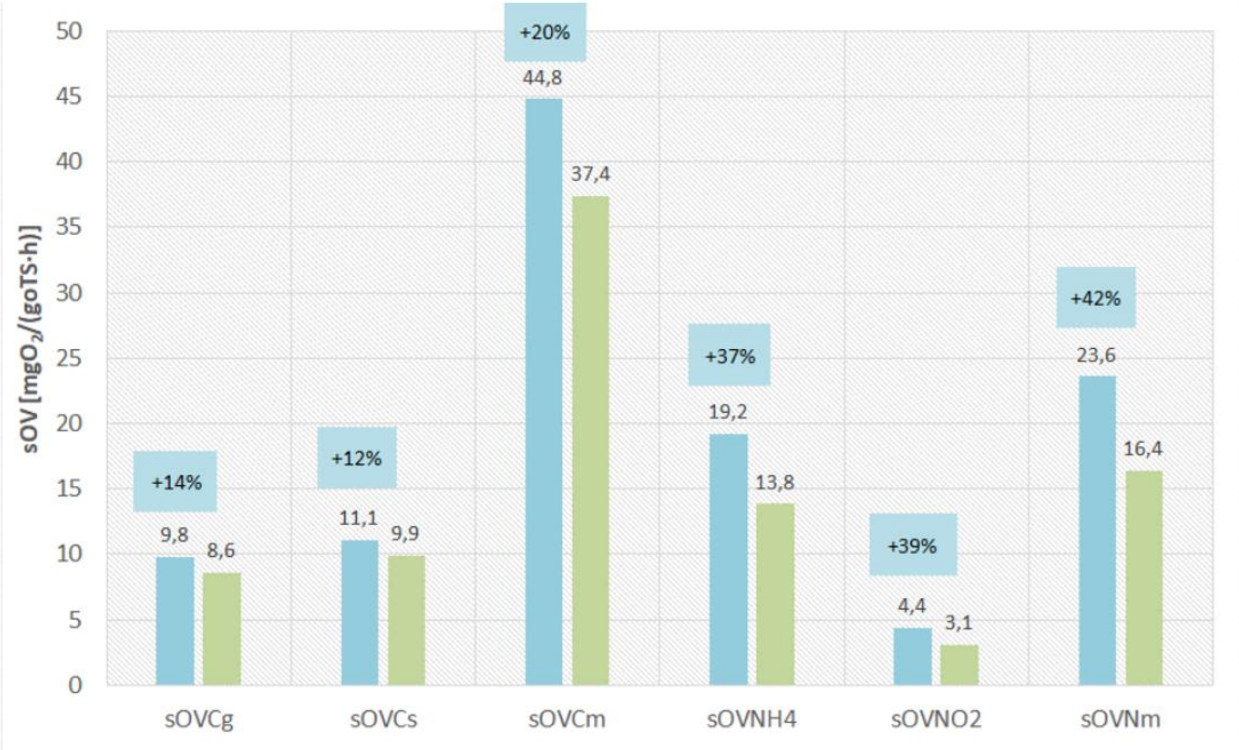

Figure 10. Oxygen uptake rates before salt dosing (green) and after 0.7 g NaCl/l (blue) (Flesch, 2020, p. 38)

As it can be seen from Figure 10, when the salt concentration was under 1 g NaCl/l, there was an increase in activity from 37% to 42% for autotrophic and from 12% to 20% for heterotrophic bacteria.

On the contrary, when the salt concentration was above 1 g NaCl/l, there were significant reductions in oxygen uptake rates. The inhibiting salt effects were affecting the WWTP only in the short and medium term. Microorganisms were able to adapt to toxic, newly created conditions relatively quickly. When the salt event has passed, there was normalization of microorganism's activity after approximately 4-5 days (Figure 11). It's also been recorded that when the salt event is passing (2 days after salt dosing), oxygen uptake rates are 50% of the oxygen uptake rates from initial salt loading (Tauber et al., 2021).

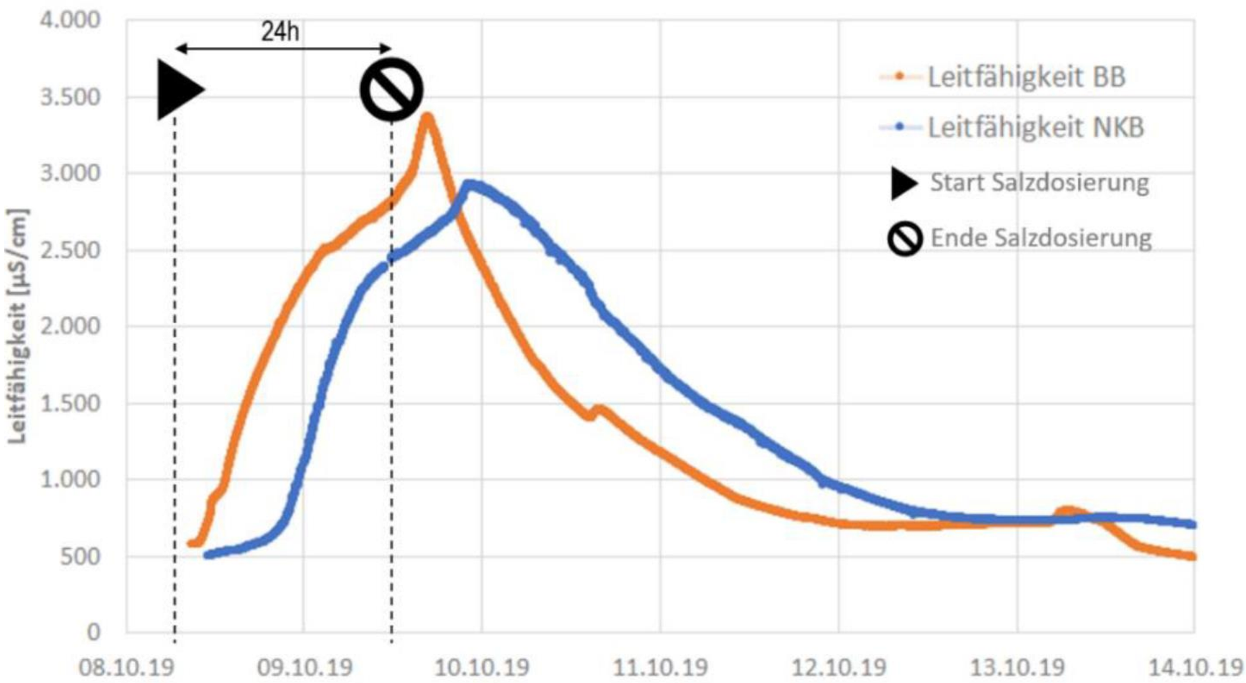

Figure 11. Conductivity measurement during the NaCl dosing on the experimental sewage treatment plant (NKB -secondary clarifier, BB – aeration tank) (Flesch, p. 35, 2020)

As mentioned before, Tauber et al. (2021) and Flesch (2020) noticed that oxygen uptake rates are dependent on salt concentration and exposure time. In the first test phase of the experimental WWTP, with a salt concentration of 0.3 g/l and an exposure time of 3 hours, there was an increase in ammonium respiration of 211% (Table 2). Furthermore, after 23 hours of exposure time and a NaCl concentration of 2.1 g/l, the NH_4 oxygen uptake rate was 152%. Only after additional 5 hours (at hour 28), the NH_4 oxygen uptake rate was 60%. This experiment showed that exposure time is an important factor in salt inhibition. Data from Tauber et al. (2021) first test phase is shown in Tables 1 and 2. The data on oxygen uptake rates from all 5 phases of the experimental WWTP can be found in appendix 1.

Table 1. Oxygen uptake rates of the first test phase (Flesch, p.31, 2021)

Datum, Zeit	NaCl Einwirkung	$OVNH_4$	$OVNO_2$	OVN_m	OVC_g	OVC_s	OVC_m	LF_{BB}	NaCl	oTS
	[h]	[mgO_2/(L·h)]	[mgO_2/(L·h)]	[mgO_2/(L·h)]	[mgO_2/(L·h)]	[mgO_2/(L·h)]	[mgO_2/(L·h)]	[µS/cm]	[g/L]	[g/L]
12.06.19 11:00	vor	21,9	7,2	29,1	9,9	16,2	175	500	0,0	5,2
12.06.19 15:30	3	37,9	12,5	50,4	33,9	40,4	153	920	0,3	5,2
13.06.19 11:30	23	28,8	9,5	38,3	22,5	28,9	152	4190	2,1	5,5
13.06.19 16:30	28	12,4	4,1	16,5	23,4	30,6	184	3840	1,9	6,0
14.06.19 09:30	45	32,2	10,6	42,8	30,3	35,5	159	1600	0,7	4,0
14.06.19 11:30	47	32,7	10,8	43,5	27,9	32,9	147	1480	0,6	4,0
17.06.19 08:30	116	24,5	8,1	32,6	13,2	26,3	123	1200	0,5	4,0

Table 2. Oxygen uptake rates of the first test phase in % (Flesch, p. 32, 2021)

Datum, Zeit	NaCl Einwirkung	$sOVNH_4$	$sOVNO_2$	$sOVN_m$	$sOVC_g$	$sOVC_s$	$sOVC_m$	LF_{BB}	NaCl
	[h]	[%]	[%]	[%]	[%]	[%]	[%]	[µS/cm]	[g/L]
12.06.19 11:00	vor	100%	100%	100%	100%	100%	100%	500	0,0
12.06.19 15:30	3	211%	218%	211%	139%	127%	75%	920	0,3
13.06.19 11:30	23	152%	157%	152%	88%	86%	71%	4190	2,1
13.06.19 16:30	28	60%	62%	60%	84%	83%	78%	3840	1,9
14.06.19 09:30	45	232%	240%	232%	161%	144%	101%	1600	0,7
14.06.19 11:30	47	236%	243%	236%	149%	134%	94%	1480	0,6
17.06.19 08:30	116	177%	182%	177%	70%	107%	78%	1200	0,5

Mean values from all 5 phases of experimental WWTP from Tauber et al. (2021) and Flesch (2020) can be seen in table 3. After the exposure time of 3 hours and the salt concentration of 0.36, the mean percentage change of NH_4 oxygen uptake rate was 49%. Likewise, on the 29th hour (with a salt concentration of 1.41 g/l) the mean percentage change of NH_4 oxygen uptake rate was -31%. After the decrease of salt concentrations below 1 g NaCl/l after 47 hours, there were again positive impacts on the NH_4 oxygen uptake rate.

Table 3. Mean percentage change of specific oxygen uptake rates from all 5 test phases (Flesch, p. 41, 2020)

mittlere NaCl-Einwirkung	NaCl	$sOVNH_4$	$sOVNO_2$	$sOVN_m$	$sOVC_g$	$sOVC_s$	$sOVC_m$
[h]	[g/L]	[%]	[%]	[%]	[%]	[%]	[%]
3	0,36	49%	54%	49%	53%	25%	-4%
29	1,41	-31%	-29%	-31%	-11%	-6%	5%
47	0,61	17%	21%	17%	23%	22%	19%
80	0,33	12%	15%	12%	15%	15%	9%

Similar microorganism behavior was also recorded in submerged biofilters. Aslan et al. (2012) have done a test with submerged biofilters and with different salt loadings (0-40 g NaCl/l). They noted that there was an increase in the activity of autotrophic and heterotrophic bacteria with a concentration of 1 g NaCl/l. Also, there was a decrease in activity at higher concentrations. At a concentration of 40 g/l, there was a 60% decrease in ammonium oxidizing rate and nitrite production rate (AOR and NPR). Removal rates of ammonium oxidizing bacteria and nitrite-oxidizing bacteria with removal efficiencies and inhibitions can be seen in Figure 12.

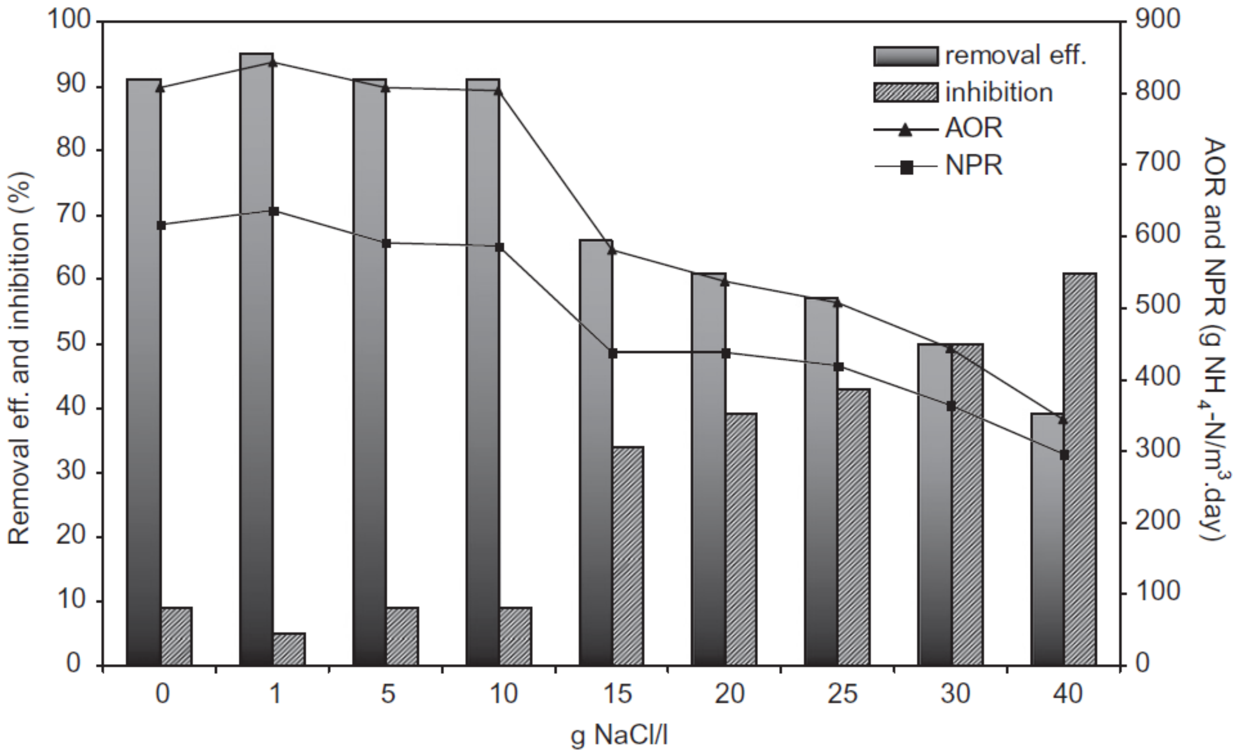

Figure 12. Removal of NH_4-N efficiency and nitrification inhibition - ammonium oxidation and nitrite production rate (AOR and NPR) (Aslan et al., p. 28, 2012)

Wang et al. (2005) showed that low salt concentrations (0.1-0.5 g NaCl/l) did not have a negative effect on oxygen uptake rates. The experimental procedure included a build of two small activated sludge tanks, that were dosed with different amounts of salt. One tank was the control tank and the other was dosed with salt. The impact of shock-like loads was investigated on oxygen uptake rates and total organic carbon removal. Also, it was shown that microorganisms can adjust their metabolism to higher concentrations of salt. Furthermore, after dosage with higher salt concentrations (> 2 g NaCl/l), a steep decline in oxygen uptake rates was recorded (Figure 13).

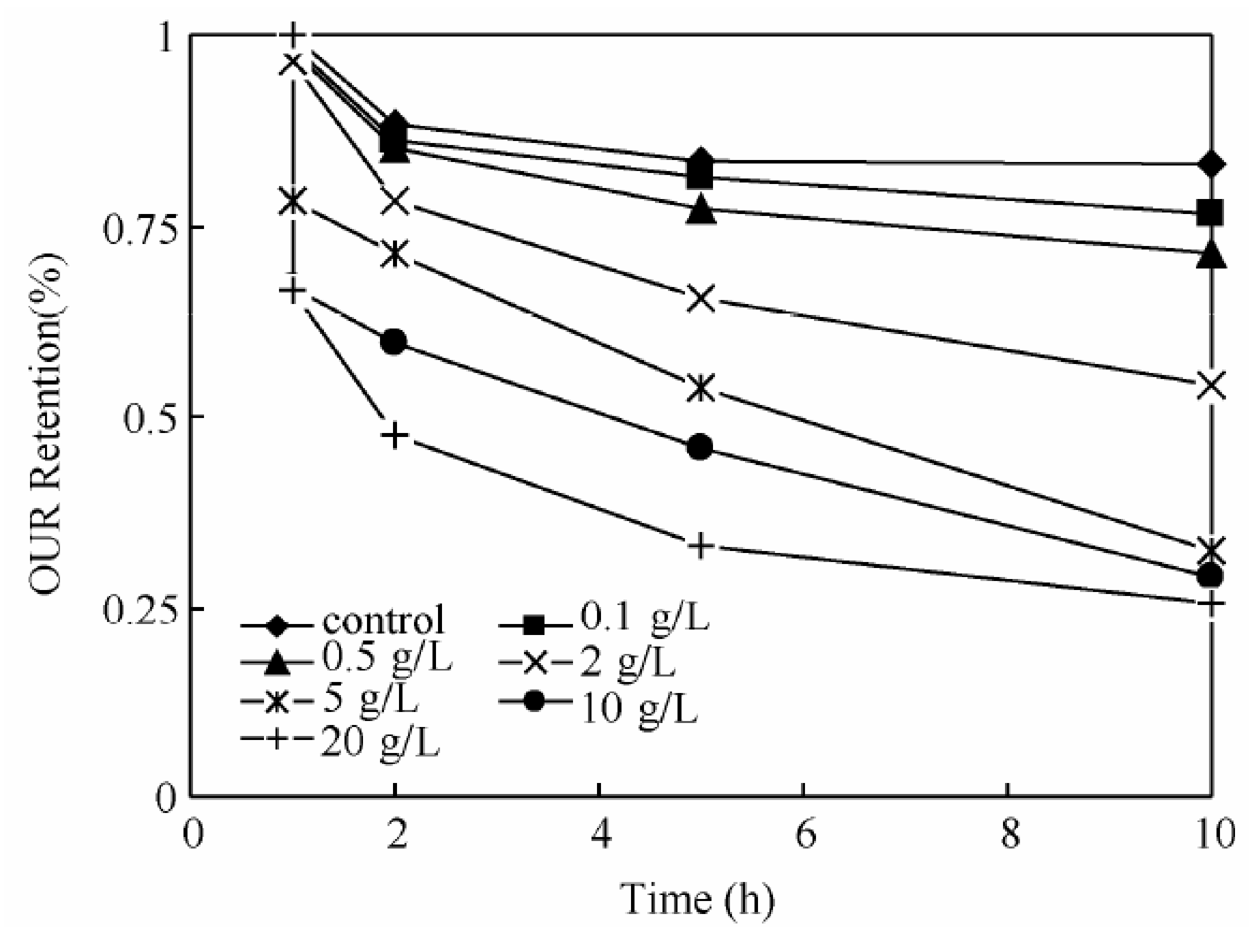

Figure 13. Oxygen uptake rates under different salt concentrations (Wang, p. 7, 2005)

Literature does not provide a clear answer for the adverse salt impact on removal efficiencies and oxygen uptake rates. Flesch (2020) states that there are 3 possible hypotheses:

1) The increase in salt concentrations leads to an increase in osmotic pressure. The increase in osmotic pressure can lead to the death of microorganisms, which are then used as food for living microorganisms. This was validated with an oxygen uptake rates measurement. With a salt shock load, there was an increase in endogenous respiration and a decrease in maximum breathing.
2) After salt shock loading, there is an increase in respiration because of toxic stress. Furthermore, there is an increase in extracellular polymer substances (EPS) to provide salvation of organisms from salt.
3) As mentioned before, an increase in salt concentration leads to an increase in osmotic pressure. In a microorganism cell, this leads to a better diffusion through a cell wall. Improved diffusion at lower concentrations (<1 g/l) also improves removal efficiencies. At concentrations higher than 1 g/l it is considered that inhibition effects are stronger than the effect of the diffusion through a cell wall.

Flesch (2020) states that bacterial growth is temperature-dependent. In the case of heterotrophic bacteria, with a temperature increase of 10 °C, there was a doubling of an activity. Autotrophic bacteria showed more reactivity with a doubling of the activity, with a temperature increase of 7 °C.

3.7.2 Impact of salt inhibition on the removal of Total Organic Carbon (TOC)

The presence of salt in the activated sludge system causes a decrease in total organic carbon removal efficiencies. Wang et al. (2005) showed that an increase in sodium chloride concentration, decreases the TOC removal efficiency. For the lower amount of salt (until 0.5 g/l) there were no apparent inhibitions, but for the larger salt concentrations (> 2g/l), there was a decrease of up to 40%. The dependency of TOC on salt concentration is depicted in Figure 14.

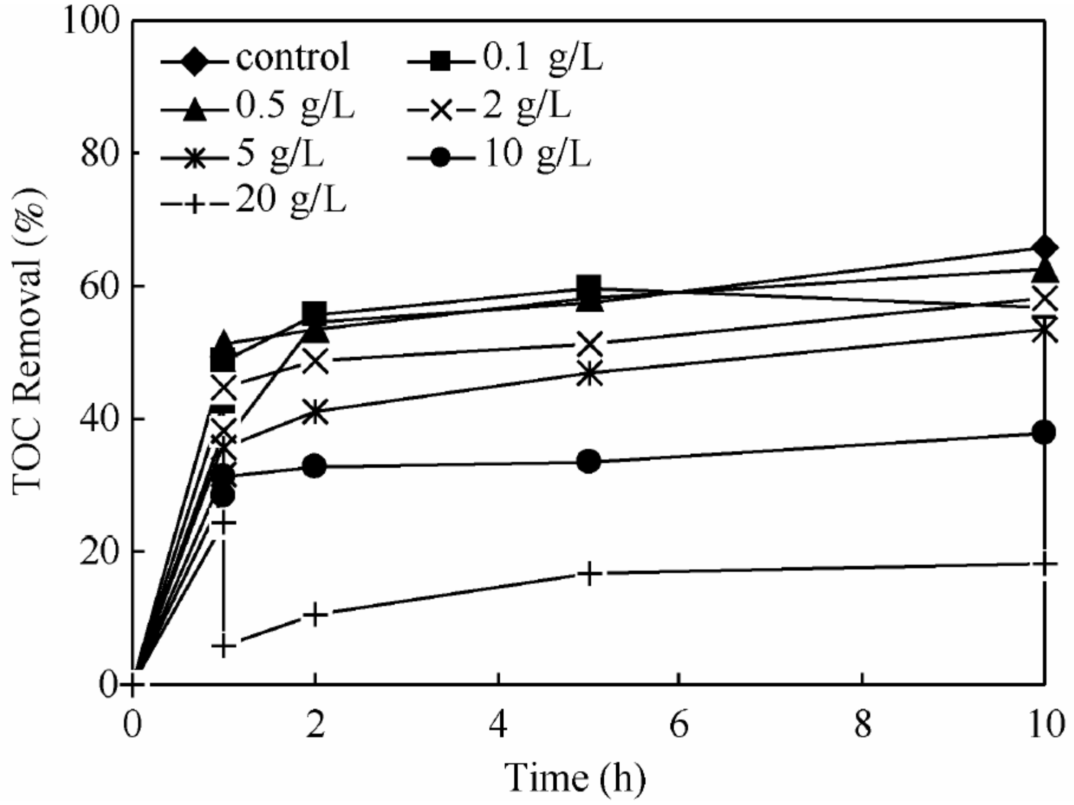

Figure 14. TOC dependency based on salt concentration (Wang et. at, p. 6, 2005)

3.7.3 Impact of salt inhibition on the sludge settling, floc size, and sludge volume index (SVI)

Operators of wastewater treatment plants reported that after salt events, there were certain operational impairments (Flesch, 2020). These impairments included the decrease of suspended solids in activated sludge tanks, which lead to an increase in the sludge volume index. It was also reported that sedimentation behavior was affected. There was a formation of floating sludge in the secondary clarifier, which lead to an increase in the concentration of suspended solids in the effluent.

Tauber et al. (2021) and Flesch (2020) state that suspended solids concentration in the aeration tank, from the experimental WWTP, experienced a decrease from 6.0 g/l to 4.9 g/l. Also, a drastic change in sludge volume index (SVI) was recorded. There was an increase in the average value of SVI from 107 ml/g to 147 ml/g during salt dosing. Furthermore, the peak value of the sludge volume index during the experiment was 346 ml/g (Figure 15).

Tauber et al. (2021) also reported the increase of suspended solids in the secondary clarifier. The salt dosing had a doubling effect on suspended solids concentration, from 10 mg/l to 15-20 mg/l. In the secondary clarifier, there was also a decrease in settling velocity from 1.7 to 0.5 m/h. This was reflected in the effluent quality, with a formation of small flocs on the surface of the secondary clarifier.

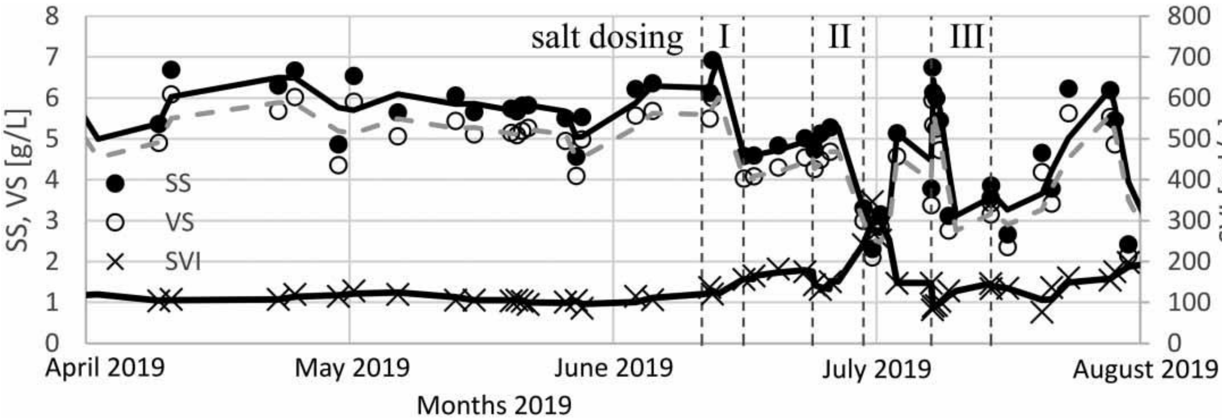

Figure 15. Sludge volume index, suspended and volatile suspended solids concentrations during salt dosing experiments (Tauber et al., p. 6, 2021)

Tauber et al. (2021) provided a possible explanation for the previously mentioned effects. The microscopic examination of the sludge flocs showed a big decrease in sludge floc size (Figure 16).

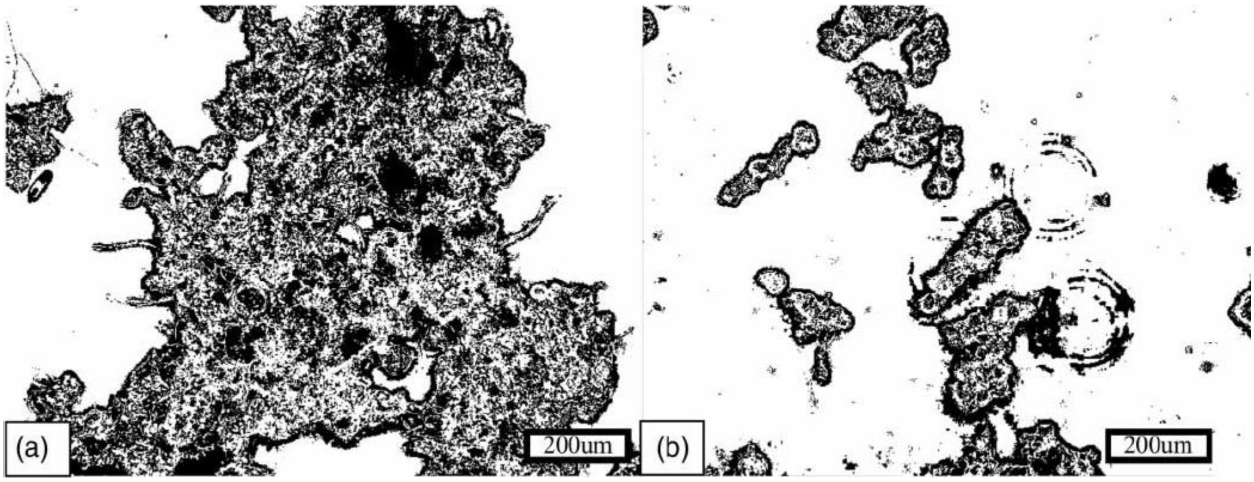

Figure 16. Activated sludge floc before salt dosing (left) and after 3 g NaCl/l dosage (right) (Tauber et al., p. 7, 2021)

The median floc particle dimension shrank from 1000 µm before the salt addition, to 200 µm with salt addition after 5 days. There was also a decrease in the statistical distribution of the size of activated sludge floc. The average diameter of floc declined from 209.5 µm to 69.4 µm (Figure 17) (Tauber et al., 2021).

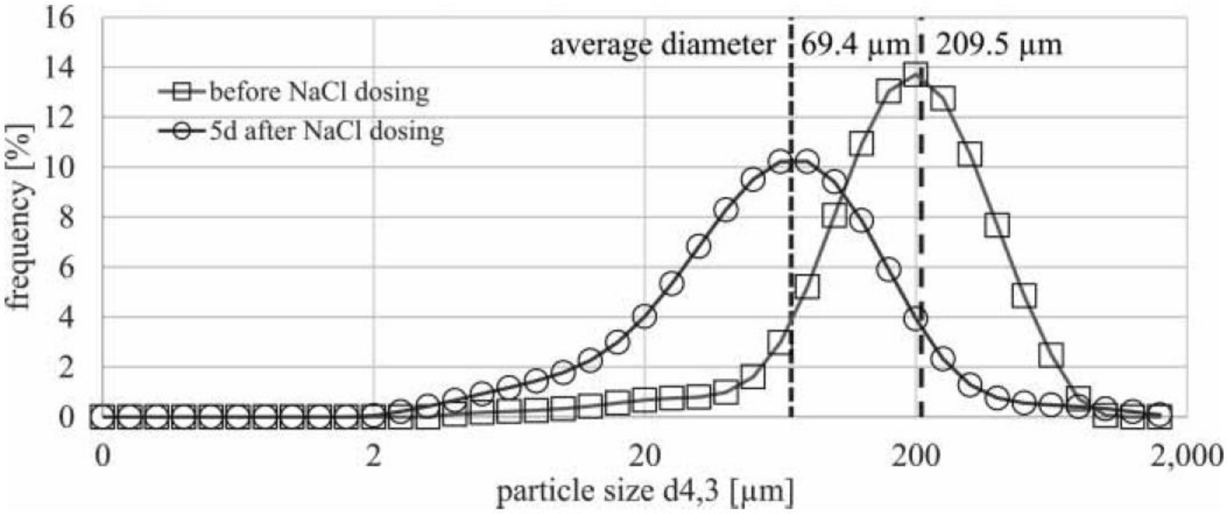

Figure 17. Floc size distribution before and after salt dosing (Tauber et al., p. 7, 2021)

3.7.4 Impact of salt inhibition on COD, Total Nitrogen (TN), Ammonium (NH_4), and Phosphorous (PO_4)

There is evidence that incoming salt concentrations, negatively impact main effluent parameters in wastewater treatment. As mentioned before, Tauber et al. (2021) and Flesch (2020) also examined the impact of salt on effluent concentration. There were both positive and negative effects.

The removal rates of chemical oxygen demand and total nitrogen increased during salt dosing (Table 4). Before the salt dosing, removal rates of COD were 94%, during dosing 98%, and 5 days after salt dosing 96%. This means that incoming salt had a positive impact on COD removal. A similar result was also with total nitrogen, with improved removal rates during salt dosing.

Ammonium and phosphorus effluent concentrations also had a positive effect during salt dosing, but had problems 5 days after the salt event. NH_4-N concentrations before the salt event were 1.76 mg/l, during 1.22 mg/l, and 2.26 mg/l 5 days after salt dosing. Phosphorous effluent concentrations also reacted in the same way (Table 4).

Table 4. Removal rates and effluent concentrations of the laboratory scale plant before, during, and after salt dosing (Tauber et al., p. 7, 2021)

Sampling time	Number of Samples –	Removal rates COD %	TN %	Number of samples –	Effluent concentration NH_4-N mg/L	PO_4-P mg/L
Before salt dosing	$n = 33$	94	81	$n = 32$	1.76	1.16
During salt dosing	$n = 7$	98	84	$n = 9$	1.22	0.76
5 days after salt dosing	$n = 5$	96	86	$n = 6$	2.26	1.40

Aslan et al. (2012) examined the impact of salt on removal efficiencies of NH_4-N, NO_2-N, and NO_3-N. The experiments were done with a partial nitrification biofilm reactor (PNBR). It was reported an increase in removal efficiencies for salt concentrations lower than 1 g NaCl/l, and inhibitions for concentrations greater than 10 g NaCl/l. For the salt concentration of 1 g NaCl/l, NH_4-N concentrations were lower than 10 mg/l. Furthermore, there was an improvement in removal efficiencies from 91% to 95% (Figures 18 and 19).

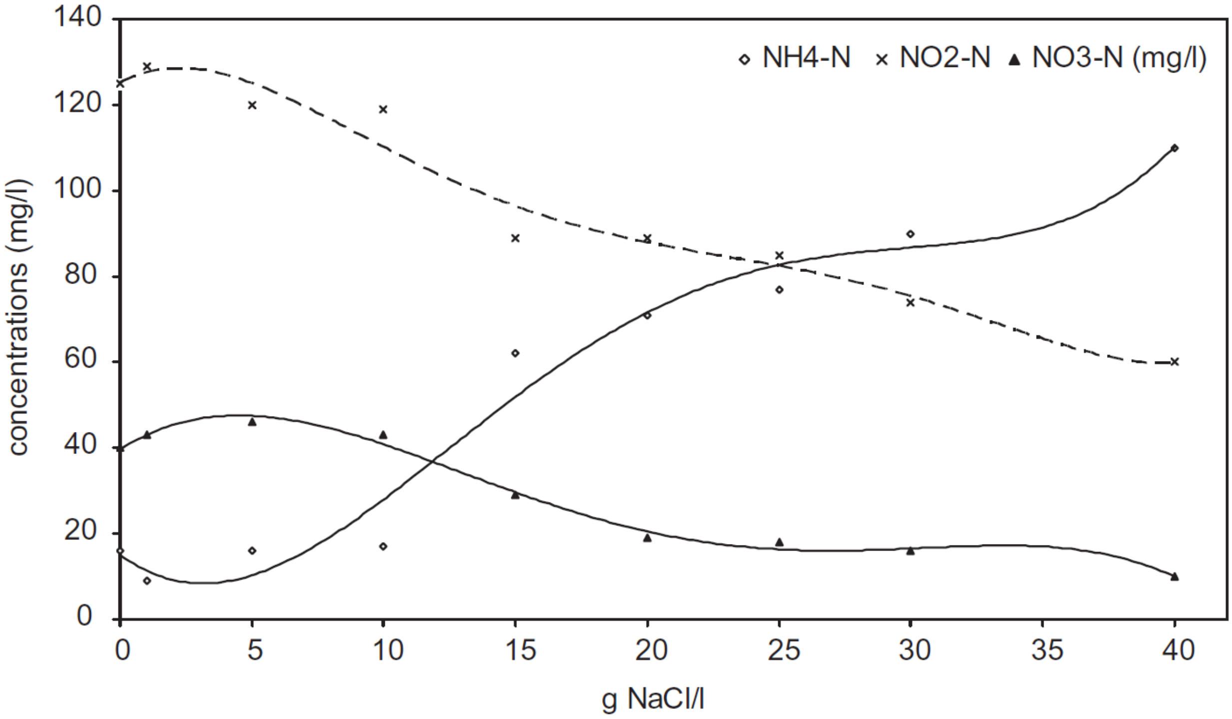

Figure 18. The effluent concentration of nitrogen compounds at various NaCl concentrations (Aslan et al., p. 27, 2012)

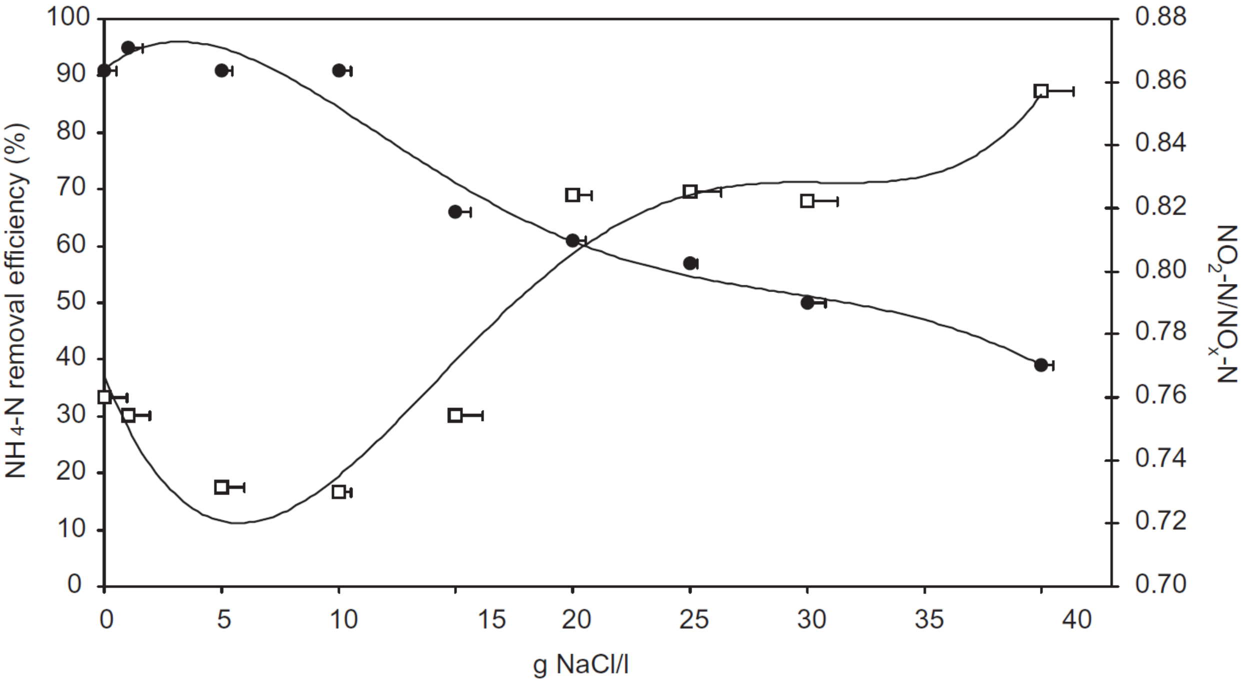

Figure 19. Removal efficiencies of nitrogen compounds at various NaCl concentrations (Aslan et al., p. 28, 2012)

4. Material and methods

4.1 Development of a numerical model for salt impacts on nitrification

A numerical model represents a set of equations that enable the conversion of the real-world problem into modelling software. SIMBA# software does not provide a direct possibility to model inhibitory chloride impacts on wastewater treatment plants. Hence, a different solution had to be made.

The first step was to find a connection between salt concentration and the removal of ammonium from wastewater. For this, the data from research done by Tauber et al. (2021) and Flesch (2020) was consulted. The data on ammonium oxygen uptake rates were used as an indicator of the activity of nitrifying bacteria. Depending on the salt concentration, the activity of nitrifying bacteria increased or decreased. Based on their activity, a set of equations was created that describes the maximum rate of nitrification (removal rates of nitrogen compound NH_4-N in activated sludge process) as a function of salt concentration. The developed numerical model is described in chapter 5.1.1.

4.2 SIMBA#

4.2.1 The SIMBA# software

The SIMBA# modelling software provides an integrated approach to modelling water, wastewater, and biogas systems. Furthermore, it offers modelling and simulation in the fields of sewer systems, rivers, anaerobic processes, drinking water networks, etc. This allows for a combined approach to the modelling of urban water and wastewater systems. It was developed by the Water & Energy department at ifak research institute in Madeburg, Germany. In the area of wastewater treatment plant modelling, SIMBA# provides dynamical modelling of activated sludge models, aeration systems, sludge digestion, and automation (ifak, 2022).

SIMBA# allows for a simplified approach to dynamical simulations of wastewater treatment plants. Its library contains predefined blocks for primary clarifiers, influent generators, nitrification and denitrification tanks, secondary clarifiers, sludge processing, control for aeration and sludge, etc. These blocks can be easily inserted and connected. SIMBA# also allows connection with external databases such as influent data, return sludge, waste sludge, aeration, temperature, etc. After the dynamical simulation is finished, SIMBA# provides an option of tabular and graphical representation of modelled results.

Dynamical modelling in this work was done in SIMBA# 4.3 version. Meanwhile, the new version 5.0 of SIMBA# was released, which offers many other additional services.

4.2.2 Implementation of the numerical model into SIMBA#

As mentioned in chapter 4.1, SIMBA# modelling software does not provide a possibility of direct modelling of chloride impacts on WWTPs. Thus, a new solution for chloride implementation in SIMBA# software had to be developed. Since nitrification is dependent on salt concentration, a new parameter had to be established that correlates salt concentration and nitrification rate. Thus, the parameter – (new) maximum rate of nitrification (m_{salt}), as a function of salt concentration was created. Development and implementation of the parameter m_{salt} into SIMBA# software are explained in detail in chapters 5.1.1 and 5.1.2.

4.2.3 Implementation of scenarios in SIMBA# software

Dynamical simulation software, such as SIMBA#, provides diverse options for the input of influent data. Particularly in SIMBA#, the following options are available as an input generator:

- Influent generator
- Advanced influent generator
- Dry weather influent generator

Depending on the influent generator type, it is required to provide specific input data files such as data on COD, total nitrogen, total phosphorus, etc. This data is usually available as an average daily value and not as an hourly (or more frequent) time step that is needed for dynamical simulation. Influent generators can compute the missing time steps to provide the model with sufficient influent data. This creates a daily fluctuation in the concentrations of influent parameters.

Whiles this is necessary for the set-up of simulation, it creates problems with the interpretation of the scenario results. Daily fluctuations in the inflow, result in the fluctuations of the outflow parameters of the WWTP and it makes the process of identifying the sole influence of inhibiting parameter difficult. This problem can be solved with dry weather influent generator, since its output creates a constant inflow of quantities and concentrations. Dry weather influent generator allows a clear representation of scenario results, since the changes in the system will only occur due to the impact of salt.

4.3 Steps of the GMP Unified Protocol

4.3.1 Project definition

As mentioned in chapter 1, salt that is applied on the road to prevent ice formation can have negative impacts on processes in wastewater treatment plants. These include inhibition of removal efficiencies, floating of sludge flocs on the surface of clarifier, etc. Since these phenomena are not yet researched and modelled, an attempt of creating a model for nitrification inhibition in wastewater treatment plants has been done.

In the area of the city of Freistadt, a new highway is planned to be built. Water runoff from the highway is designed to be drained to the Freistadt WWTP. Freistadt WWTP is designed for

30 000 PE and it is operating on the edge of capacity. Since the WWTP is operating on the edge of capacity, there was a question of what possible impact could this additional road salt have on nitrification at the WWTP.

For this to be done, after the literature review, the following steps need to be made:

- Development of numerical model – This step consists of the creation of a set of equations that describe the nitrification rate depending on the salt concentration.
- Data collection and reconciliation
- Plant model Set-up in SIMBA# software
- Calibration and Validation
- Implementation of the numerical model and scenario simulation

4.3.2 Data collection and reconciliation

Freistadt WWTP collects operational data on regular basis. The data on basic parameters like water quantities and flows, COD, BOD, nitrogen and phosphorous compounds, pH, temperature, etc. were available. However, the Freistadt WWTP does not record the data on Sodium-chloride (NaCl) measurements. Data on chloride measurements would be very valuable for this thesis, but since the additional measuring campaigns were not planned, the work had to be done without this data. This poses a significant limit to the accuracy of this work.

As mentioned in chapter 3.5.3, for the model development, the following data are needed: Input data, Physical data, Operational settings, Performance data, and Other additional data. This data was collected from the master thesis of Matzinger (2017) and the data set acquired from Freistadt WWTP personnel. The data set acquired from Freistadt WWTP personnel is the basic operational parameters for the year 2020 (Table 5).

Table 5. Operational data from Freistadt WWTP

Wastewater Quantity	Q_{inflow}, $Q_{dry\ weather}$, $Q_{rain\ weather}$, Q_{max}, Q_{min}
pH	Inflow - minimal and maximal Outflow - minimal and maximal
Temperatur	Median inflow Median outflow
Settleable Solids	Inflow and Outflow
BOD_5	Inflow, Inflow Biological Outflow, Removal efficiency
COD/TOC	Inflow, Inflow Biological Outflow, Removal efficiency
Nitrogen N	Inflow - Total N, NH_4-N, NH_4-N Biological Outflow - NH_4-N, NO_3-N, NO_2-N, Total N, Total N Removal efficiency
Phosphorus	Total P_{inflow} Total $P_{outlfow}$, Removal efficiency
Influent load	BOD_5, COD, NH_4-N, Total N, PO_4-P, Total P
Organic load	BOD_5, COD
Effluent load	BOD_5, COD, NH_4-N, Total N, PO_4-P, Total P
Aeration Tank Parameters	Sludge volume (AT1, AT2, AT3, and AT4) Total solids (AT1, AT2, AT3, and AT4) Sludge index (AT1, AT2, AT3, and AT4)
Return Sludge	Sludge volume, Total solids, Quantities (SC1, SC2, SC3), $Q_{Waste\ sludge}$

After the acquisition of the operational plant parameters, the data reconciliation has been done. To create as accurate a model to the reality as possible, this step is essential before model calibration. Since the calibrated model was available from the master thesis of Matzinger (2017), and the data used in that thesis was already verified, the process of verifying the data on this thesis was much simplified.

The available data from the Freistadt WWTP was inserted into the SIMBA# software and the simulation was performed. The results of the model showed that the used data sets fit very well to the calibrated model and that no further work on data reconciliation is needed.

4.3.3 Plant model Set-up in SIMBA# software

SIMBA# software allows an integrated approach to water, wastewater, and biogas systems modelling. It is generally used for teaching and research in universities, but in recent times also in engineering offices.

The first step in modelling in SIMBA# software, or any other WWTP simulation software, is to choose the appropriate activated sludge model. The goal of the work dictates the choice of the activated sludge model. For this project, activated sludge model 3 (ASM3h) was chosen. ASM3 was chosen because it represents an improved ASM1 and there is no need for phosphorous modelling.

After the choice of the activated sludge model, the work on setting up the model can begin. To represent reality, the model in SIMBA# software was set up, in the same way, to mimic reality as accurately as possible. The following sub-models have been included:

- Influent generator
- Primary clarification
- Activated sludge tanks
- Secondary clarification
- Controls – aeration, waste sludge, return sludge
- Digestion

On Figure 20 is represented the model in SIMBA#. It is important to note that this model was created by Matzinger (2017) as a part of his master thesis. Thus, his model was slightly adapted and used also in this thesis.

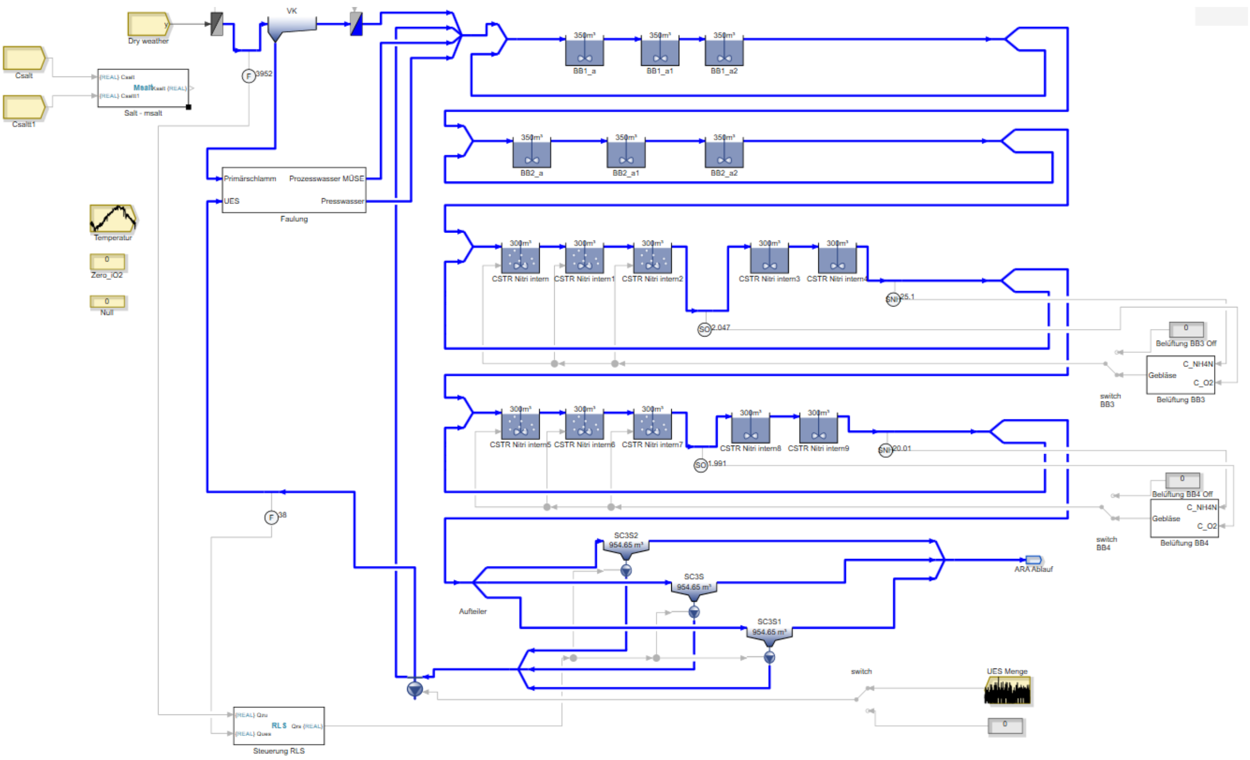

Figure 20. SIMBA# model of Freistadt WWTP (screenshot from SIMBA# software)

4.3.4 Calibration and validation

As mentioned in chapter 4.3.2, in this master thesis the model from Matzinger (2017) was used. Thus, the model was already calibrated and did not need any additional calibration. This means that steps of calibration and validation could be skipped. However, since the model was done in an older version of Simba# software, some blocks did not work in a new version of the software, and they needed to be exchanged. These blocks are activated sludge tanks - "CSTR nitri extern" and secondary clarifiers "SC3S". Because of this change, the calibrated model was checked again.

The process of calibration involves the comparison of modelled effluent values and measured values from the Freistadt WWTP. The following parameters have been checked:

- COD influent and effluent concentrations
- NH_4-N influent and effluent concentrations
- NO_3-N effluent concentration
- Total Nitrogen – TKN influent and effluent concentrations

The calibration step is finished when "Stop Criteria" is reached. Stop criteria is a limit, usually defined as a quantitative concentration limit, after which the model is deemed fit for modelling of scenarios. Rieger et al. (2013) give a guideline on "Stop criteria" limits for different effluent parameters based on the application matrix. In table 6 is represented the acceptable error range for nitrogen removal calibration parameters.

Table 6. Target nitrogen calibration parameters and proposed error range (Rieger et al., 2013, p. 98)

Calibration parameter	**Target variable**	**Error range**
Nitrogen removal	NHx-N NOx-N Ntot	1,0 mg/l

It is important to note that the error range is proposed as a guide to modelling, and that also other error ranges are acceptable based on the type of a project and stakeholder agreement.

Since the model for this thesis was already available from Matzinger (2017) master thesis, his model and adjoining parameters were taken for this thesis. Matzinger (2017) stated that certain parameters needed to be changed to get better matching of modelled and measured COD effluent values. These parameters include a fraction of inert soluble COD, a fraction of inert COD from particulate COD, and a fraction of SS from biodegradable COD. The previously mentioned parameters are represented in Figure 21.

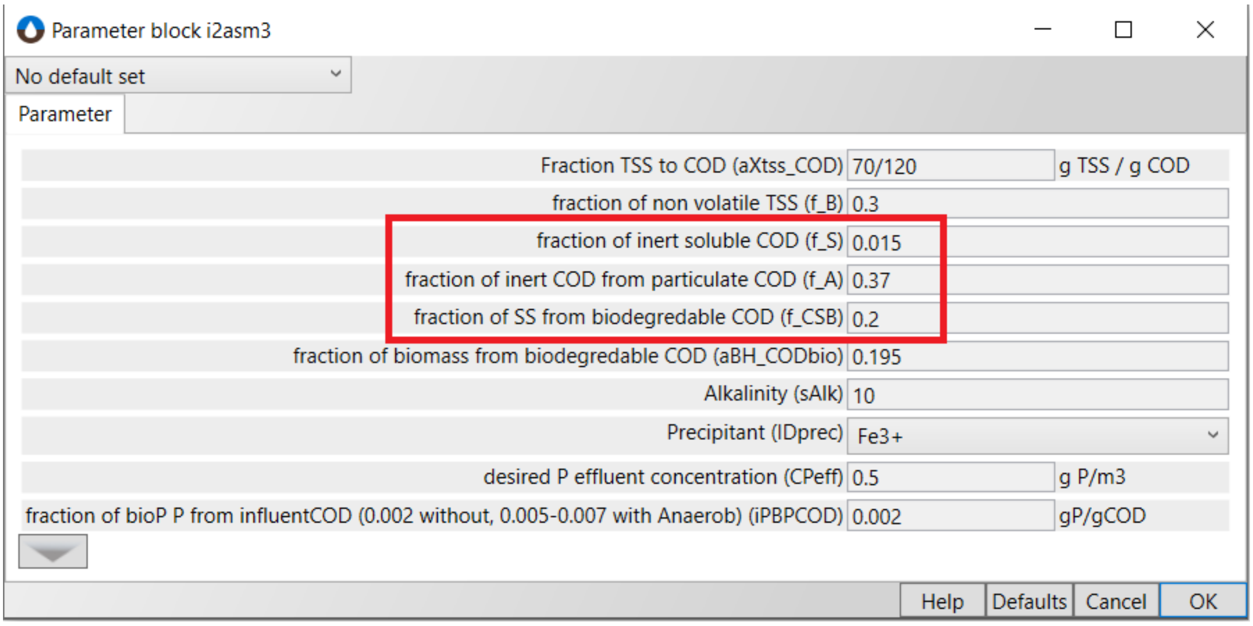

Figure 21. COD fractions changed for COD effluent calibration (screenshot from SIMBA# software)

4.3.5 Scenarios and Results

After literature review, the following parameters are identified as possible impactors on activated sludge inhibition processes:

- salt concentration
- duration of salt dosing
- water temperature
- inflow quantity

Because of this, previously mentioned parameters were chosen for further investigation and scenario development.

Scenario 1 – Varying of salt concentrations

The following scenarios of salt concentrations have been investigated:

- 0.5 g NaCl/l
- 1.0 g NaCl/l
- 1.5 g NaCl/l
- 2.0 g NaCl/l

These scenarios were made to describe the impact of a shock-like salt dosing on the ammonium removal efficiencies at the Freistadt WWTP. All the different salt scenarios were done with the salt dosing duration of 24h on day 10 of modelling. The salt dosing was kept constant during these 24 hours (Figure 22). Besides the changes in effluent quality, special attention was put on the time the activated sludge system needs, to go back to the state before salt dosing.

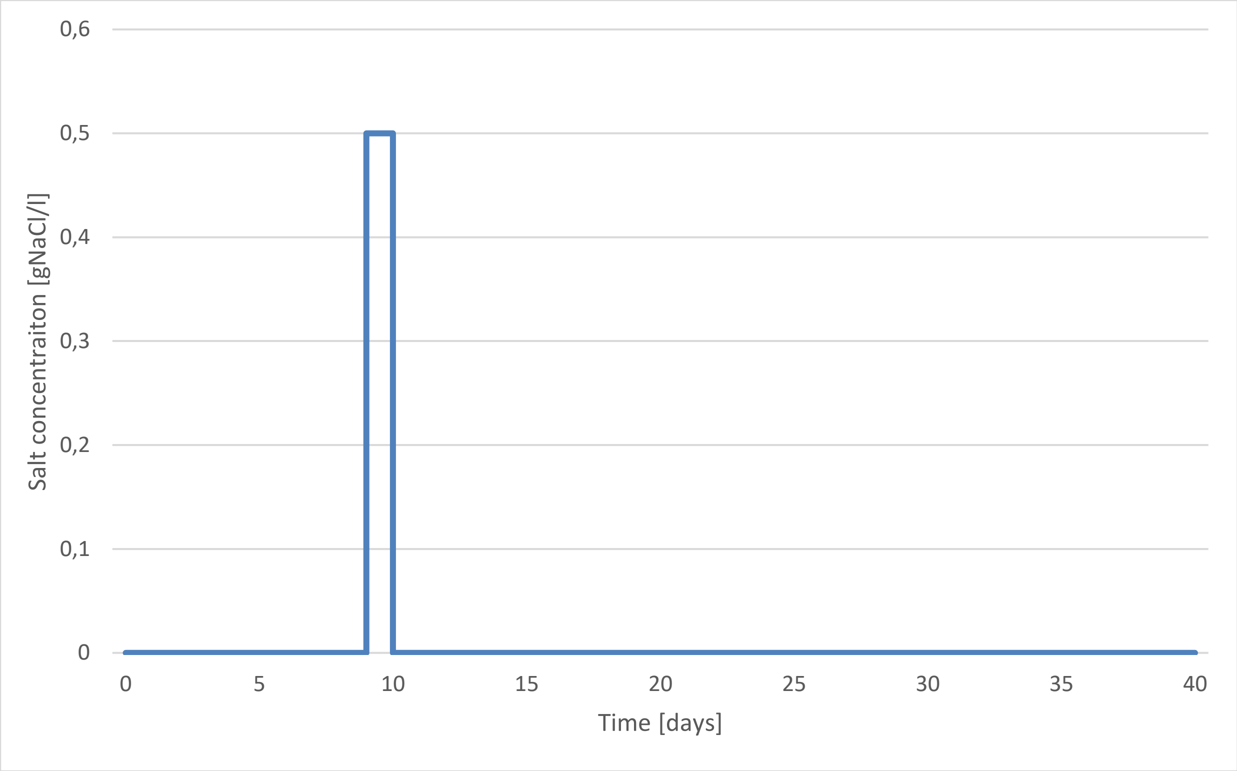

Figure 22. Salt dosing for 24 hours on day 10 of modelling

Scenario 2 - Longer duration of salt

The duration of exposure of activated sludge microorganisms to the salt can also have a significant impact. Because of this, the time of salt exposure was increased from 24 hours to 48. As in the previous scenario, all salt dosings were done on day 10 of modelling. The following scenarios of prolonged salt dosing have been investigated:

- 0.5 g NaCl/l for 48 hours
- 1.0 g NaCl/l for 48 hours
- 1.5 g NaCl/l for 48 hours
- 2.0 g NaCl/l for 48 hours

Scenario 3 - Lower inflow temperatures

The processes in activated sludge plants are highly dependent on inflow water temperature. Lower water temperatures can inhibit microorganism activity and higher temperatures can improve it. It's also important to note that oxygen is more dissolvable in colder water and thus are the aeration costs lower.

The scenarios in SIMBA# software were done with alternating inflow water temperatures and constant salt dosing of 2.0 g NaCl/l. The temperature was slowly decreased from the default value of 7.3 °C and the NH_4 effluent changes were tracked. The scenarios were done with a water temperature of:

- 4.0 °C
- 5.0 °C
- 6.0 °C

Scenario 4 - Increased inflow water quantities

Since the appearance of salt in wastewater treatment plants is usually due to a snow melting event or rain event, another scenario was needed to examine its impacts. Consequently, three scenarios were created. The default dry weather inflow was 3951.90 m^3/day and all scenarios were done with a salt concentration of 2.0 g NaCl/l for 24 hours. The scenarios were done with an inflow of:

- 5 000 m^3/day
- 6 000 m^3/day
- 7 000 m^3/day

The increased inflow was kept for 5 days from day 10 till day 15 of modelling.

5. Results and discussion

5.1 Numerical model for salt impacts on nitrification

5.1.1 Development of numerical model for salt impacts on nitrification

As mentioned in chapter 3.7.1, the removal of nitrogen compounds is dependent on salt concentration. For the concentrations below 1 g NaCl/l, there were positive effects on wastewater treatment plants and above 1 g NaCl/l there were inhibitory effects. For the concentration lower than 1 g/l, the increase in activity of microorganisms was up to 200%. For the concentration higher than 1 g/l, there were inhibitions of activity for up to 48% of the original (starting) value. Also, as mentioned in chapter 3.7.1, the reaction of microorganisms is more severe for the incoming concentration, as the bacteria can get used to chloride concentration relatively fast. Because of this, three sets of equations were created. The data from research done by Tauber et al. (2021) and Flesch (2020) were plotted on the graph (blue triangles in Figures 23, 24, and 25), and functions with formulas that approximate the maximum rate of nitrification were compiled using Microsoft Excel (orange line on Figure 23, 24, and 25).

The first equation (1) describes the behavior of the nitrifying organisms for the incoming (shock-like) salt loads, for the concentrations of salt lower than 1.1 g NaCl/l (Figure 23).

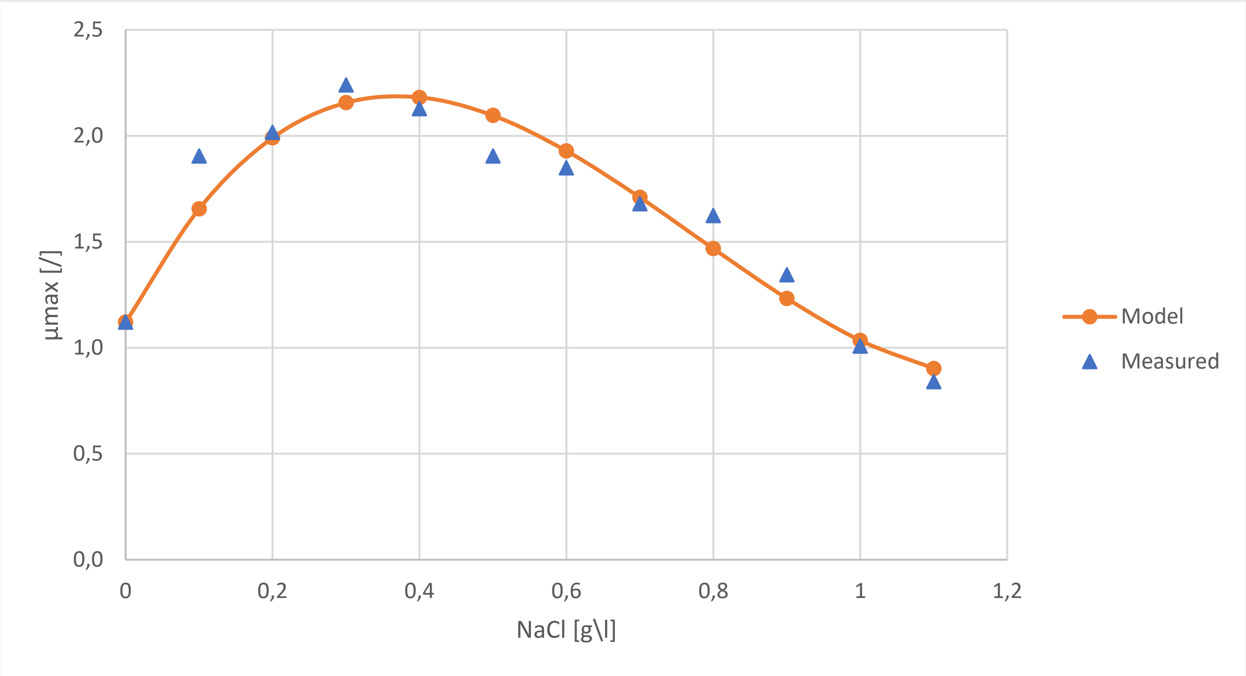

Figure 23. Maximum rate of nitrification for the salt concentration from 0.0 to 1.1 g NaCl/l

Results and discussion

$$\mu_{salt} = 4.9114\ C_{salt}^3 – 11.44\ C_{salt}^2 + 6.4432 * C_{salt} + 1.12 \qquad (1)$$

where,

μ_{salt} – maximum rate of nitrification depending on salt concentration

C_{salt} – salt concentration

The second equation (2) describes the behavior of organisms for the concentrations of salt higher than 1.1 g NaCl/l (Figure 24).

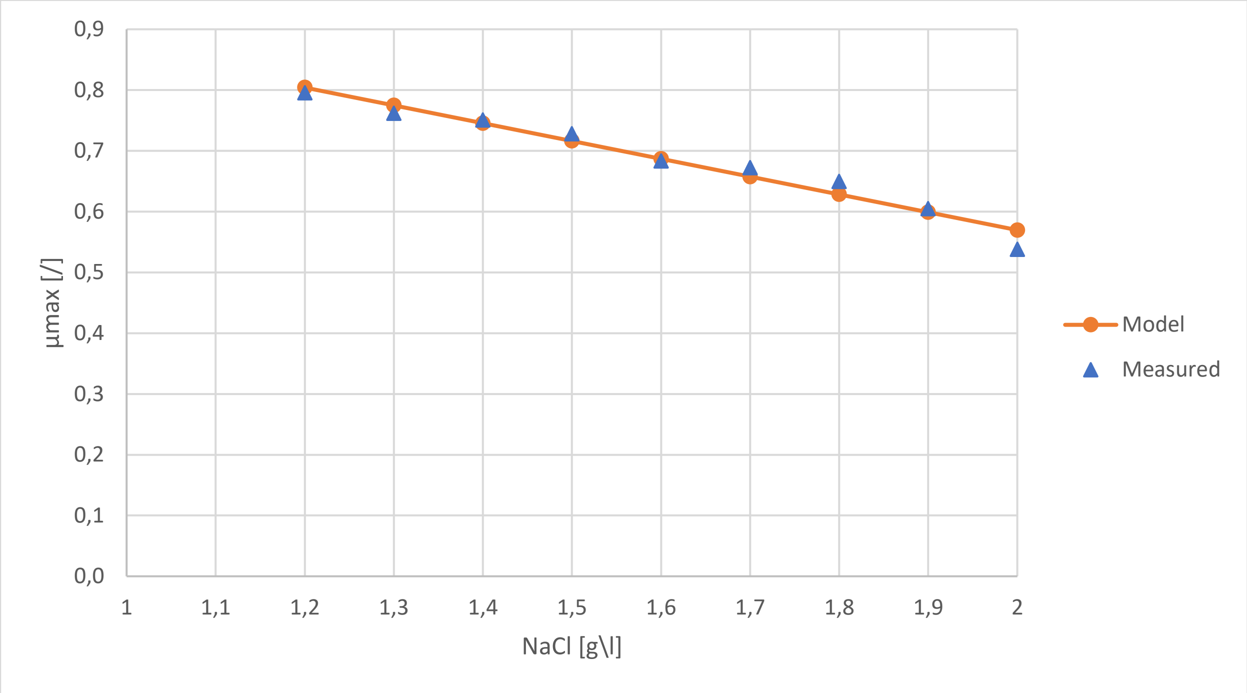

Figure 24. Maximum rate of nitrification for the salt concentration from 1.2 to 2.0 g NaCl/l

$$\mu_{salt} = -0.2931\ C_{salt} + 1.1558 \qquad (2)$$

The third equation (3) describes the behavior of the nitrifying organisms after the shock-like salt dosing, when the salt concentration is slowly decreasing (Figure 25). This equation is for the salt concentration from 2 g NaCl/l to 0 g NaCl/l.

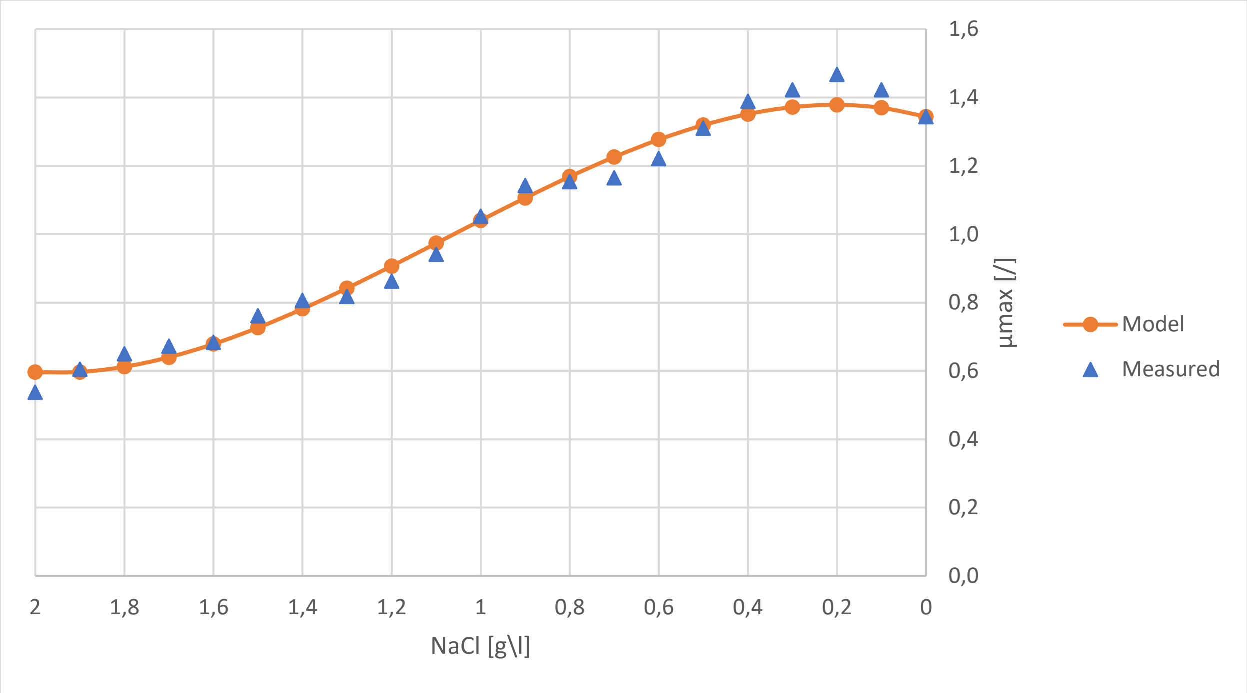

Figure 25. Maximum rate of nitrification for the salt concentration from 2.0 to 0.0 g NaCl/l

$$\mu_{salt} = 0.2919\ C_{salt}^{3} - 0.9462\ C_{salt}^{2} + 0.3508 * C_{salt} + 1.344 \qquad (3)$$

A combined overview of the maximal rate of nitrification depending on the salt concentration with incoming (increasing) and outgoing (decreasing) salt concentrations is represented in Figure 26.

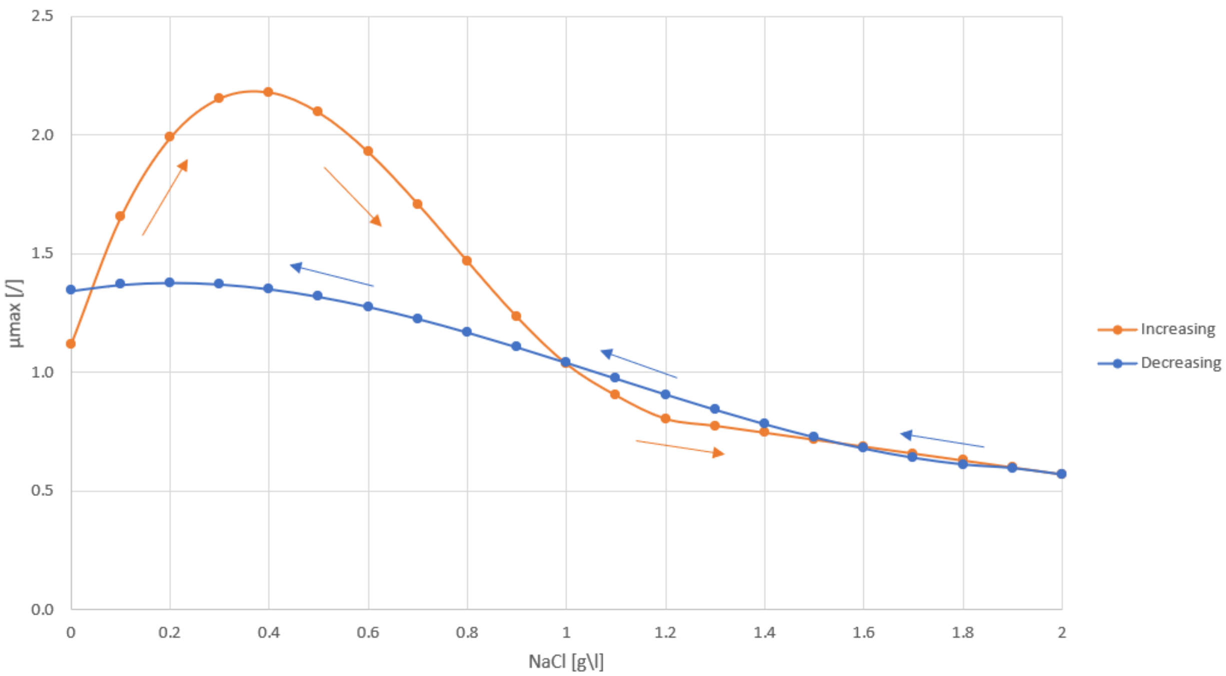

Figure 26. Maximal rate of nitrification with increasing (orange) and decreasing (blue) salt concentration

Implementation of the above-mentioned equations (1), (2), and (3) in SIMBA# modelling software are explained in chapter 5.1.2.

5.1.2 Implementation of the numerical model in SIMBA# software

SIMBA# software does not provide a direct possibility to model inhibitory chloride impacts on wastewater treatment plants. Hence, a new numerical model had to be created. Implementation of the equations created in chapter 5.1.1 in SIMBA# modelling software was done in the following way. Because SIMBA# does not have a parameter for salt inhibition, a new parameter had to be created. In the "IEC Code" block, the 3 equations were inserted, and m_{salt} as an output parameter was created. Since the parameter m_{salt} is dependent on the salt concentration, the blocks that define salt concentration ("Csalt" and "Csalt1" blocks) were connected to the "IEC Code" block and used as an input for all of the scenarios (Figure 27).

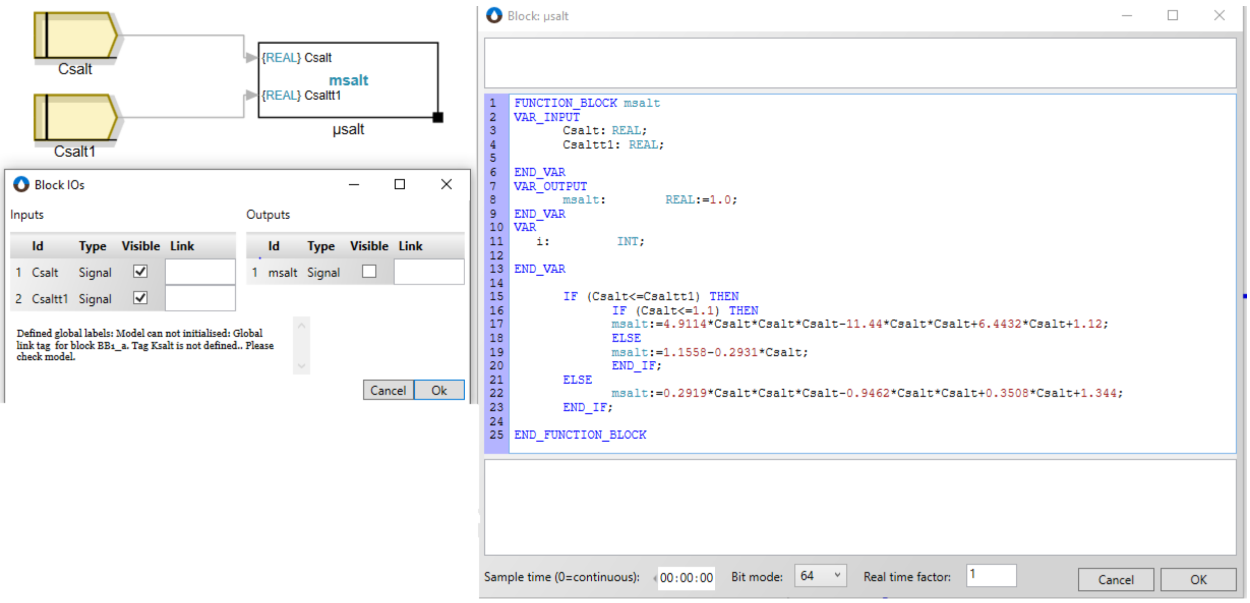

Figure 27. Implementation of m_{salt} parameter (screenshot from SIMBA# software)

As a second step for the m_{salt} parameter implementation, a modification in the stoichiometric ASM3h matrix was required. In the SIMBA# ASM editor, a parameter $muAUT_{20}$ (5) was changed for a parameter m_{salt} (Table 7). This was done because ASM3h describes the rate of nitrification (RN) with the following formulas (4) and (5):

$$RN = muAUT \, \frac{SO}{SO+KNO2} \, \frac{SNH}{SNH+KNNH4} \, \frac{SALK}{SALK+KNALK} \, XA \qquad (4)$$

where,

$$muAUT = muAUT20 * ft105 \qquad (5)$$

*muAUT_{20} in the stoichiometric matrix represents the maximum rate of nitrification.

Table 7. Modified ASM3h stoichiometric matrix (screenshot from SIMBA# software)

Rate
$Kh20\,ft_{04}\frac{\frac{XS}{XH}}{\frac{XS}{XH}+KX}XH$
$k_{sto}\frac{SO}{SO+KHO2}\frac{SS}{SS+KHSS}XH$
$k_{sto}\,etaHNO3\frac{KHO2}{SO+KHO2}\frac{SS}{SS+KHSS}\frac{SNO}{SNO+KHNO3}XH$
$muH\frac{SO}{SO+KHO2}\frac{SNH}{SNH+KHNH4}\frac{SALK}{SALK+KHALK}\frac{\frac{XSTO}{XH}}{\frac{XSTO}{XH}+KHSTO}XH$
$muH\,etaHNO3\frac{KHO2}{KHO2+SO}\frac{SNH}{KHNH4+SNH}\frac{SALK}{KHALK+SALK}\frac{XSTO}{XH}\frac{1}{KHSTO+\frac{XSTO}{XH}}\frac{SNO}{KHNO3+SNO}XH$
$bH\frac{SO}{SO+KHO2}XH$
$bH\,etaHend\frac{KHO2}{SO+KHO2}\frac{SNO}{SNO+KHNO3}XH$
$bH\frac{SO}{SO+KHO2}XSTO$
$bH\,etaHend\frac{KHO2}{SO+KHO2}\frac{SNO}{SNO+KHNO3}XSTO$
$\boxed{msalt\,ft_{105}\frac{SO}{SO+KNO2}\frac{SNH}{SNH+KNNH4}\frac{SALK}{SALK+KNALK}XA}$
$bAUT\frac{SO}{SO+KHO2}XA$
$bAUT\,etaNend\frac{SNO}{SNO+KHNO3}\frac{KHO2}{SO+KHO2}XA$
$\frac{iO2}{V}1000$

5.2 Simulation of salt impact at the WWTP Freistadt

5.2.1 Calibration and validation

COD parameter

After the change of COD fractions, shown in chapter 4.3.4, much better results in COD effluent concentrations were acquired. The average concentration of measured COD effluent values was 24.5 mg/l and 20.9 mg/l for modelled effluent values. The peak in modelled values at the beginning of the simulation was most likely due to the initial state of the model and they are excluded from the calculation. The result of COD effluent concentrations is shown in Figure 28.

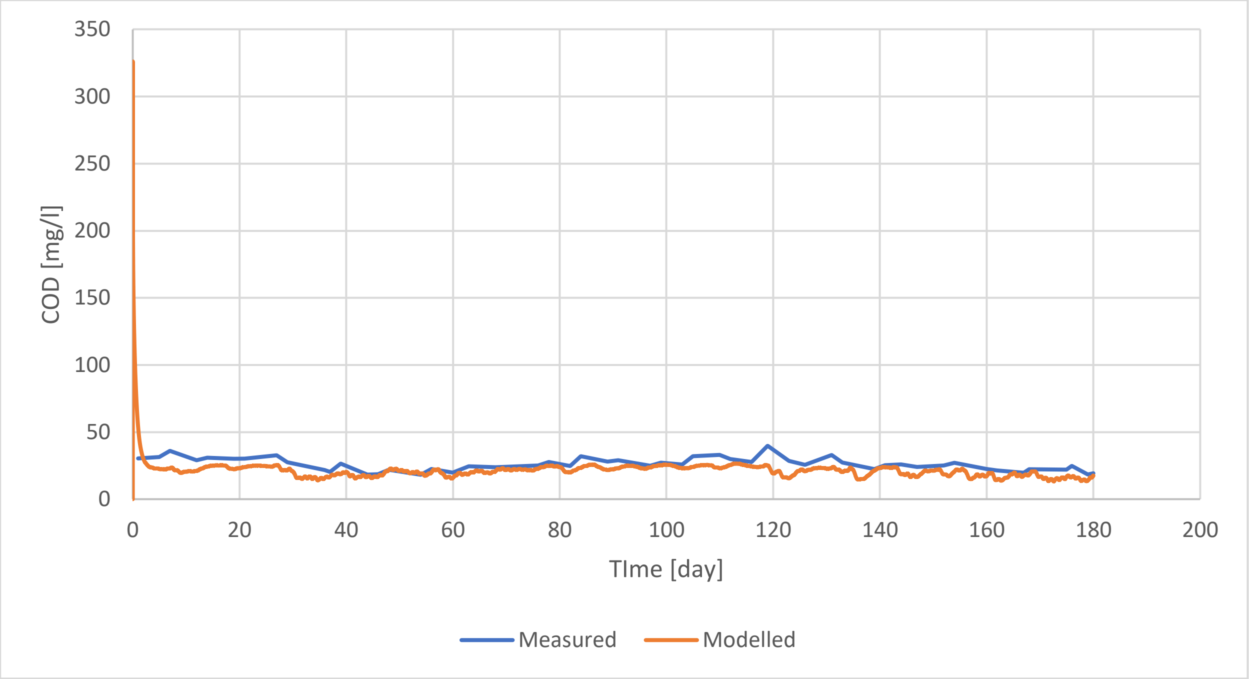

Figure 28. COD measured and modelled effluent concentrations

<u>NH_4-N parameter</u>

Average measured ammonium-nitrogen effluent concentrations were 0.58 mg/l and modelled were 1.70 mg/l. This exceeds the above-mentioned error range of ±1 mg/l, but with the consent of a stakeholder, this value was accepted as a stop criteria. At the beginning of the simulation, a peak of almost 16 mg/l is observed. This peak has the same cause as in the COD effluent calibration step. Result of ammonium-nitrogen effluent concentrations is shown in Figure 29.

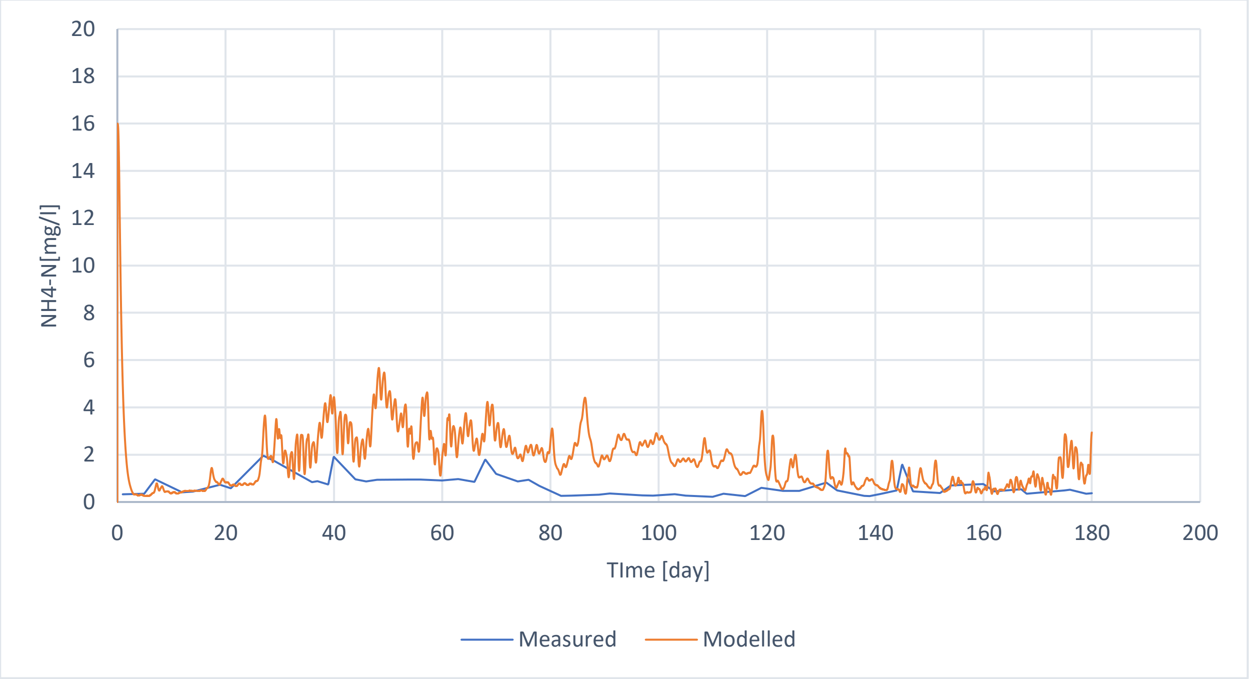

Figure 29. NH4-N measured and modelled effluent concentrations

NO$_3$-N parameter

In the nitrate-nitrogen effluent, there is the biggest difference between measured and modelled data. The average measured NO_3-N concentration is 4.81 mg/l and modelled is 9.15 mg/l (Figure 30). According to Matzinger (2017) in the Freistadt WWTP, the return of NO_3-N after NH_4-N degradation is done solely through return sludge. Since this could not be represented in SIMBA#, an attempt was made to recircle the NO_3-N concentrations back to upstream denitrification reservoirs with a flow split. Even through this method, the improvement was only a minor success. In this step, the stakeholder approval was also acquired to continue with work.

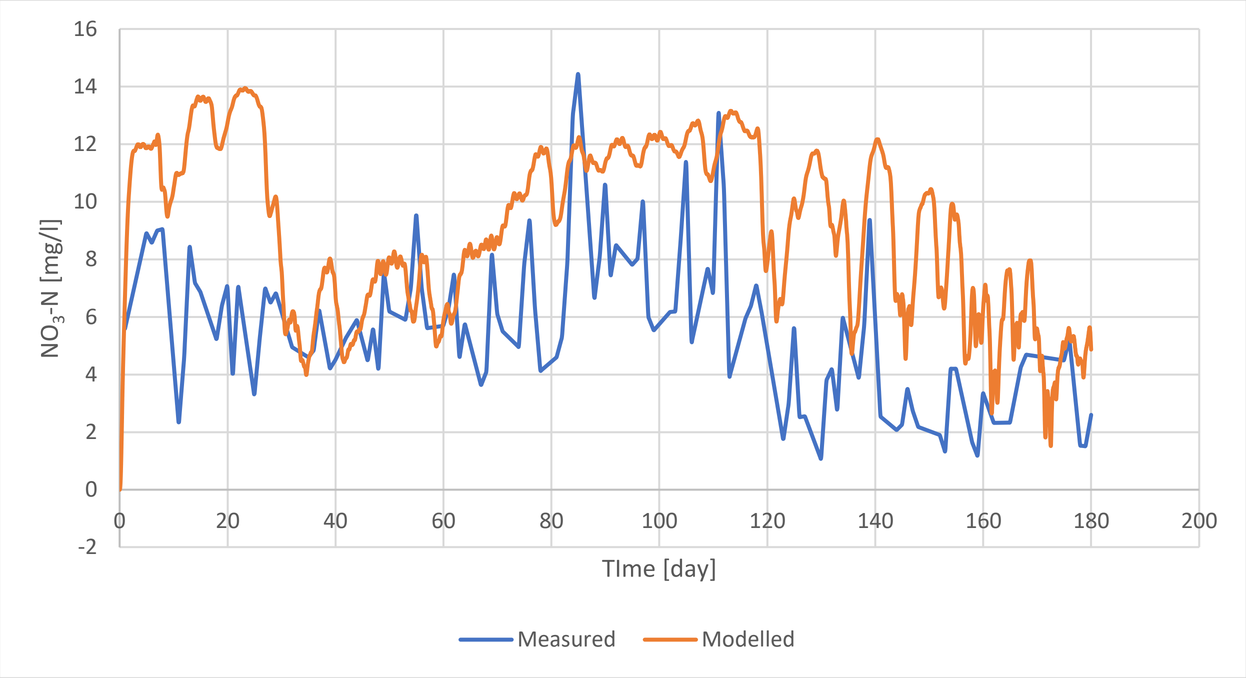

Figure 30. NO_3-N measured and modelled effluent concentrations

Total nitrogen parameter

Since there was an increase in modelled NO_3-N concentrations, these results also reflect on total nitrogen concentrations. The average measured NO_3-N concentration is 7.08 mg/l and modelled 11.26 mg/l (Figure 31).

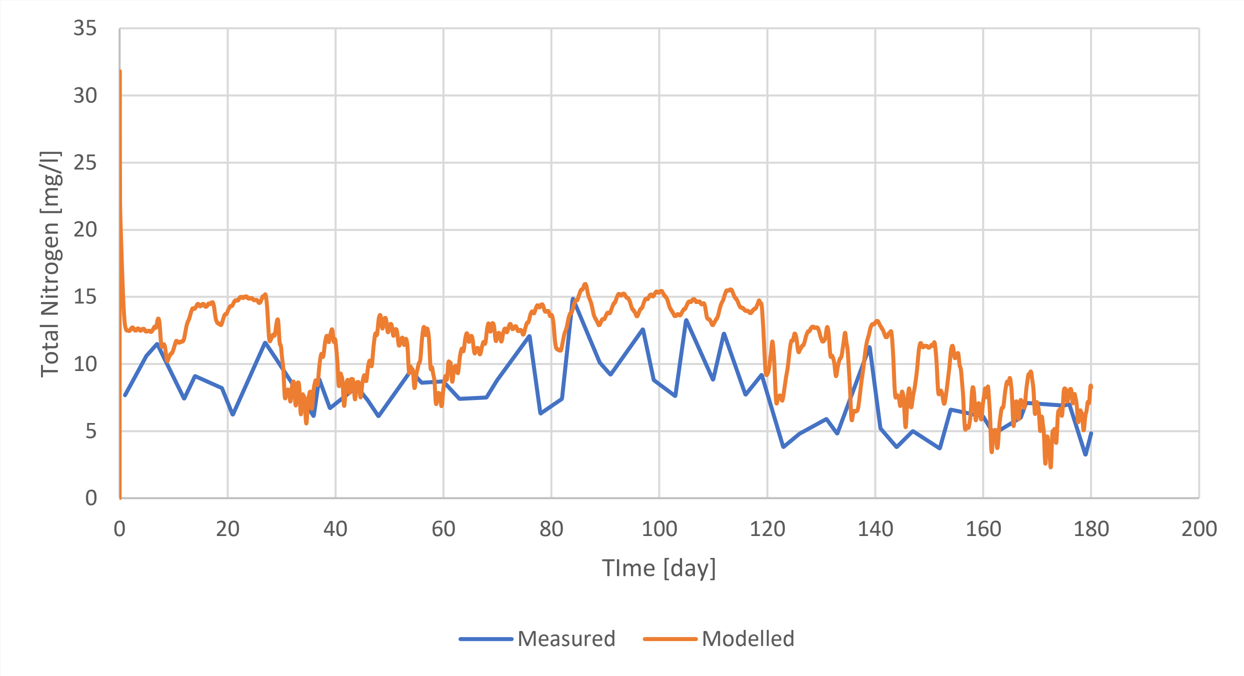

Figure 31. Total Nitrogen measured and modelled effluent concentrations

5.2.2 Implementation of scenarios in SIMBA# software

To represent solely the impact of road salt, a slight adjustment was made to the calibrated model. This reflects in the change of the influent generator (Figure 32). The model for scenarios was changed from the advanced influent generator to a dry weather inflow generator. A dry weather inflow generator creates an influent with constant flow quantities and constant concentrations. This allows a clear representation of salt inhibition in the effluent parameters, and not due to fluctuations of inflow quantities and concentrations.

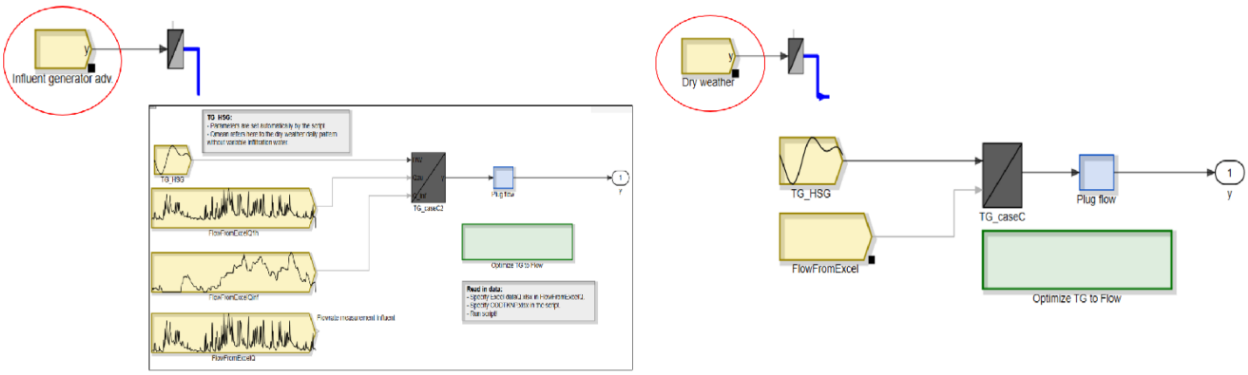

Figure 32. Changed influent generator (screenshot from SIMBA# software)

Since there is no available data on chloride influent in the Freistadt WWTP, the investigatory work on identifying the possible days of snow melt was performed (higher inflow salt concentrations reach WWTP as a result of street runoff due to snow melt or rain event). The snowfall (and snow melt) usually occurs in the months of December, January, and February and thus these were the investigated months. The investigation was done in the following way. The average monthly influent water temperatures were calculated and then compared with the minimum influent water temperature of the month. For the month of February, the average influent water temperature was 8.7 °C and the minimum temperature was 7.3 °C on the 11th of February (Figure 33). This was the biggest deviation from the average temperature in all of the months. Thus, the 11th of February was selected as the day of the salt dosing in models. Also, since the 1st of February is day 0 of the modelling, the 11th of February is considered as day 10 of modelling in SIMBA#.

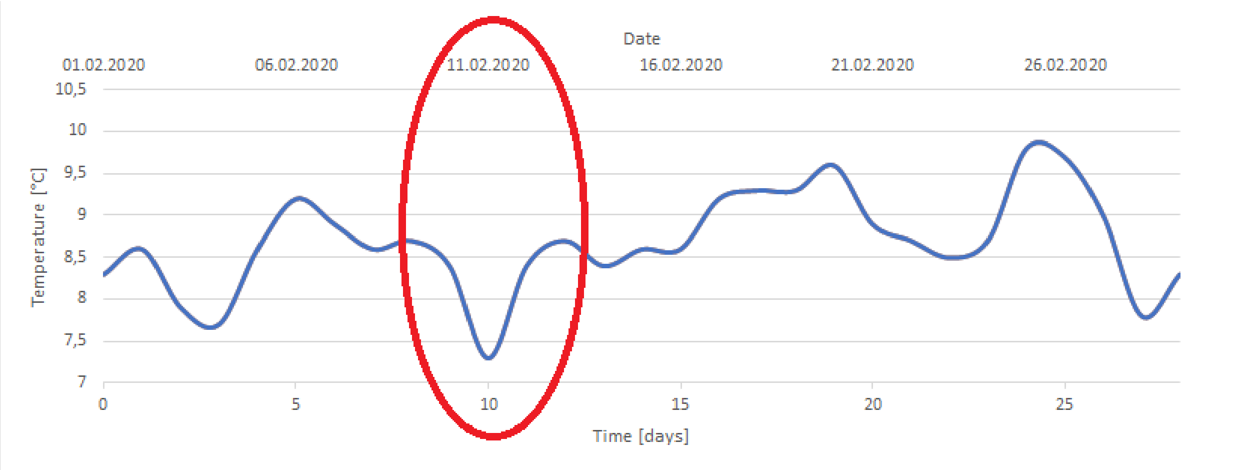

Figure 33. Influent water temperature in the month of February

5.2.3 Scenarios and Results

After the literature review, the following parameters are identified as possible impactors on activated sludge inhibition processes: salt concentration, duration of salt dosing, water temperature, and inflow quantity. That's why, these parameters were chosen for further investigation and scenario creation.

<u>Scenario 1 – Varying of salt concentrations</u>

The following scenarios of salt concentrations have been investigated:

- 0.5 g NaCl/l
- 1.0 g NaCl/l
- 1.5 g NaCl/l
- 2.0 g NaCl/l

Results and discussion

1) <u>0.5 g NaCl/l</u>

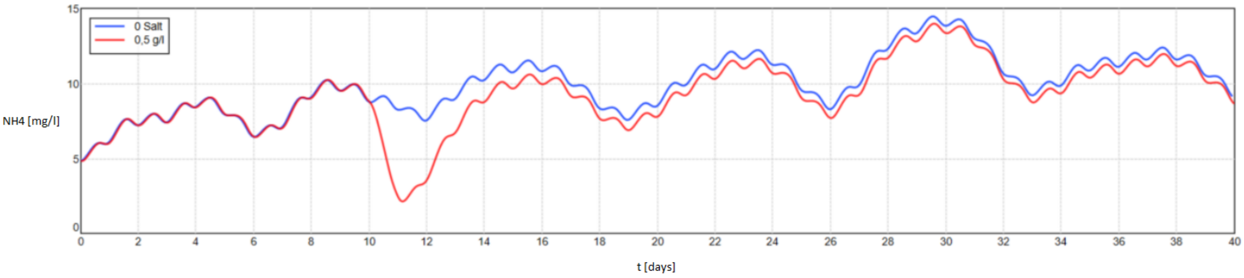

Figure 34. NH_4 effluent concentrations with dosing of 0.5 g NaCl/l for 24 hours

With a low salt concentration of 0.5 g NaCl/l, there was an improvement in NH_4 removal efficiencies. The effluent concentration before salt dosing was 9 mg/l and during the salt dosing, it fell to 2.5 mg/l (Figure 34).

It is also worth mentioning that after a conversation with different wastewater treatment personnel, it was reported that usually, incoming salt concentrations are higher than 0.5 g/l and that these improved NH_4 removal efficiencies are rarely taken advantage of.

2) <u>1.0 g NaCl/l</u>

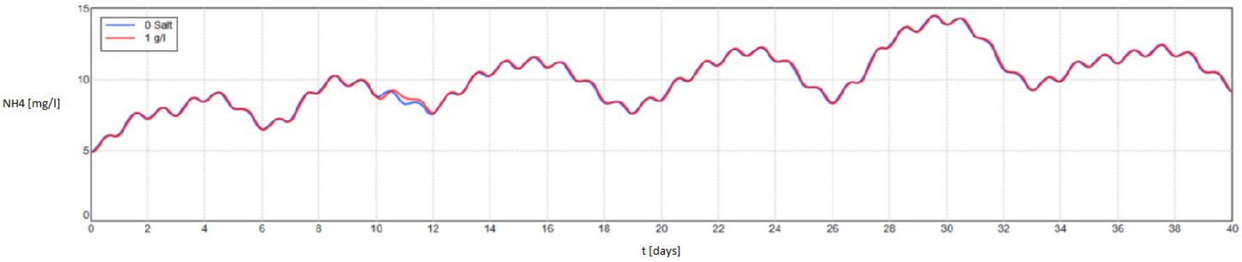

Figure 35. NH_4 effluent concentrations with dosing of 1.0 g NaCl/l for 24 hours

The salt concentration of 1,0 g/l is a tipping point between improved removal efficiencies and inhibition. Figure 35 shows that there was no noticeable effluent quality change. Below 1.0 g/l, as seen in Figure 34, there was an improvement in NH_4 removal and above 1.0 g/l there were noticeable inhibitions (Figure 36).

3) <u>1.5 g NaCl/l</u>

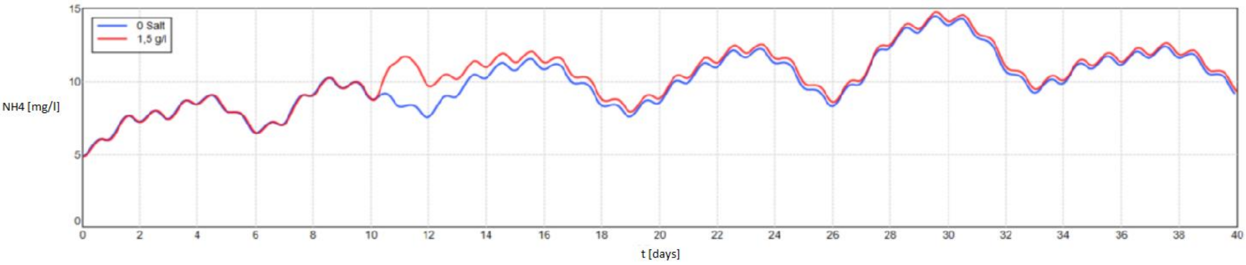

Figure 36. NH_4 effluent concentrations with dosing of 1.5 g NaCl/l for 24 hours

With an increase in salt concentrations, there is a strong trend toward worsening of effluent NH_4 quality. With a salt dosing of 1.5 g/l for 24 hours, there was an increase of 25% in NH_4 effluent.

4) <u>2.0 g NaCl/l</u>

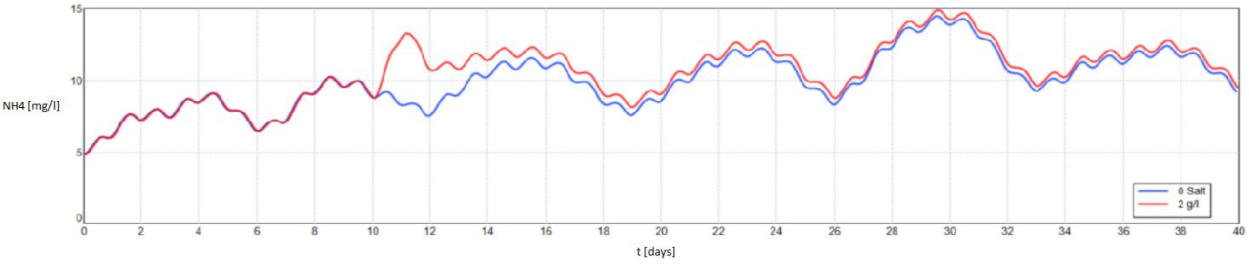

Figure 37. NH_4 effluent concentrations with dosing of 2.0 g NaCl/l for 24 hours

The highest modelled salt concentration of 2.0 g/l had a severe negative effect on NH_4 removal efficiencies. As it can be seen from Figure 37, the increase in salt concentrations brings more inhibition to the rate of nitrification.

For all the salt dosing cases, the activated sludge system went back to its normal state after 5-15 days. Similar results were also recorded in the literature, where Tauber et al. (2021) and Flesch (2020) reported normalization of the activated sludge process after 5 days.

<u>Scenario 2 - Longer duration of salt</u>

The following scenarios of prolonged salt dosing have been investigated:

- 0.5 g NaCl/l for 48 hours
- 1.0 g NaCl/l for 48 hours
- 1.5 g NaCl/l for 48 hours
- 2.0 g NaCl/l for 48 hours

1) 0.5 g NaCl/l for 48 hours

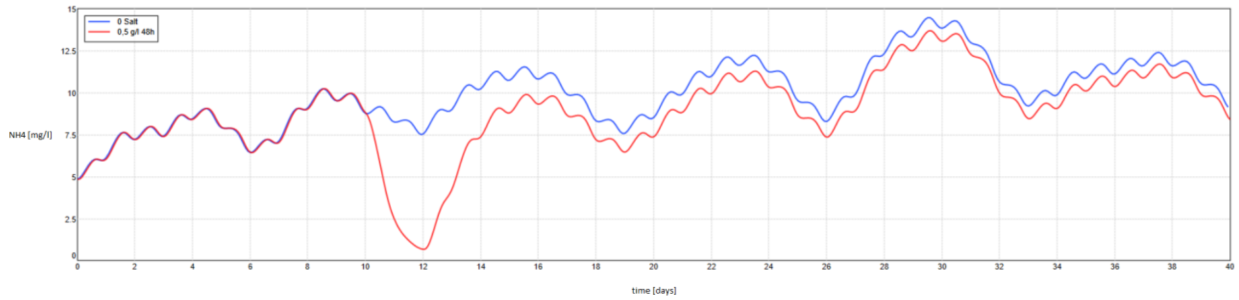

Figure 38. NH_4 effluent concentration with 0.5 g NaCl/l for 48 hours

After the salt dosing of 0.5 g/l for 48 hours, there was a significant increase in the removal of ammonium (Figure 38). Compared to the duration of the salt dosing for 24 hours (Figure 34), where the minimum effluent concentration was 2.3 mg/l, the effluent concentration improved with a minimum value of 0.9 mg/l.

2) 1.0 g NaCl/l for 48 hours

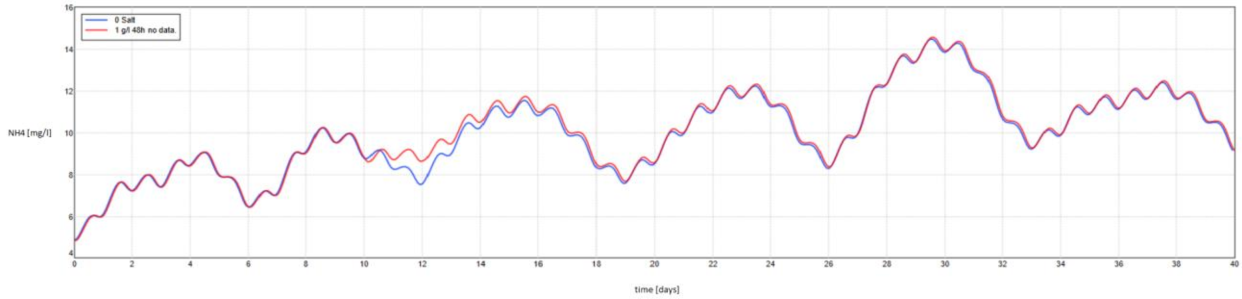

Figure 39. NH_4 effluent concentration with 1.0 g NaCl/l for 48 hours

As Figure 39 shows, similarly to a previous scenario, the salt dosing with a concentration of 1.0 g/l, had no significant effect on removal ammonium efficiencies.

3) 1.5 g NaCl/l for 48 hours

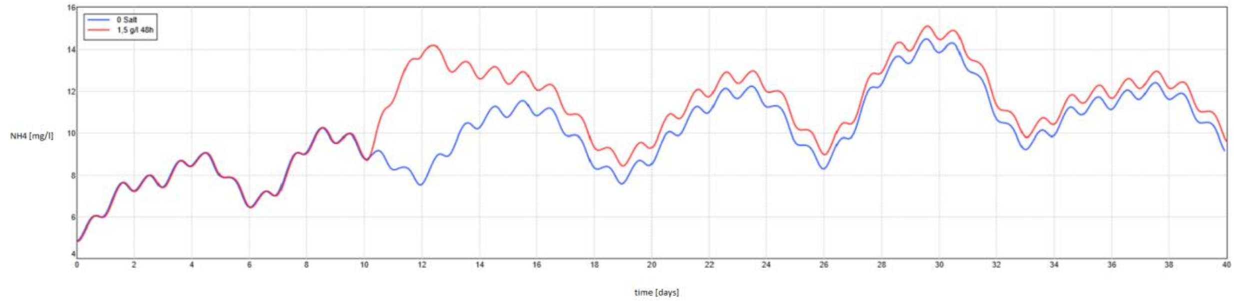

Figure 40. NH_4 effluent concentration with 1.5 g NaCl/l for 48 hours

Prolonged salt dosing in this scenario led to the dire deterioration of ammonium removal efficiencies. The maximum value of ammonium effluent, for the 24-hour dosing scenario, was around 12 mg/l. In this scenario, with the salt dosing for 48 hours, the maximum effluent concentration was 14.1 mg/l (Figure 40).

4) 2.0 g NaCl/l for 48 hours

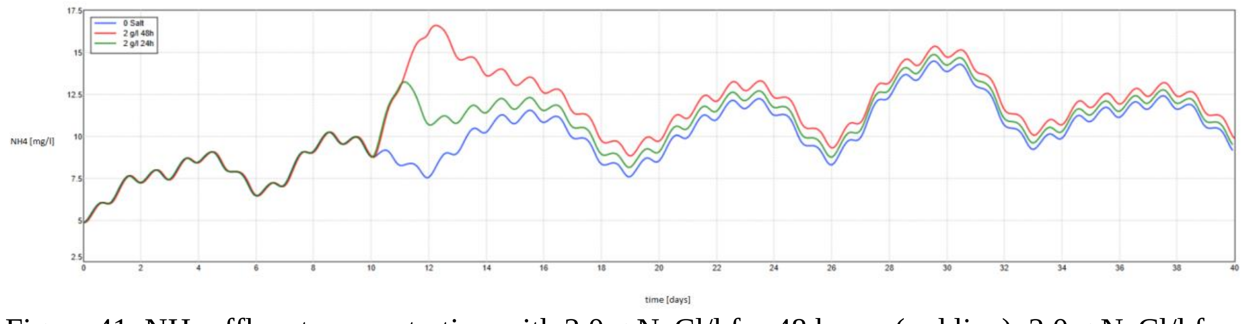

Figure 41. NH_4 effluent concentration with 2.0 g NaCl/l for 48 hours (red line), 2.0 g NaCl/l for 24 hours (green line), and before salt dosing with 0 g NaCl/l (blue line)

On Figure 41 is represented the difference between different salt dosing duration times. When the salt dosing time was increased, more severe inhibition of nitrifying bacteria occurred. This led to an increase in ammonium effluent concentration.

Scenario 3 - Lower inflow temperatures

The scenarios were done with a water temperature of:

- 4.0 °C
- 5.0 °C
- 6.0 °C

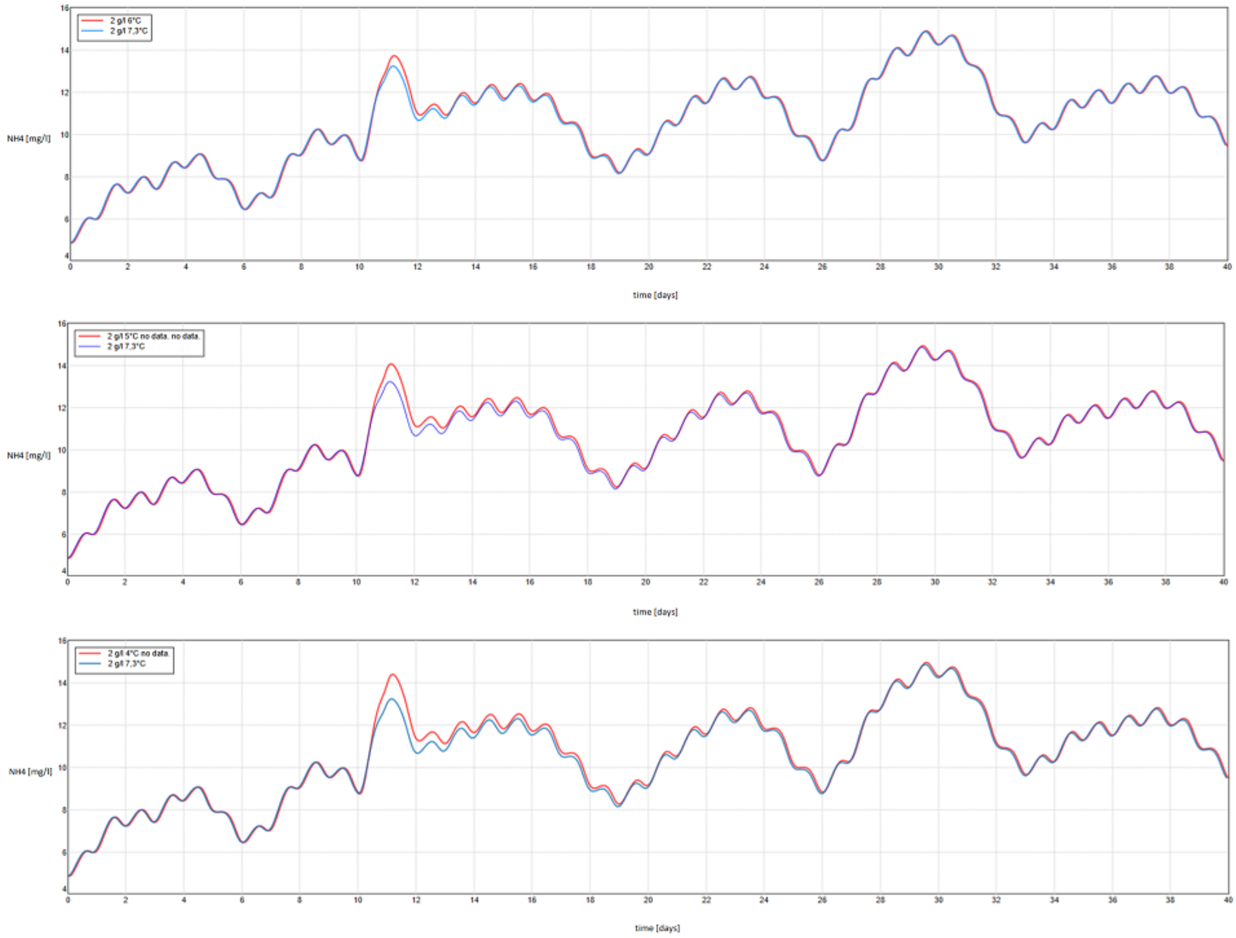

Figure 42. NH_4 effluent concentration with variable inflow temperatures of 6.0, 5.0, and 4.0 °C

Figure 42 shows how an activated sludge system with higher salt content reacts to an inflow water temperature decrease. The default value, before temperature decrease, was 7.3 °C. The decrease of 1.3 °C did not have a significant impact on the wastewater treatment. When the temperature dropped to 4°C, there was a 10% decrease in removal efficiencies.

It is important to note here also that ASM3h is limited to the minimum temperature of 8.0 °C. In order for this data to be used, they should be first compared with data from a real WWTP.

Scenario 4 - Increased inflow water quantities

The scenarios were done with an inflow of:

- 5 000 m³/day
- 6 000 m³/day
- 7 000 m³/day

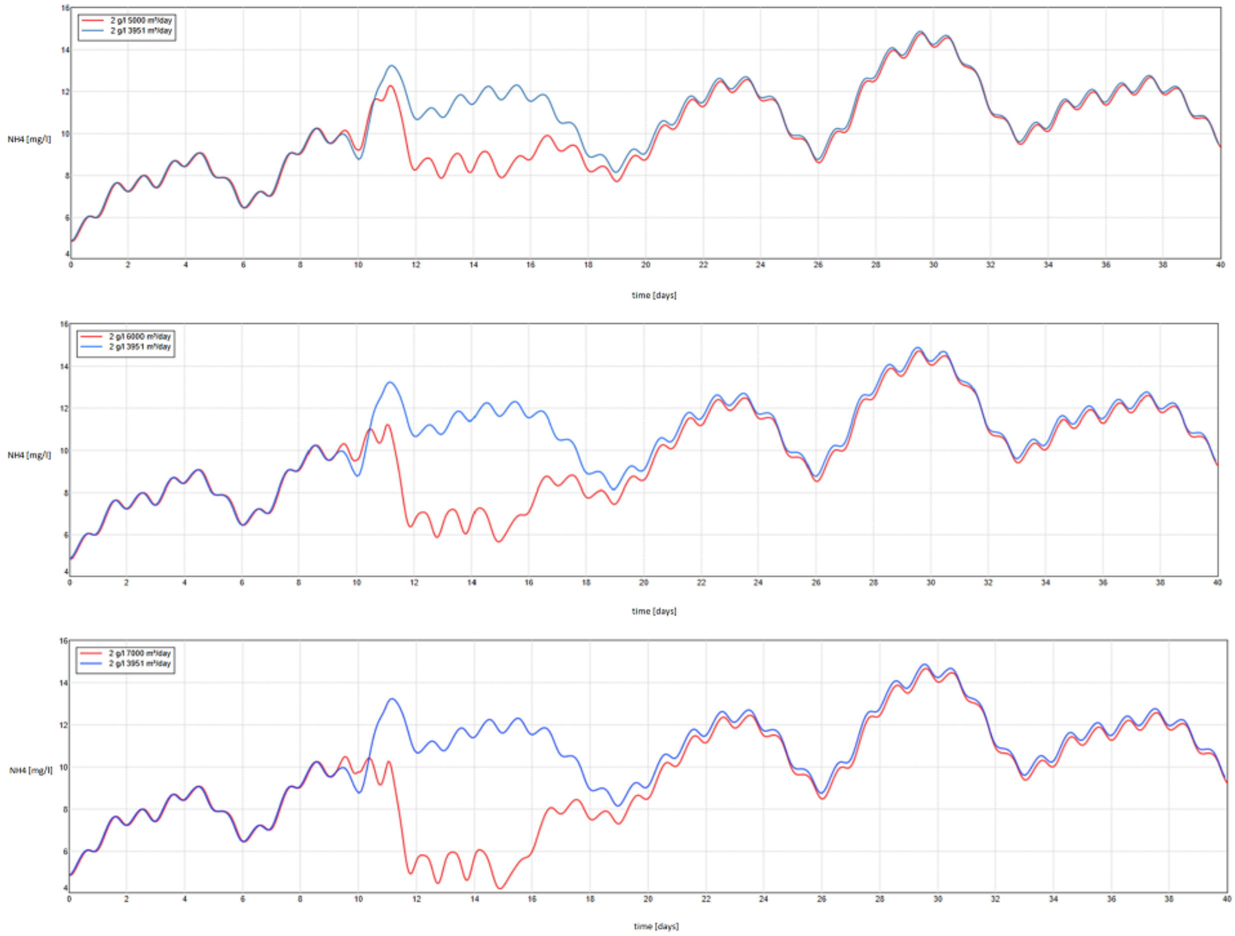

Figure 43. NH_4 effluent concentration with fluctuating inflow quantities of 5 000, 6 000, and 7 000 m³/day

A temporary inflow increase due to a rain or snow melting event would not cause impairment in nitrification processes. On the contrary, short-term elevated inflow quantities improved the NH_4 removal. For the scenario where inflow was increased from original 3951 m³/day to 7 000 m³/day for 5 days, there were improved removal efficiencies from the average of 12 mg/l to 4.5 mg/l (Figure 43).

5.3 Interpretation

Modelling of scenarios gave a good insight into the salt-nitrification rate dependencies. Scenario 1 showed that salt concentration is one of the most important factors that influence the rate of nitrification. Varying the salt concentrations from 0.0 to 2.0 g NaCl/l brought positive and negative effects on removal rates of ammonium. Until the value of around 1.0 g NaCl/l, there were significant improvements in the nitrification rate. The scenario with 0.5 g NaCl/l and salt dosing of 24 hours, brought improved the effluent NH_4 quality from 9.0 mg/l to 2.5 mg/l. The salt concentration of 1.0 g NaCl/l is described in the numerical model as a tipping point between positive effects and inhibition. This is also reflected in modelled results, as there was no significant change in effluent concentrations. When the tipping point of 1.0 g NaCl/l was exceeded, inhibition started to occur. Inhibition correlated nicely with salt concentration. As the salt dosing increased, the inhibition also increased.

The increase in salt dosing exposure times, brought weighty changes to modelled results. When the salt dosing exposure time was increased from 24 hours to 48 hours, there was a magnification of both positive and negative effects. This scenario showed that the duration of salt dosing exposure is also a significant impactor on the nitrification rate.

Since road salt dosing events only occur in the winter months, the impact of lower influent water temperatures was also examined. The simulation showed that lower influent temperatures don’t significantly impact the activity of autotrophic nitrifying bacteria. It is important to note here, that ASM3h used in this work is limited to the temperature range of 8.0 – 23.0 °C. It is possible that because of this constraint, modelled results are not accurately represented. To combat this problem, SIMBA# offers a plug-in to the ASM3h, which could be used for temperatures lower than 8 °C.

Salt that is being dispersed on roads, ends up in the sewer system through a snow melting or rain event. Both events, bring an increase in the influent water quantities. Modelled results showed that an increase in the inflow quantity brings improvement to NH_4 effluent concentrations. The possible reason for this is that the dilution factor increases with a larger inflow quantity. The increased dilution does not create operational problems, as long there is enough capacity in the WWTP to process the wastewater with designed sludge retention time.

6. Conclusion and outlook

The impact of salt on wastewater treatment plants is still a highly unresearched topic. The literature review did not provide enough information, since the available papers for the concentration of salt up to 2-3 g NaCl/l are very scarce. From the available literature, it was concluded that salt concentration and length of exposure time are the most important factors that influence nitrification rate.

Salt concentrations that are less than 1.0 g NaCl/l have a positive effect on the nitrification rate. There was up to a 200% increase in the activity of autotrophic bacteria when the salt concentration was 0.7 g NaCl/l. On the contrary, when the concentrations exceeded the threshold of 1.0 g NaCl/l, inhibition started to occur. The inhibition in bacterial activity reached up to 50% of the original value for the concentration of 2 g NaCl/l. This behaviour was also modelled and validated in a dynamical simulation.

In this thesis, a numerical model for salt impacts on nitrification was developed (see chapters 4.1 and 5.1.1) and implemented the SIMBA# software (chapter 5.1.2). Since different salt concentrations have a positive and inhibitory effect on the WWTP, steps in chapters 4.1 and 5.1 could be adapted to other possible case uses. This process can be used for other inhibitory substances in dynamical wastewater treatment modelling, when the impact on operational parameters is known and quantifiable.

As a final note, it is important to note that there were no available data in the Freistadt WWTP that could confirm the results of this work. There were no measurements of influent chloride concentrations and there was no recorded impact that a salt event had on a WWTP. Thus, the results of this work still need to be validated with an additional measuring campaign.

7. Summary

Road salt that is dispersed on the roads during the winter, prevents the formation of ice and snow on top of the asphalt surfaces. However, during snow and ice melting events, this salt drains into the sewer system and eventually ends up in the wastewater treatment plant. Due to the increase in chloride concentration, WWTP operators reported deterioration of effluent concentrations and hindrance in plant operation.

The Freistadt WWTP collects wastewater from 5 municipalities: Freistadt, Lasberg, Rainbach, Grünbach, and Waldburg. The WWTP is located in Upper Austria and has a capacity of 30 000 population equivalent. The plant is comprised of the following cleaning stages: Mechanical cleaning, Biological cleaning, and Sludge stabilization.

<u>A numerical model for salt impacts on nitrification</u>

Based on a literature review of salt impacts on wastewater treatment plants, a set of equations were created that describe the maximal nitrification rate based on salt concentration. In the ASM3h, the parameter of maximal rate of nitrification ($muAUT_{20}$) was adapted to include the influence of salt. Thus, a new parameter (μ_{salt}) for the maximal rate of nitrification, dependent on the salt concentration was created.

To describe the impact of salt on nitrification in activated sludge treatment plants, three equations were created:

1) Salt concentration for increasing salt concentrations between 0,0 – 1,1 g NaCl/l

   $$\mu_{salt} = 4.9114\ C_{salt}^3 - 11.44\ C_{salt}^2 + 6.4432 * C_{salt} + 1.12 \qquad (1)$$

2) Salt concentration for increasing salt concentrations between 1,1 – 2,0 g NaCl/l

   $$\mu_{salt} = -0.2931\ C_{salt} + 1.1558 \qquad (2)$$

3) Salt concentration for decreasing salt concentrations between 2,0 – 0,0 g NaCl/l

   $$\mu_{salt} = 0.2919\ C_{salt}^3 - 0.9462\ C_{salt}^2 + 0.3508 * C_{salt} + 1.344 \qquad (3)$$

<u>Implementation of numerical model into SIMBA# software</u>

In the “IEC Code” block, the 3 equations were inserted and m_{salt} as an output parameter was created. Since the parameter m_{salt} is dependent on the salt concentration, the blocks that define salt concentration (“Csalt” and “Csalt1” blocks) were connected to the “IEC Code” block and used as an input for all of the scenarios (Figure 44).

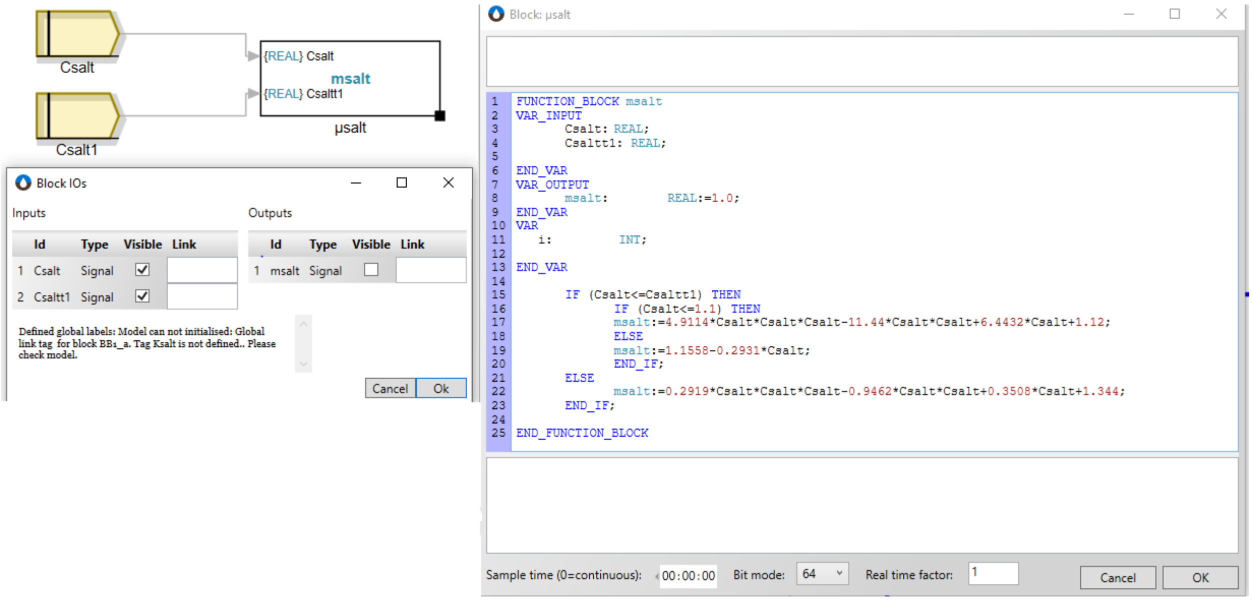

Figure 44. Implementation of m_{salt} parameter (screenshot from SIMBA# software)

As a second step, in the ASM editor, a parameter $muAUT_{20}$ (5) was exchanged for a parameter m_{salt}.

Scenarios and result interpretation

In total four different scenarios have been examined:

1) Varying of salt concentrations (0.5, 1.0, 1.5, 2.0 g NaCl/l) with a salt dosing time of 24h
2) Longer duration of salt dosing (48 hours)
3) Lower inflow water temperature (6, 5, and 4 °C)
4) Increased inflow water quantities (5000, 6000, and 7000 m^3/day)

Modelling of scenarios showed that salt concentration from 0.0-1.0 g NaCl/l has a positive effect on nitrification removal efficiencies, but salt concentration from 1.0-2.0 g NaCl/l has a negative effect. Longer exposure times brought amplification of impacts, both for positive and inhibitory effects. Lowering the inflow water temperature posed no significant impact on the nitrification processes. Finally, there was an improvement in NH_4-N efficiencies with an increase in inflow water quantities.

The model created in this thesis is developed solely through the data from literature review. Since there were no data from Freistadt WWTP on chloride concentrations and its possible impacts on effluent and operational parameters, the modelled results could not be verified.

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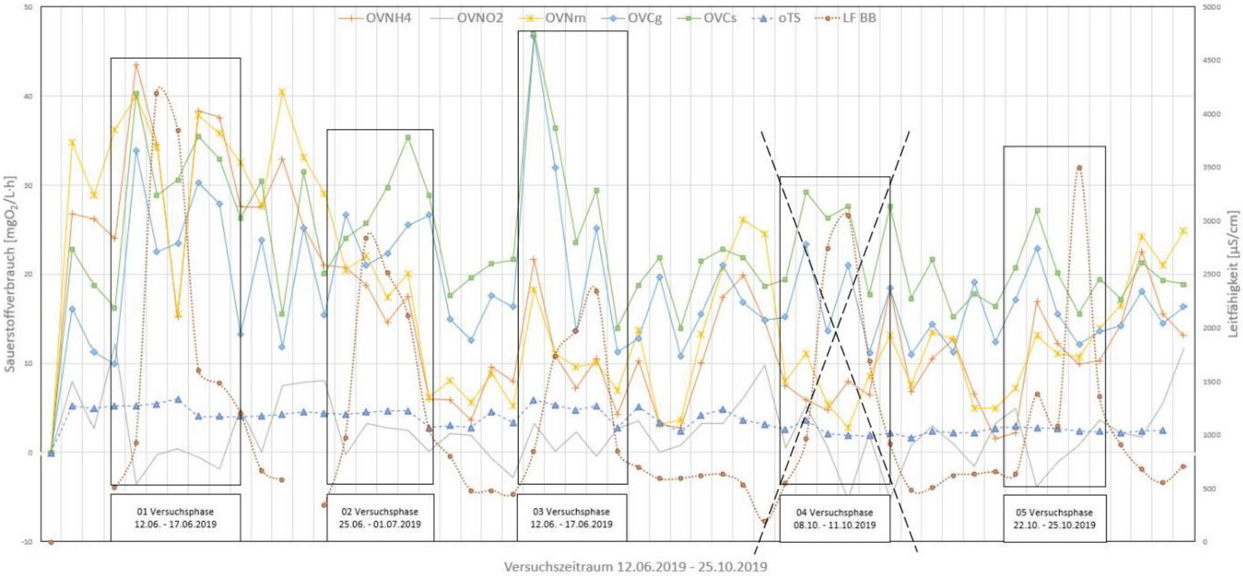
9. List of tables

10. List of figures

12. Appendix



Appendix 1. Oxygen uptake rates in all 5 phases of experimental WWTP (Flesch, p. 40, 2020)

13. Curriculum Vitae

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WORK EXPERIENCE

From Aug 2021 — Water and Sanitary Engineer

Lugitsch und Partner Ziviltechniker GmbH, Vienna (Austria)

- Planning of wastewater treatment plants
- Planning of drainage systems
- Design and review of pipeline information systems
- 3D surveying
- Photogrammetry
- Execution of sewer and manhole inspections

Jun - Okt. 2019 — Environmental and Sanitary Engineer

BMD Bau, Belgrade (Serbia)

- Design of sanitary landfills
- Preparation, review and compilation of projects and technical reports
- Leachate modelling
- Closure, remediation and reclamation of non-sanitary landfills
- Earthwork calculations
- Sanitary engineering design
- Supervision of field operations
- Interaction with field staff, clients, and contractors

July - Aug. 2017 — Engineering Internship

Lindner, Belgrade (Serbia)

- Support in the daily tasks of hydraulic engineers and architects
- AutoCad

EDUCATION

Okt. 19– Sep. 22 — Master studies - Water Management and Environmental Engineering

University of Natural Resources and Life Sciences (BOKU), Vienna (Austria)

Master thesis: Modelling the effect of salt from road runoff on nitrification at Freistadt Wastewater Treatment Plant

Okt. 13–Jun 19 — Bachelor studies – Hydrotechnical and Environmental Engineering

University of Belgrade, Faculty of Civil Engineering, Belgrade (Serbia)

Bachelor Thesis: Leachate modelling from sanitary landfill in Subotica

Sep. 09–Jun 13 **Telecommunications Technician**

Technical school PTT, Belgrade (Serbia)

PERSONAL SKILLS

Native language: Serbian

Languages

	UNDERSTANDING		TALKING		WRITING
	Listening	Reading	Taking part in conversations	Coherent speaking	
German	B2	B2	B2	B2	B2
English	C1	C1	C1	C1	C1
	TOEFL iBT Total Score: 93				

Driving licence: B