CHALMERS
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Coagulation and Flocculation Optimization for Sustainable Wastewater Treatment

Investigation of coagulation methods and predictive modelling to reduce chemical consumption and carbon footprint

Master’s thesis in Industrial Ecology

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Optimizing Coagulation and Flocculation for Sustainable Water Treatment
Optimization of chemical dosing strategies for more climate efficient wastewater treatments
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Cover:
Experimental jar test for determining the efficiency of polymer dosage in industrial wastewater.

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Abstract

This thesis investigates opportunities for optimizing the primary coagulation and flocculation process at the company that treats industrial wastewater. The treatment process handles highly variable incoming raw water, where chemical dosing is currently based on fixed dosages. These variations in incoming water quality create opportunities to proactively improve resource efficiency and process stability, with a primary focus on reducing environmental impact.

The aim of this work was to investigate how variations in raw water quality influence the efficiency of the coagulation and flocculation process and to examine how a data driven approach can support and improve chemical dosing. The objective was to reduce chemical consumption and its associated carbon footprint while maintaining or improving treatment performance.

This thesis was based on laboratory jar tests using wastewater collected from the inlet of the treatment process following initial sedimentation. A range of experimental conditions were tested and evaluated, including the current performance of TOC, absorbance and turbidity removal, pH adjustments for ferric chloride, polymer addition, mixing strategies and dilution series. The dilution series was evaluated based on the measurement error between the instruments used at Chalmers and at the company's lab. Key water quality and performance parameters for the coagulation and flocculation process were measured, including TOC, turbidity, absorbance, conductivity and sludge production. In addition, a linear model was developed in Python to predict TOC removal from SUVA. Based on this model, an algorithm was proposed to predict the coagulation outcome. The algorithm suggests an optimal chemical dose based on these raw water quality parameters.

The results show that the performance of the treatment process is influenced by several operational conditions, such as pH and mixing strategies, and by how these are managed in relation to variations in the incoming raw water quality, which directly affects the efficiency of contaminant removal. The study also demonstrates that the characteristics of the raw water influence the required treatment level, highlighting the importance of an adaptive and flexible approach to chemical dosing.

Furthermore, the findings indicate that transitioning from a fixed dosing strategy to a more adaptive approach can improve both plant stability and chemical use efficiency, resulting in reduced carbon footprint. By combining experimental and modelling approaches, this thesis demonstrates how treatment performance can be better understood and managed under varying operating conditions.

Keywords: Wastewater treatment, coagulation, flocculation, pH optimization, jar tests, SUVA, polymer, process optimization, TOC.

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Declaration of AI Use

AI tools were used to support language refinement and to assist with Python scripting for the generation of figures and visualization of results.

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1 Introduction

This section of the thesis contains information about wastewater treatment at the company. The problem definition aims, research questions and delimitations of this thesis.

1.1 Overview

Industrial wastewater treatment plays a significant role in reducing environmental impact and supporting the transition towards a more circular and sustainable economy (UNESCO, 2017). Industries generate complex wastewater streams, and there is an increasing need to optimize treatment processes, not only to improve treatment performance but also to reduce greenhouse gas (GHG) emissions. Wastewater treatment involves several processes, such as coagulation and flocculation, which are effective for contaminant removal. However, these treatment plants are associated with substantial chemical consumption, sludge production and indirectly high CO_2 emissions (United Nations Environmental Programme, 2023).

At the company hazardous and industrial wastewater are treated, which focused this thesis on optimizing the coagulation and flocculation process referred as Coagulation & Flocculation Treatment Stage (CFT) and which is one of the initial stages of the treatment process, where chemical dosing is currently fixed or experience based despite substantial variations in incoming water quality. This may result in inefficient chemical usage and unnecessary environmental impact.

The fixed dosing strategy raises the question of whether chemical dosing can be optimized to reduce chemical consumption, improve process stability and lower GHG emissions. By developing a more data driven approach, this study contributes to a more resource efficient wastewater treatment process and supports the company's environmental and sustainability objectives.

1.2 The Plant

The plant is a specialized facility that mainly processes and recycles hazardous waste. The facility focuses on the import, storage and processing of different types of industrial waste and wastewater. Figure 1 provides an overview of the facility.

Within the plant, dedicated wastewater collection and treatment systems are used to manage different wastewater streams. Coagulation and flocculation methods are applied together with filtration systems and biological treatment processes to separate oil, water and other valuable resources, enabling their return to circular flows or safe disposal.

The wastewater treatment facility consists of multiple treatment stages. First, tankers carrying wastewater are weighed upon entry to and exit from the facility to calculate the amount of wastewater transported. The wastewater is then sucked or pumped into one of the two drainage pits, where it is sedimented for one day to remove the majority of the larger particles from the wastewater. This treatment facility receives highly variable industrial wastewaters, including streams originating from car washes, waste management activities and other miscellaneous industries. The sludge from the drainage pits is transported to external partners for incineration and energy recovery.

The wastewater from the drainage pits is subsequently transported to the CFT facility, where the inflows differ significantly in composition, particularly in terms of total organic carbon (TOC), conductivity, turbidity and the presence of oil. The CFT facility utilizes coagulation and flocculation with the primary objective of removing TOC and heavy metals. The focus of this study is to optimize this treatment step, as discussed later in the thesis. In the CFT process, different chemicals are added to the wastewater to promote coagulation and flocculation. The wastewater pH is regulated during this process, both before entering CFT and before exiting the treatment step.

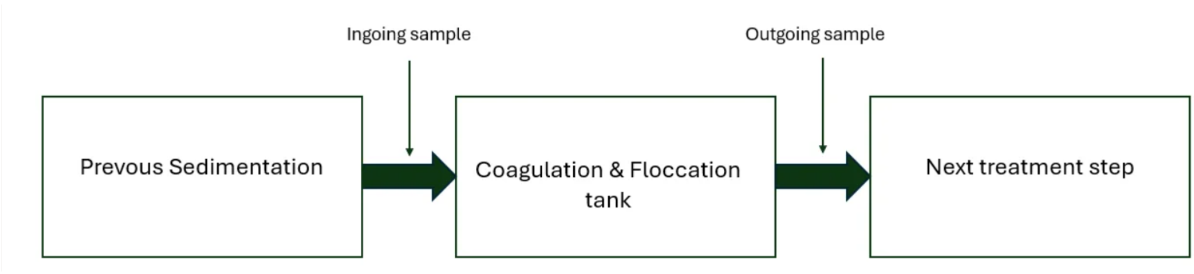

Figure 1. Sampling and treatment stages in the CFT process.

1.3 Problem Description

The inflows differ significantly in composition, particularly in terms of total organic carbon (TOC), conductivity, turbidity and the presence of oil. As a result, the raw water quality entering CFT fluctuates substantially over time.

The current CFT process applies a fixed or "experience based" dosage of acid and ferric chloride. Because the composition of the incoming water changes daily, this approach does not adequately reflect the optimal dosing of chemicals for the wastewater. Consequently, the system experiences both underdosing and overdosing of chemicals. Underdosing results in insufficient coagulation and poor removal of dissolved and particulate organic carbon. Overdosing, on the other hand, leads to increased sludge volumes, higher conductivity due to excess dissolved ferric chloride and hence increased operational costs.

Furthermore, the CFT process involves several chemical reactions, including acidification, emulsion breaking, coagulation and flocculation. Each of these processes is sensitive to incoming pH levels, mixing conditions and chemical ratios. Small variations in one process may disturb and negatively affect subsequent process steps. As the current operation is primarily based on fixed setpoints rather than adaptive dosing strategies, the operators have limited insight into which parameters are most suitable for controlling and improving process performance.

Data are collected by personnel at the company, including TOC, pH and conductivity measurements, but these data are currently not utilized to understand how raw water characteristics correlate with optimal chemical dosing and sludge quality. The CFT process currently functions "adequately", where operators mainly respond to symptoms rather than addressing underlying causes. With more structured laboratory testing and process related data, it could become easier to identify the key factors governing CFT performance, creating opportunities for a more consistent, chemically efficient, and cost effective process.

This project will provide a foundation for a simple predictive linear regression model capable of recommending chemical dosing based on water quality parameters. Such a model could support the company's transition towards a more data driven and environmentally efficient process control strategy.

1.4 Aim

The aim of this thesis is to investigate how variations in raw water quality affect the performance of the coagulation and flocculation process. This includes investigating how the process can be improved to optimize chemical consumption, enhance cost efficiency and reduce GHG emissions without compromising treatment performance.

The expected outcome is a methodology for selecting optimal chemical dosing strategies for different types of incoming water. By enabling more precise and adaptive chemical dosing, the results are expected to contribute to more stable process performance, reduced chemical consumption and sludge production, as well as lower overall resource usage. These improvements support environmental objectives by reducing the demand for chemical production and associated transportation, thereby lowering GHG emissions linked to the treatment process. Furthermore, more efficient coagulation and flocculation are expected to improve the removal of organic contaminants, contributing to enhanced water quality and more sustainable operations.

To achieve this, three research questions were formulated:

1.5 Research Questions

1. What methods and operational strategies can improve chemical dosing and treatment performance in coagulation and flocculation processes under varying wastewater conditions?
2. What is the current performance of the coagulation and flocculation process under varying raw water qualities?
3. How can the facility improve its coagulation–flocculation process to enhance stability, reduce chemical consumption, increase cost efficiency, and reduce environmental impact, without compromising treatment performance?

1.6 Delimitations

The project did not include the full scale implementation of optimized dosing strategies at the company’s operational facility; instead, all optimization work was based on laboratory scale experiments. The study focused exclusively on the coagulation and flocculation steps within CFT, while downstream treatment processes were not examined. The development of the linear regression model was intentionally kept relatively simple, as the primary focus was on generating the necessary underlying data and improving the understanding of the relationship between raw water quality and chemical dosing. The project did not include a complete economic assessment, such as investment calculations, labor costs or redesign considerations, and was therefore limited to evaluating the potential for chemical savings. Furthermore, the study did not address the upstream processes responsible for generating the incoming wastewater streams, and the raw water was treated as a given input to CFT. All laboratory experiments were conducted at the Chalmers Wet Lab facilities primarily using the existing equipment available at the facility.

2 Literature review

Here, literature about the key aspects of the thesis is explained and sources are noted.

2.1 Sustainability and Resource Efficiency

Chemical usage in industrial processes is directly associated with climate impact and operational costs, as chemical production contributes to overall greenhouse gas (GHG) emissions. From a life cycle perspective, emissions are linked to raw material extraction, processing and market supply chains, highlighting the importance of improving material efficiency within large scale treatment systems. The system also provides information regarding specific geographical regions, where RER represents Europe and ROW represents the Rest of the World.

Based on the Ecoinvent 3.11 database using the Environmental Footprint 3.1 method (100 year climate change potential), ferric chloride production (iron (III) chloride production, product in 40% solution state (RoW)) has an impact of 0.803 kg CO_2e/kg. Sodium hydroxide (market for sodium hydroxide, without water, in 50% solution state (RER)) has an impact of 0.915 kg CO_2e/kg, while sulfuric acid (market for sulfuric acid (RER)) has an impact of 0.122 kg CO_2e/kg (Ecoinvent Association, 2026), which are the chemicals used in CFT.

To compare the chemical demand within the CFT process, the following dosages were applied: ferric chloride: 0.9 mL/L; sodium hydroxide: applied for pH adjustment as a diluted solution, with the impact calculated per equivalent chemical mass where applicable; and sulfuric acid: used for pH reduction, with the impact similarly calculated per equivalent chemical mass where applicable.

Assuming typical solution densities, the contributions from ferric chloride and sodium hydroxide dominate the overall chemical footprint due to their higher dosing requirements and higher emission factors. Sulfuric acid contributes comparatively less because of its lower emission intensity and generally lower dosage volumes required for pH control.

2.2 Chemical Wastewater Treatment and Coagulation Flocculation

Chemical treatment is one of the most established and widely applied methods for removing solids, emulsified oils, dissolved organic matter, metals and other contaminants from industrial wastewater (Lucas, 2025). According to Bratby (2016), chemical coagulation is used to destabilize dissolved matter in water through the addition of metal salts, most commonly ferric- or aluminium based coagulants. Colloids also influence the treatment process and consist of small particles between 1 µm and 1 nm with very low sedimentation rates. The most effective method for removing colloids is through coagulation and flocculation, where the electrostatic charges are destabilized to promote particle collisions and aggregation (Lenntech, n.d.).

Coagulation and flocculation are central steps in chemical wastewater treatment processes and refer to the separation of small, suspended particles. These particles are negatively charged and therefore repel each other. Chemicals are consequently added to the water with opposite surface charges to neutralize the particles and initiate chemical reactions (Midwest Rural Water Association, n.d.).

In the CFT system, ferric chloride is used as the primary coagulant. When ferric ions are introduced into the water and the pH is subsequently increased using sodium hydroxide, iron (III) hydroxide precipitates are formed. These hydroxide flocs act as highly absorptive surfaces that capture organic matter, emulsified oils and both dissolved and particulate contaminants. This mechanism is consistent with classical descriptions of hydroxide precipitation in water treatment processes (Stumm & O'Melia, 1968).

Chemical coagulation and flocculation generally occur in four stages (Henze et al., 2002):

1. Precipitation (hydrolysis of metal salts)
2. Coagulation (destabilization of colloids)
3. Flocculation (aggregation under gentle mixing)
4. Solid–liquid separation (settling or filtration)

In practice, the first two stages occur almost simultaneously because ferric chloride hydrolyses rapidly once added to water. The CFT process also includes an initial pH reduction step using acid. This is particularly important for breaking oil water emulsions commonly found in car wash effluents and industrial wash waters (Oriekhova & Stoll, 2014). The pH is adjusted using sodium hydroxide (NaOH) and sulfuric acid (H_2SO_4).

To achieve effective coagulation, rapid and short term mixing is required in order to homogenize the coagulant and increase particle collisions. Typical mixing times range between 1–3 minutes, and insufficient mixing may result in incomplete coagulation, while over mixing generally has no significant negative physical or chemical effect on the process (Midwest Rural Water Association, n.d.).

Flocculation is most effective under slow and gentle mixing conditions, which promote collisions between colloidal particles and lead to the formation of larger flocs, commonly referred to as pin flocs. These flocs continue to grow as additional particles collide, eventually forming larger macroflocs. When the suspended flocs have reached an optimal size, they are allowed to sediment to achieve efficient treatment performance (Midwest Rural Water Association, n.d.).

The flocculation process requires carefully controlled mixing conditions to avoid excessive shear forces, allowing the flocs to maintain their structure and preventing them from breaking apart during mixing. As the flocs increase in size and volume, the mixing intensity must gradually be reduced. If the flocs are exposed to excessive shear forces, they may disintegrate, making it difficult for them to retain their optimal size and structure. Typical flocculation contact times range between 15–20 minutes but may, in certain cases, exceed one hour depending on the wastewater characteristics and the treatment equipment available on site. Once the flocs have reached an optimal size, the sludge is removed (Midwest Rural Water Association, n.d.).

2.3 Metal Salt Coagulants

Metal based coagulants are generally divided into two main categories: aluminium based and iron based coagulants. Other coagulants are also used, such as hydrated lime and magnesium carbonate. Aluminium and iron coagulants are the most widely applied due to their high availability, relatively low cost and effective performance in wastewater treatment processes (Bratby, 2016).

The coagulation process depends on the ability of these metal salts to form positively charged hydrolysis products and polynuclear complexes when dissolved in water. These complexes possess strong adsorption properties, allowing them to interact with colloidal and suspended particles in the wastewater. Since many particles in wastewater carry negative surface charges, the positively charged coagulant species neutralize these charges when adsorbed onto the particle surfaces. This destabilization enables the particles to aggregate into larger flocs that can be more easily separated from the water (Bratby, 2016).

The formation and charge density of these complexes are strongly influenced by the pH of the system. Consequently, pH adjustment can significantly affect the chemical form of the coagulant and, therefore, the overall efficiency of the coagulation process (Bratby, 2016).

2.4 Ferric Chloride as Coagulant

Ferric chloride, also known as iron (III) chloride ($FeCl_3$), is widely used in wastewater treatment for the removal of suspended solids, organic matter and heavy metals. Due to its strong coagulation properties, ferric chloride is commonly applied in both industrial and municipal wastewater treatment processes (Bratby, 2016).

Ferric chloride is an inorganic iron salt and acts as a Lewis acid, meaning that it can accept electron pairs during chemical reactions. When ferric chloride is added to water, it hydrolyzes and forms positively charged iron complexes and iron hydroxide flocs. These species neutralize negatively charged particles and dissolved organic matter in the wastewater, which allows the particles to aggregate into larger flocs that can later be separated from the water (Bratby, 2016).

The coagulation performance of ferric chloride is strongly dependent on pH because the chemical form and charge density of the iron species vary with the water chemistry. During hydrolysis, hydrogen ions are released, which can significantly reduce the pH of the treated water. The pH therefore has a major influence on coagulation efficiency and floc formation (Bratby, 2016).

Commercial ferric chloride solutions typically contain between 40 and 43% $FeCl_3$ and are characterized by high viscosity and a dark brown color. According to Bratby (2016), a typical ferric chloride solution contains approximately 628 g $FeCl_3$ per liter and has a density of approximately 1.45 kg/L at 20°C.

Equation 1 shows the reaction between ferric chloride ($FeCl_3$) and calcium bicarbonate ($Ca(HCO_3)_2$) during the coagulation–flocculation process. The reaction forms ferric hydroxide ($Fe(OH)_3$), calcium chloride ($CaCl_2$), and carbon dioxide (CO_2). The ferric hydroxide precipitates as insoluble flocs that capture suspended particles and other contaminants, facilitating their removal in subsequent treatment stages.

$$2FeCl_3 + 3Ca(HCO3)_2 \rightarrow 2Fe(OH)_3 + 3CaCl_2 + 6CO_2$$

Equation 1. Hydrolysis and precipitation reaction of ferric chloride

2.6 The Effect of pH

According to Lucas (2025) describes the importance of pH in wastewater treatment processes. In relation to inorganic coagulants and flocculants, such as ferric chloride used in the CFT process, pH directly influences hydrolysis, floc formation and the charge density previously discussed. The optimal pH range varies depending on the metallic salt applied in the treatment process.

Figure 2 illustrates how ferric iron undergoes hydrolysis and forms different hydroxyl complexes depending on the pH conditions. At low pH values, Fe^{3+} is the dominant species, while increasing pH promotes the formation of hydrolyzed species such as $Fe(OH)_3$, which becomes the predominant species. This is associated with effective coagulation and floc formation. At higher pH values, negatively charged species such as $Fe(OH)_4^-$ are formed. These observations demonstrate that pH plays a crucial role in controlling iron speciation and coagulation performance, as ferric salts undergo hydrolysis resulting in different species that influence particle destabilization and aggregation (Oriekhova & Stoll, 2014).

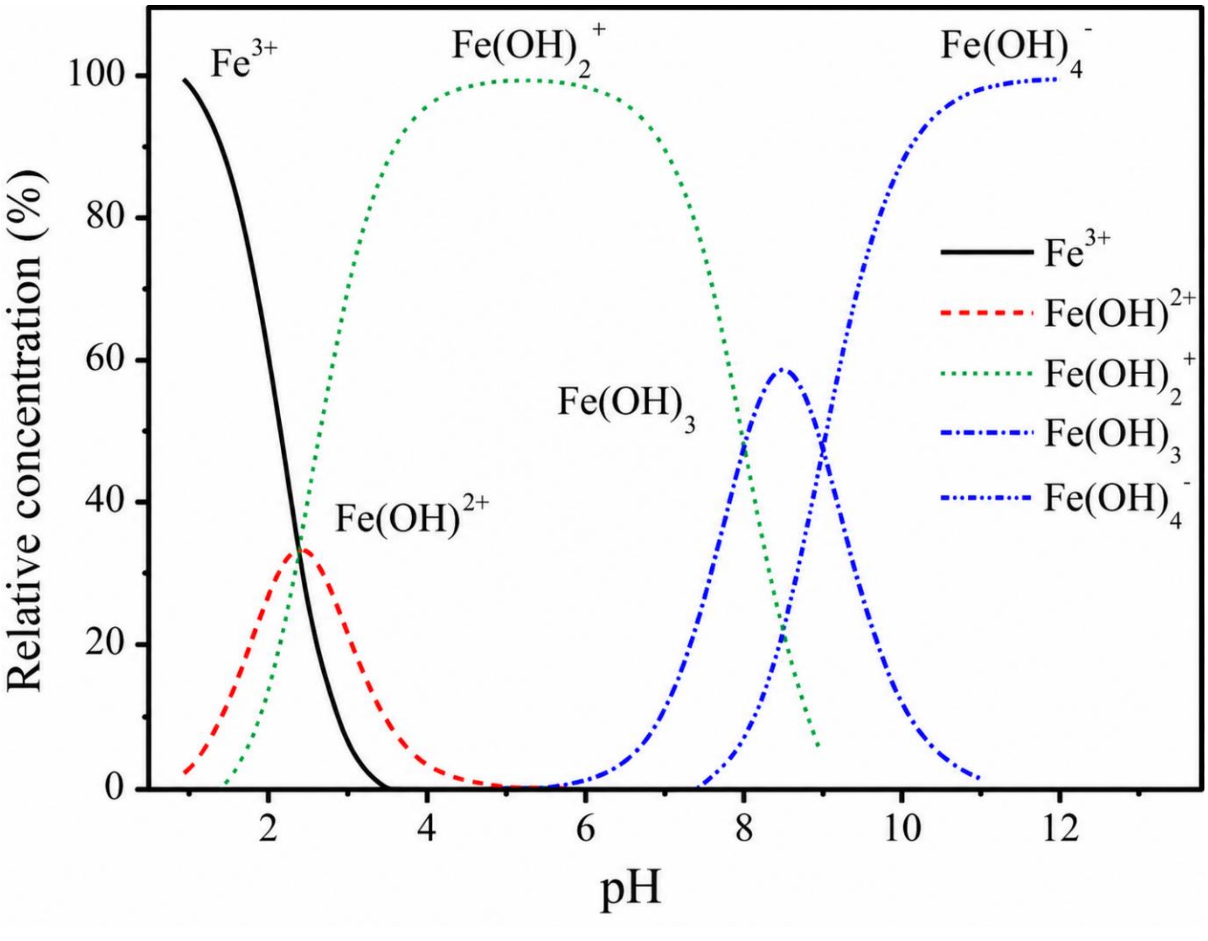

Figure 2. Fe^{3+} species distribution as a function of pH. (from Oriekhova & Stoll, 2014).

2.7 Polymers as Coagulation Aid

Polymers represent a broad group of macromolecular compounds that can be either natural or synthetic. They consist of repeating chemical units connected through covalent bonds. Depending on the composition of these chemical units, polymers can be classified as homopolymers when consisting of identical repeating units, or copolymers when consisting of different repeating units (Bratby, 2016). Polymers used in water treatment are generally soluble and can be applied to destabilize particles or enhance flocculation in processes.

Bratby (2016) states that synthetic polymers are widely used and are more common in industrial and commercial applications than natural polymers. Synthetic polymers generally exhibit a higher degree of effectiveness and can be designed almost specifically for a particular industrial process by controlling the number of charged units and the molecular weight, making them more effective as flocculation aids.

Bratby (2016) further explains that polyelectrolytes consist of long, stretched polymer chains containing charged units. When calculating polymer dosage, the molecular weight affects the charge density, also referred to as the degree of hydrolysis of the polyelectrolytes, which in turn influences the polymer configuration in the solution. As the molecular weight increases, both the charge density and viscosity increase. The polymer chains become increasingly stretched due to stronger electrostatic repulsion between the charged units. This affects the ionic strength of the polyelectrolyte solution through the increased charge density and consequently influences the destabilization process when polymers are added to wastewater. The destabilization process directly affects the resulting floc formation but remains dependent on the properties of the solution in which the polymer is applied.

When adding polymers, there is theoretically no upper dosage limit for achieving optimal floc formation when considering molecular weight (Kitchener, 1972). However, according to Bratby (2016), there are practical limitations associated with polymer usage. The long polymer chains require sufficient time to disentangle, and excessive shear mixing cannot be applied, as it may break down the flocs and negatively affect sludge properties.

2.8 Wastewater Variations and Treatment

The quality of the water delivered to the CFT treatment step can vary substantially over time, particularly because the system receives industrial wastewater streams that may include wash water, oily effluents and surfactant discharges. This variation is a key factor contributing to fluctuations in coagulation and flocculation performance, since coagulant demand and floc formation are strongly dependent on the concentration and characteristics of organic matter, suspended particles and dissolved ions (Oriekhova & Stoll, 2014). Bratby (2016) emphasizes that coagulation and flocculation performance is highly sensitive to water chemistry and that variations in raw water properties often require adaptive process control rather than fixed dosing strategies.

Industrial wastewater generally exhibits greater variability in composition and concentration than municipal wastewater because it is influenced by varying industrial operations, cleaning cycles, chemical usage and batch discharges. Standard wastewater engineering literature (e.g. Metcalf & Eddy, Inc. 2004) describes municipal wastewater as comparatively more predictable in composition due to its primarily domestic origin, whereas industrial wastewater streams may vary considerably depending on the industry type and the processes contributing to the system.

For the CFT process, this implies that a “one-size-fits-all” dosing strategy is unlikely to perform robustly across all incoming wastewater types, particularly when the influent alternates between relatively dilute streams and high load oily or surfactant rich streams.

2.9 Water Quality Parameters Affecting Coagulation

Factors affecting wastewater treatment and the corresponding approaches for achieving stable and efficient coagulation and flocculation performance through process control have been widely described in the literature. By utilizing measurable water quality parameters, it became possible to improve the understanding of process variability and relate these factors to variations in the incoming raw water quality. This section discussed literature that provided the foundation for predictive and more efficient management of adaptive and optimized chemical dosing strategies based on relevant water quality parameters.

2.9.1 TOC

Total organic carbon (TOC) is widely used as an indicator of the overall organic load in water and consists of different fractions, including humic substances, colour and UV-absorbing natural organic matter (García, 2005). According to Bratby (2016), TOC concentrations in natural waters may vary between 1 and 20 mg/L, while industrial wastewater can contain significantly higher concentrations, for example in heavily oil contaminated water. Variations in TOC are important because they are generally associated with changes in the overall organic loading, which directly influences the coagulant demand. However, the composition and characteristics of the TOC also play a significant role in determining the required coagulant demand (Bratby, 2016).

2.9.2 Turbidity

Turbidity is a key parameter widely used for monitoring coagulation performance. Bratby (2016) explains that turbidity instruments measure scattered light using a nephelometer, often at a 90° angle, as this approach compensates for the effect of dissolved colour and reports results in Nephelometric Turbidity Units (NTU), which is the preferred modern unit. Bratby (2016) further emphasizes that turbidity can serve as a proxy indicator for particle concentration. This is consistent with the standard methods description of nephelometry, where turbidity is determined from the intensity of light scattered by the sample relative to a standard suspension (National Health and Medical Research Council, 2011).

In the CFT process, fluctuations in turbidity are important because higher particle loads may increase the amount of coagulant required to destabilize and remove suspended material. In addition, turbidity is one of the fastest indicators of whether the coagulation and flocculation process is operating effectively at a given moment (Bratby, 2016).

2.9.3 Conductivity

Conductivity is an indicator of the concentration of dissolved ions (salts) present in water and can therefore be used to measure the ionic strength of wastewater. Bratby (2016) explains, through double layer theory, that increasing ionic strength compresses the electrical double layer surrounding suspended particles. This reduces the electrostatic repulsion between particles and can promote destabilization and aggregation.

In other words, variations in conductivity can influence how easily colloids are destabilized and how sensitive the system becomes to chemical dosage and pH conditions. This is particularly relevant in industrial wastewater streams where the salt content may vary due to detergents, cleaning agents and processing chemicals, causing the optimal coagulation pH window to shift over time.

2.9.4 Oil Contamination

Industrial wastewater often contains mixtures of emulsified oils and surfactants originating from detergents, degreasers and cleaning agents. These components interact to form highly stable oil/water emulsions, where surfactants reduce the interfacial tension and surround oil droplets with electrostatic or steric barriers that prevent coalescence. This limits the effectiveness of conventional coagulation processes because metal salts cannot easily neutralize or bridge these stabilized droplets (Tadros, 2013).

For treatment processes such as CFT, these effects result in practical operational challenges. Variations in oil and detergent loads can increase the required degree of acidification, alter the optimal ferric chloride dosage and affect the structure of the formed flocs. Consequently, oily and surfactant rich wastewater streams contribute to substantial process variability, making laboratory jar testing and adaptive dosing strategies essential for maintaining stable treatment performance.

2.9.5 Process Instability

Changes in TOC, turbidity, conductivity and the presence of oils or surfactants alter the chemical conditions required for colloid destabilization and floc formation. Higher TOC concentrations increase particle surface charge and strengthen electrostatic repulsion, resulting in a higher coagulant demand. Variations in conductivity affect the electrical double layer, where high ionic strength compresses the layer and improves coagulation efficiency, while low ionic strength reduces particle destabilization (Bolto & Gregory, 2007).

Variations in dissolved organic matter and surfactants also influence polymer performance by blocking adsorption sites and reducing the efficiency of polymer bridging. In some cases, overdosing may even lead to particle restabilization (Nasser & Twaiq, 2014). Additionally, wastewater streams containing high concentrations of oils and surfactants tend to form weaker and more shear sensitive flocs with poorer settling properties and lower dewaterability, thereby increasing process variability (Yin et al., 2014).

Together, these factors make coagulation performance highly sensitive to variations in raw water composition, resulting in fluctuating sludge characteristics and inconsistent treatment efficiency.

2.10 Data Driven Predictive Process Management

Measurable water quality parameters are commonly used as input variables in predictive treatment models due to their relationship with treatment performance (Zhu et al., 2022). In modern wastewater treatment plants, online measurements of parameters such as pH, conductivity and UV254 absorbance, which measures ultraviolet light absorption at 254 nm. An indication of the presence of organic matter, can support predictive process management because they can be monitored continuously and in real time. These parameters can therefore be linked to operational variables such as coagulant dosage, polymer dosage and pH adjustment.

In this project, TOC, UV254 absorbance, conductivity and pH were selected as key input variables for evaluating coagulation and flocculation performance. TOC was used as the primary indicator of organic load, while UV254 absorbance provided additional information regarding aromatic organic compounds. Conductivity was included as an indicator of ionic strength and variations in dissolved substances, which may influence coagulation conditions and chemical demand. Since ferric chloride coagulation is strongly dependent on pH, pH was also considered a critical operational parameter.

In addition to these parameters, SUVA (Specific UV Absorbance) was evaluated as a potential predictor of treatment efficiency. SUVA is calculated as UV254 absorbance divided by TOC and provides information regarding the characteristics of organic matter rather than only its concentration. Higher SUVA values are generally associated with more aromatic and hydrophobic organic compounds, which are often more effectively removed through coagulation. Previous studies have demonstrated that coagulation performance may correlate more strongly with SUVA than with TOC alone (Ghernaout & Elboughdiri, 2013).

3 Methods

Experimental design is described and explained in this section, including the needed tools methods for data collection and procedures for laboratory tests.

3.1. Instruments and Analytical Equipment

The experiments were performed using a FC6S jar test flocculator from VELP Scientifica. TOC concentrations were measured using a Shimadzu TOC-V CPH analyzer, while UV254 absorbance was analyzed using a Shimadzu UV-1800 spectrophotometer. pH, turbidity and conductivity were measured using a VWR pH110 pH meter, a Xylem Turb 430 IR turbidity meter and a VWR HCO 304 conductivity meter.

3.2. Dilution Series for Calibration

To evaluate the accuracy and reproducibility of the TOC measurements, dilution series tests were conducted using wastewater collected from the facility before entering the CFT process. The purpose of the experiments was to compare the manual dilution procedure performed at Chalmers with the automatic dilution procedure used at the company.

The wastewater samples were diluted manually to dilution factors of 1:10, 1:25, 1:50, 1:100, 1:150 and 1:200. TOC concentrations were then measured and compared between the different dilution factors and laboratories to evaluate the measurement uncertainty and calibration differences between the TOC instruments.

3.3 Full-scale Coagulation Evaluation at the Company

After the dilution series experiments, a baseline evaluation of the existing full-scale treatment process was performed. Incoming and outgoing water samples from the CFT facility were collected during 37 sampling days between 9 February and 2 April 2026 while the process was operating under normal full-scale treatment conditions. The samples were analyzed for TOC, turbidity and UV254 absorbance removal. These measurements were used to evaluate the baseline performance and variability of the existing coagulation and flocculation process. All sampling dates and test numbers can be found in Appendix A59–A62.

3.4 Coagulation pH Optimization

Jar tests were conducted to evaluate the effect of pH on ferric chloride coagulation performance. The experiments were performed using ferric chloride with dosages of 1.5 mL/L and 3 mL/L. The pH range tested was between 3.0 and 5.5 with increments of 0.5 pH units across six jar tests. pH was adjusted using sulfuric acid and sodium hydroxide.

The purpose of the experiments was to identify the optimal pH range for ferric chloride coagulation regarding TOC, turbidity and UV254 absorbance removal. All coagulation procedures, mixing conditions and settling times followed the procedure described in sections 3.6 and 3.7.

3.5 Optimization of Polymer Dosing

The polymer experiments were performed after the pH optimization experiments, where pH 4.5 was identified as the target pH for ferric chloride coagulation. Based on the previous experiments, a ferric chloride dosage of 1.5 mL/L wastewater was initially selected for polymer optimization tests.

The polymer used in the experiments was polyacrylamide (PAM) prepared as a 0,1% solution. Polymer dosages between 2.4 and 12 mL were evaluated to investigate the effect of polymer dosage on TOC, turbidity and UV254 absorbance removal in the jar tests.

3.5.1 Effect of Ferric Chloride Dose

Additional jar tests were conducted to evaluate the effect of ferric chloride dosage on treatment performance. The experiments were performed at the target pH of 4.5 using a polymer dosage of 6.4 mL.

Ferric chloride dosages between 0.3 and 1.8 mL/L wastewater were tested with increments of 0.3 mL/L. The purpose of these experiments was to investigate how variations in coagulant dosage influenced the removal of TOC, turbidity and UV254 absorbance. The pH after ferric chloride addition was estimated using drop tests. To ensure consistent pH conditions during the rapid mixing phase, preliminary trials were conducted to determine the amount of acid or base required for each sample, based on its initial pH and coagulant dose. In these pretrials, samples were dosed accordingly, and the necessary volume of acid or base to reach the target pH was recorded empirically. During the actual experiments, the pH was adjusted to the target value using sulfuric acid and/or sodium hydroxide prior to dosing the coagulant.

3.6 Mixing Schemes

The next experiment investigated the effect of different stirring schemes and how these three mixing strategies influenced the efficiency of TOC, absorbance and turbidity removal, while also comparing them to the mixing scheme previously applied in the full-scale process. For jars 5 and 6, the conditions of the full-scale plant were mimicked to evaluate the difference between the currently applied mixing strategy and how an alternative mixing scheme could affect the removal efficiency. In these experiments, 0.9 mL/800 mL ferric chloride and 6.4 mL PAM were used. The mixing rates are presented in Table 1. This experiment provided data regarding the effect of mixing conditions on treatment performance.

Table 1. Mixing conditions used in the experiments.

Jar	Rapid mixing	Slow mixing	Settling time
1 & 2	300rpm 2min	15rpm 20min	30min
3 & 4	45rpm 2min	10rpm 20min	30min
5 & 6	200rpm 2min	-	30min
Previously used mixing	200rpm 2min	45rpm 20min	30 min

3.7 Coagulation and Flocculation Efficiency at Different $FeCl_3$ Doses

After these tests were conducted, all the data required for the experiments investigating different ferric chloride dosages under fixed conditions had been collected. The following 10 experiments consisted of applying optimal mixing techniques, polymer dosages and pH conditions, while using ferric chloride dosage as the only variable. Ferric chloride dosages between 0.3 and 1.8 mL/L were tested with increments of 0.3 mL/L. Wastewater samples were collected from the CFT process and used for the experiments. The sampling and testing procedures were repeated at least ten times to obtain ten different data points for the analysis and conclusions of the thesis. The final experiment compared the optimal dosage and mixing conditions with a simulation of the current full-scale operation to provide a visual comparison for the final presentation. The samples were collected every Tuesday and Thursday between 09:00 and 12:00 during the period from 19 March to 23 April 2026.

3.8 Data Processing

To complement the experimental jar testing, a data driven predictive model was developed in Python using the libraries Pandas, NumPy, Matplotlib and Scikit-learn. The purpose of the model was to investigate whether raw water characteristics could be used to estimate suitable ferric chloride dosages and expected treatment performance. Experimental data from all performed jar tests were exported from Excel and used as input data for the model.
The dataset included ferric chloride dosage, raw water TOC, conductivity, initial pH, SUVA, TOC removal, turbidity removal, absorbance removal, and chemical consumption of sulfuric acid and sodium hydroxide. Before modelling, the dataset was cleaned by removing missing values and converting numerical parameters into consistent formats.

Linear regression was used to investigate the relationship between SUVA and TOC removal for different ferric chloride dosages. Separate regression models were generated for each ferric chloride dosage level according to Equation 2.

$$TOC\ Removal = b_0 + b_1 \cdot SUVA$$

Equation 2. Linear regression model

Here $b_0$represents the intercept and $b_1$the slope of the regression coefficient describing the influence of SUVA on TOC removal.

The predicted TOC removal was further used to estimate the final TOC concentration after treatment according to Equation 3.

$$TOC_{final} = TOC_{initial} \cdot \left(1 - \frac{Removal}{100}\right)$$

Equation 3. TOC concentration after coagulation treatment

To support process optimization, the model also included a simplified chemical minimization strategy. If several ferric chloride dosages resulted in predicted TOC removal values within 4% of the highest achievable removal, the lower chemical dosage was selected. This approach was implemented to reduce chemical consumption, operational cost and environmental impact while maintaining acceptable treatment performance.

The model further included a simplified chemical cost index based on ferric chloride, sulfuric acid and sodium hydroxide consumption. The index was used for relative comparison between dosing strategies rather than absolute economic evaluation.

3.9 Carbon Footprint Estimation

A simple cradle-to-grave carbon footprint assessment (excluding end-of-life treatment) was conducted based on the data described in Section 2.1 in order to summarize the annual chemical consumption and the associated greenhouse gas (GHG) emissions, both under business-as-usual conditions and under the optimal chemical dosages identified in this thesis. The methods used for estimating chemical consumption are discussed further in Section 5.

To calculate the emissions associated with chemical transportation, the following equation was applied (Culture for Climate Scotland, n.d.).

$$kg\ of\ chemical \times emission\ factor = kgCO2e$$

Equation 4. Transport CO_2 calculation

Which later corresponds to the following equation for this case.

$$CO2e = 1000kg \times km \times emission\ factor$$

Equation 5. Applied transport equation

Using the collected data from the company's receipts over a one-year period, transport related emissions were calculated using an emission factor of 958 g CO_2-e per 10 km for large trucks with trailers (Swedish Transport Administration, 2026). The transport distance to the Netherlands, where the chemicals were assumed to be produced, was estimated to be approximately 1000 km.

4 Results

Here all tests are interpreted, and the most important findings are explained.

4.1 Dilution Series

The dilution series was performed to evaluate the uncertainty and accuracy of manual dilution compared to the automatic dilution system used at the facility. Since several wastewater samples exceeded the TOC measurement range of the instrument at Chalmers, manual dilution was required before analysis.

Different dilution factors between 10 and 200 were tested. For each dilution factor, the diluted samples were analyzed and compared to the mean TOC concentration after correction using the dilution factor. The percentage error was calculated as the difference between the measured and the mean TOC concentration.

Each dilution factor was tested four times for both the manual dilution performed at Chalmers and the automatic dilution system at the company. The reported error values represent the average error calculated from these repeated measurements.

Table 2 presents the average percentage error for each dilution factor for both the manual dilution performed at Chalmers and the automatic dilution system used at the company. The overall measurement error remained relatively low for most dilution factors. The error values presented are average errors calculated from four repeated measurements for each dilution factor. The total average error was 7.7% for the manual dilution performed at Chalmers and 9.6% for the automatic dilution system at the company. However, the dilution factor of 150 at the company showed a significantly higher error compared to the other dilution factors. Since most dilution factors resulted in relatively low deviations, the results indicate that manual dilution could be used for the jar tests without significantly affecting the TOC measurements. These results indicate that the pre-dilution procedure performed in the company's system was functioning as intended.

Table 2. TOC measurement error for different dilution factors.

Dilution Factor	Average Error [%] (Chalmers)	Error [%] (The Company)
10	8.082	8.430
25	3.706	0.910
50	9.577	8.460
100	8.643	2.160
150	10.131	34.360
200	6.284	3.140
Error [%]	7.737	9.577

4.2 Effect of pH on Performance and Efficiency

Jar tests were conducted to evaluate the effect of pH on coagulation performance using a fixed ferric chloride dose of 1.2 mL. The results shown in Figure 3 indicate that the optimal pH range for TOC, absorbance, and turbidity removal was between pH 4 and 5, which is consistent with the findings presented in Section 2.5 of the literature review.

Within this pH interval, TOC removal varied between approximately 30% and 35%, while absorbance removal ranged between approximately 51% and 69%. In contrast, turbidity removal remained consistently high between approximately 95% and 99% across all tested pH levels. These results indicate that pH had a greater influence on TOC and absorbance removal than on turbidity removal.

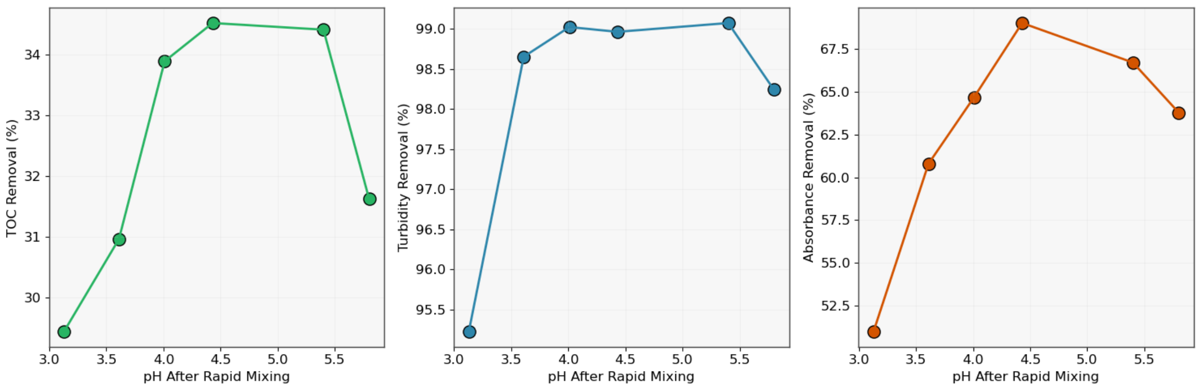

Figure 3. Effect of pH on treatment performance at 1.2 mL/L $FeCl_3$.

For the second pH experiment, the ferric chloride dose was doubled (2.4mL) to investigate whether the optimal pH range was similar at higher coagulant dosage. The results indicated that treatment performance was overall highest at pH 4 with an upgoing trend for all data points, as seen in Figure 4. Despite a higher dose the optimal pH followed a trend. The TOC removal decreased above pH 4.

This work showed that ferric chloride coagulation performed most efficiently at a targeted pH of approximately 4.5, with an operational margin of ±0.5. This suggested maintaining a pH range between 4 and 5 for optimal treatment performance considering all tests. In comparison, the company's system targeted a pH reduction to approximately 4 prior to the addition of ferric chloride.

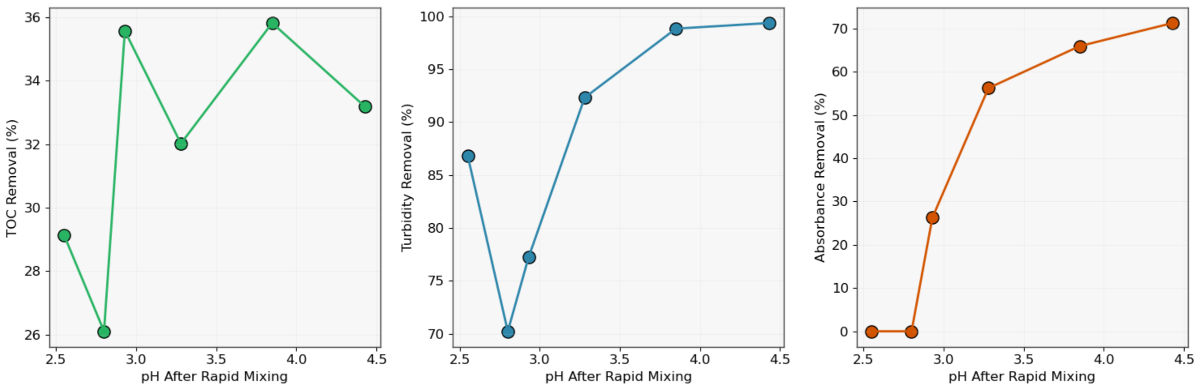

Figure 4. Effect of pH on treatment performance at 2.4 mL/L $FeCl_3$.

4.3 Optimizing Polymer Dosage

For the first polymer experiment, the role of polymer as both a supporting flocculant and as a standalone treatment chemical was evaluated. As shown in Figure 5, the tests using only polymer without ferric chloride resulted in significantly lower TOC, turbidity and absorbance removal compared to the tests where ferric chloride was included. The tests using 4 mL polymer and no ferric chloride achieved TOC removals of approximately 14%, while the combined ferric chloride and polymer tests achieved removals close to 40%. Similar differences were observed for turbidity and absorbance removal. This indicates that the polymer alone is not sufficient as a primary coagulant and mainly functions as a supporting flocculant in combination with ferric chloride. These findings correlate with the literature presented in section 2.7.

When evaluating increasing polymer dosages together with ferric chloride, shown in Figure 5, higher polymer dosages resulted in gradual improvements in TOC removal. TOC removal increased from approximately 47% at 2.4 mL polymer to approximately 59% at 12 mL polymer. However, the improvement became increasingly limited at higher polymer dosages, indicating that the treatment performance approached a plateau rather than continued proportional improvements. At the same time, turbidity removal slightly decreased under overdosing conditions. This may indicate the presence of residual polymers in the treated water, which is undesirable before the biological treatment step due to potential negative effects on bacterial activity.

Because the polymer (PAM) dosages of 4 mL and 6.4 mL achieved relatively similar TOC, turbidity and absorbance removal compared to higher dosages, these levels were selected for the following experiments. Lower polymer dosage was preferred due to lower chemical consumption, reduced environmental impact and lower risk of residual polymer remaining in the treated water.

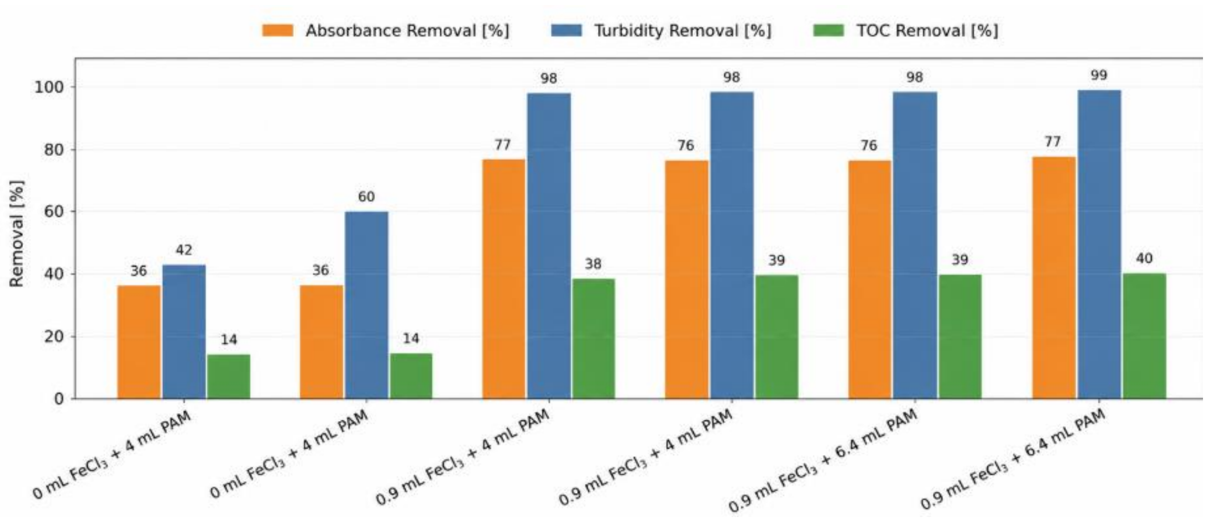

Figure 5. Effect of polymer dosage on treatment performance.

For the second polymer experiment, the effect of polymer dosage was further evaluated together with different ferric chloride conditions, shown in Figure 6. The tests using ferric chloride together with polymer resulted in substantially higher TOC, turbidity and absorbance removal compared to the tests using polymer alone. The tests with 4 mL and 6.4 mL polymer showed relatively similar treatment performance, while the differences between these dosages remained limited for all measured parameters.

The results further support that polymer mainly acts as a supporting flocculant rather than a standalone coagulant. Lower polymer dosages achieved treatment results similar to the higher dosages. Therefore, a lower polymer addition is preferable due to lower chemical consumption, reduced carbon footprint and lower risk of residual polymers leaving the treatment step.

The absorbance removal remained relatively stable above approximately 85% throughout the polymer experiments and was therefore not further prioritized in the following optimization tests.

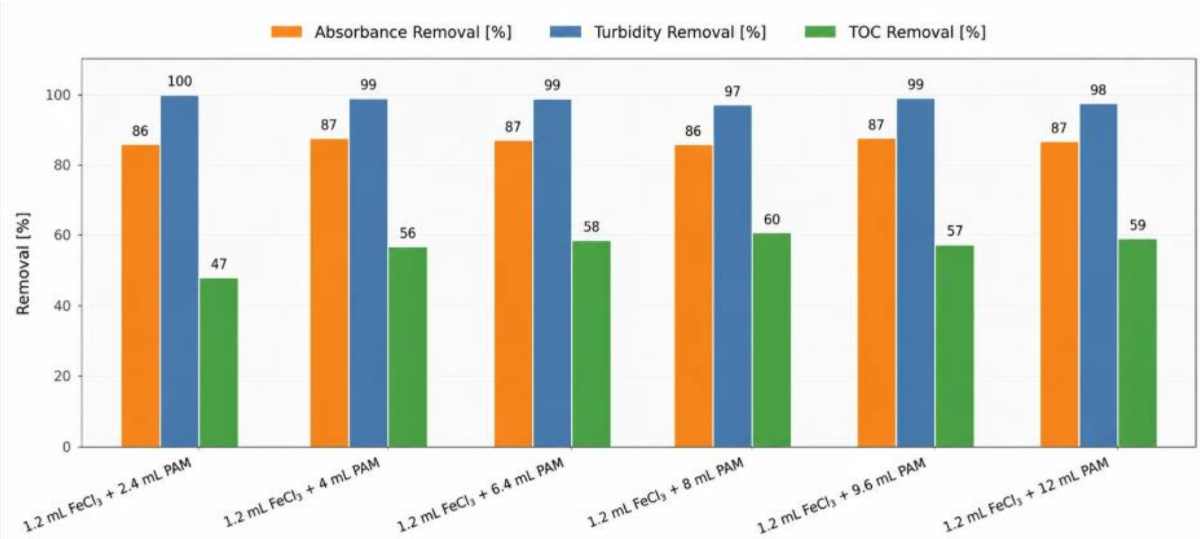

Figure 6. Polymer dosage combined with ferric chloride coagulation.

4.4 Impact of Mixing Conditions

The mimicked mixing of the current state, in the full-scale plant as described in section 1.3, in the test called “200rpm”. As seen in Figure 7 below, this test does not differ substantially from the test called “300 → 15 rpm” nor the test “45 → 10 rpm” which all resulted in a TOC removal of 10 to 15%. On the other hand, the test called “Optimal mixing” which used a rapid mixing of 300 rpm in 2 minutes to a slow mixing in 20 minutes and a settling time of 30 minutes had significantly higher removal of about 46% TOC removal. This indicates that the mixing highly affects the TOC removal and is important to consider in the final testing when comparing the result. This test was constructed to try to include all variables of the coagulation and flocculation process, and their effects towards the end goal of reducing TOC.

The current state is represented by the test labeled “200 rpm” which can be found in the figure 7 below. This test does not differ significantly from the test labeled “300 → 15 rpm” or “45 → 10 rpm” regarding TOC removal of approximately 10-15%.

In contrast, the test labeled as “Optimal mixing” which used rapid mixing at 300 rpm for 2 minutes followed by slow mixing for 20 minutes and a settling time of 30 minutes, achieved a significantly higher TOC removal of about 46%.

These results highlight the importance of using “optimal mixing” strategy, indicating that the mixing conditions have a strong influence on TOC removal and should be prioritized for the final testing.

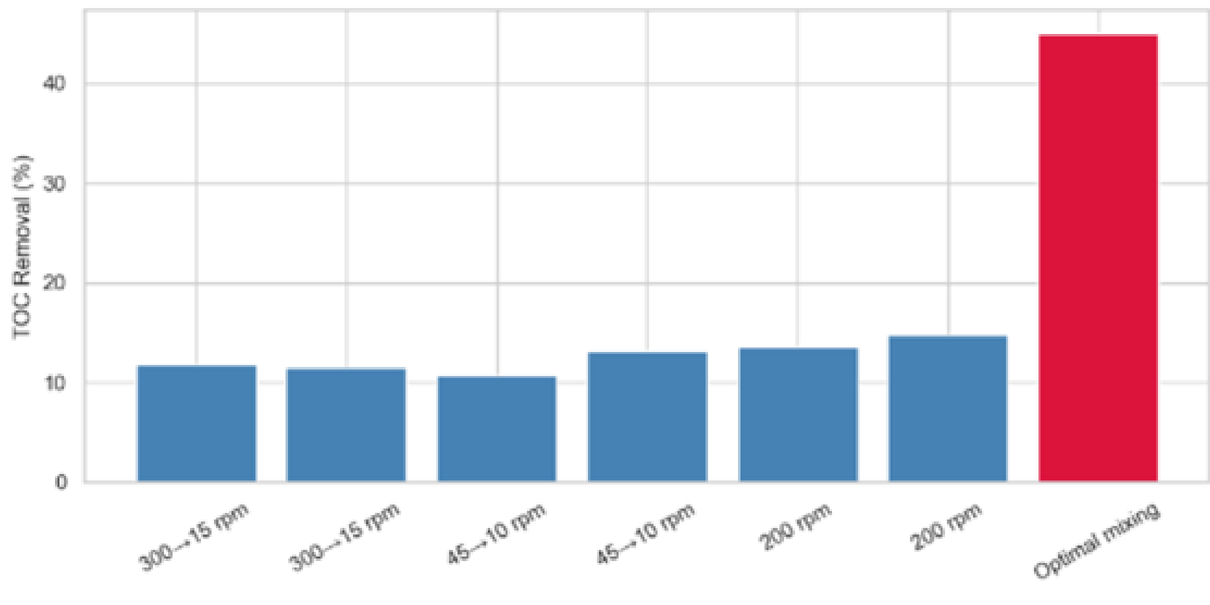

Figure 7. Effect of mixing schemes on TOC removal.

4.5 Baseline Performance and Variability

When evaluating the incoming and outgoing water at the company, the TOC removal exhibited substantial variability over the sampling period, as shown in Figure 8. The TOC removal ranged from approximately −140% up to nearly 80%. Several negative TOC removal values were observed during the baseline measurements, particularly during sample days with incoming TOC concentrations above approximately 1200 mg/L. Negative TOC removal indicates that the measured TOC concentration after treatment was higher than the incoming TOC concentration. This may suggest negative impact of coagulation under certain wastewater conditions, release of dissolved organic matter during treatment, or variations in sampling and process conditions during full-scale operation. The results indicate that variations in incoming wastewater characteristics can significantly influence the treatment performance under the current operating conditions.

In contrast, the turbidity removal shown in Figure 9 remained relatively stable during most sample days. Most measurements achieved turbidity removals between approximately 80−97%. However, some deviations were observed, including one measurement close to 0% removal around 1000 mg/L TOC and several measurements below 60% at higher incoming TOC concentrations.

The absorbance removal at 254 nm, presented in Figure 10, also showed more stable behavior compared to TOC removal. Most absorbance removal values ranged between approximately 45−75%. Despite this, several lower removal values below 30% were observed, particularly at incoming TOC concentrations above approximately 1300 mg/L. This indicates that UV-absorbing organic compounds became more difficult to remove during certain periods with higher organic loading.

Figure 8 further illustrates the fluctuations in TOC removal over time and highlights the unstable treatment performance during several sampling dates. While some measurements achieved removals above 50%, other dates resulted in strongly negative TOC removal values. Together, these results demonstrate that the current treatment process lacks sufficient adaptability to handle the large variations in incoming industrial wastewater quality.

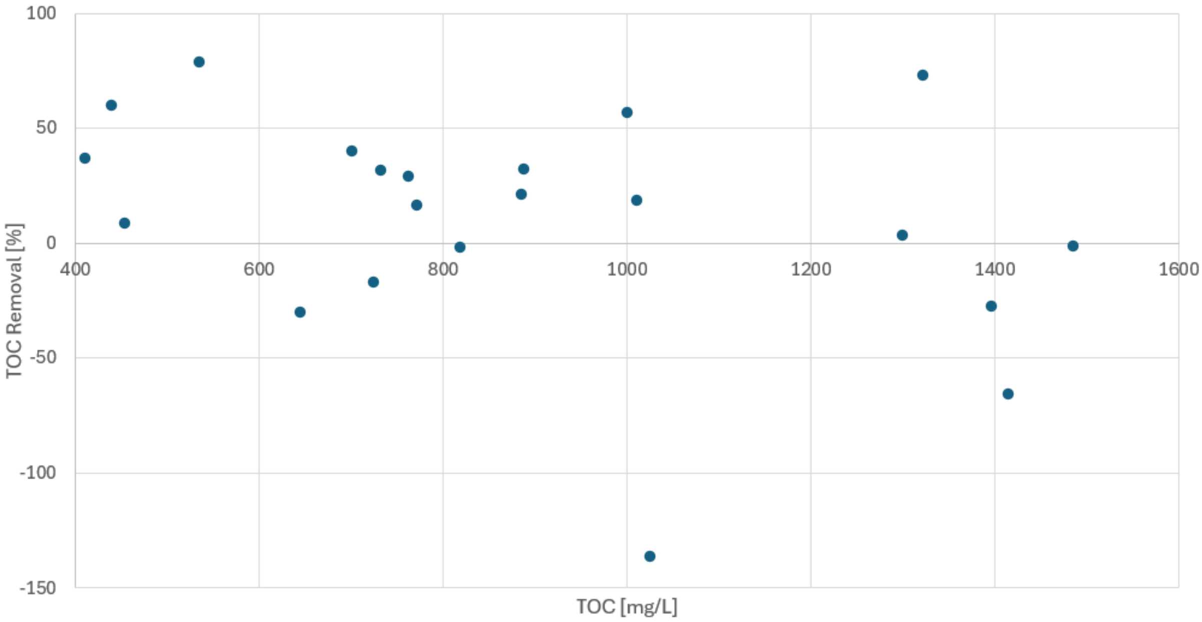

Figure 8. TOC removal during baseline operation.

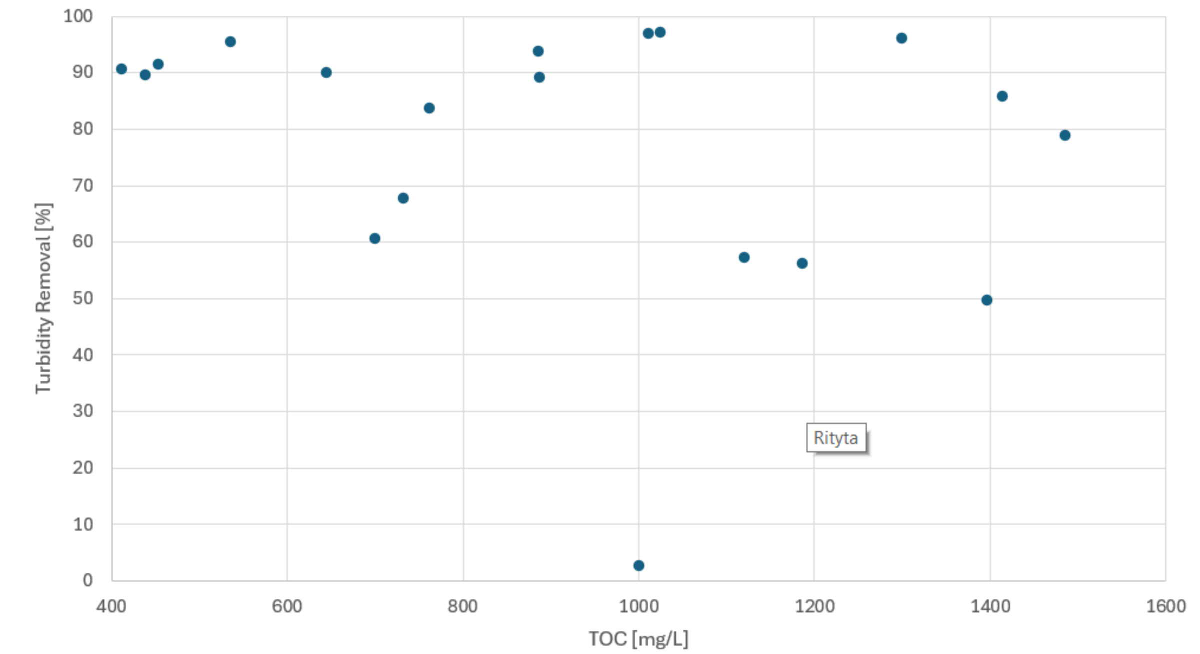

Figure 9. Turbidity removal during baseline operation.

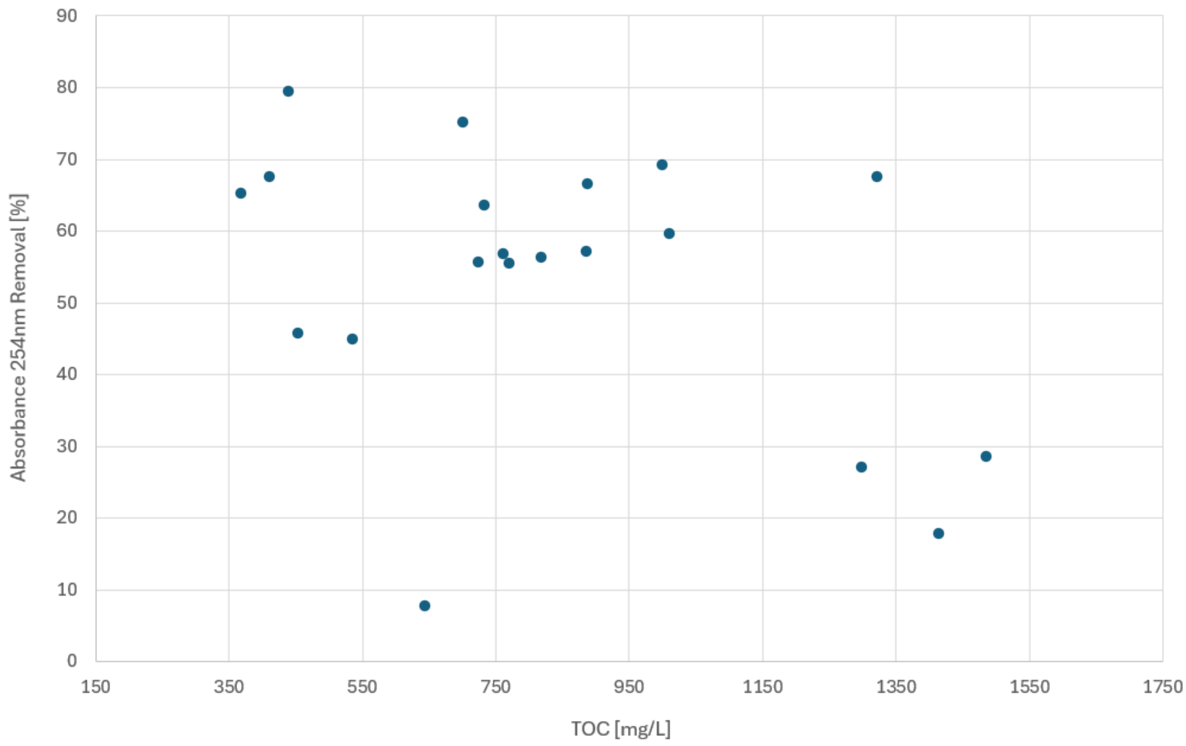

Figure 10. UV254 absorbance removal during baseline operation.

Figure 11 illustrates the variation in incoming and outgoing TOC concentrations during the sampling period. Large fluctuations were observed both in the incoming wastewater quality and in the achieved TOC removal, which is consistent with the results presented in Figure 8.

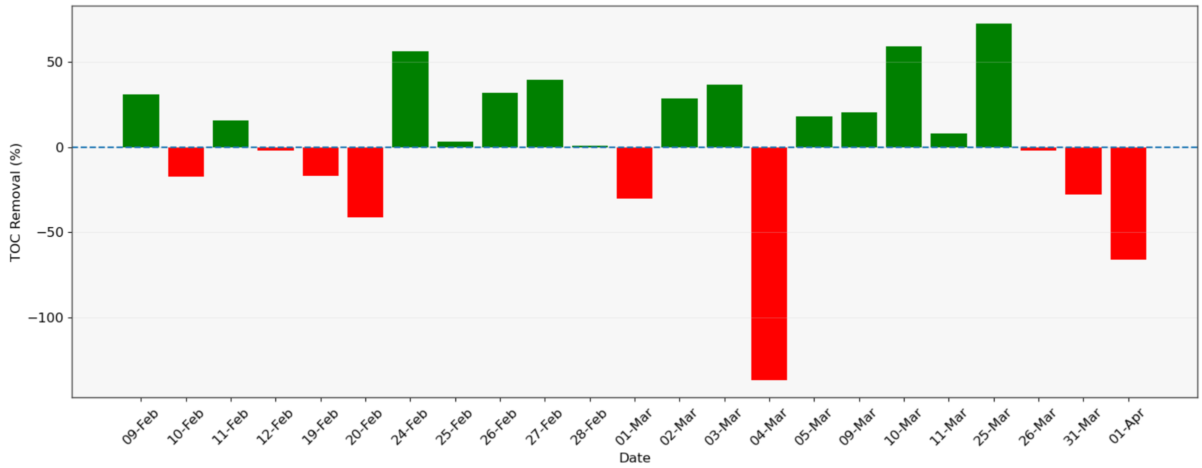

Figure 11. Incoming and outgoing TOC during baseline sampling.

4.6 Effect of Ferric Chloride on Removal Efficiency

For all jar tests, the removal of TOC, turbidity and absorbance varied depending on the characteristics of the raw water. The results from one raw water sample are presented in Figures 12-14, while all conducted jar tests are presented in Appendix A1–A33 together with the corresponding sampling dates and test numbers.

The results demonstrated that increasing ferric chloride dosage generally improved the TOC removal efficiency. However, the improvement observed between certain dosage levels was relatively limited compared to the corresponding increase in chemical consumption. For the raw water sample presented in Figures 12–14, a ferric chloride dosage of 1.5 mL achieved the highest overall removal performance in terms of TOC, turbidity and absorbance.

Despite this, lower dosages such as 0.9 mL and 1.2 mL also achieved relatively similar removal efficiencies in several experiments while requiring lower amounts of ferric chloride, sulfuric acid and sodium hydroxide. This indicates that the selection of an optimal dosage may depend not only on the targeted removal efficiency but also on operational factors such as chemical consumption, treatment costs and environmental impact.

These observations were further considered during the development of the Python prediction tool, where lower chemical dosages were prioritized when the predicted treatment performance remained close to the maximum achievable removal efficiency.

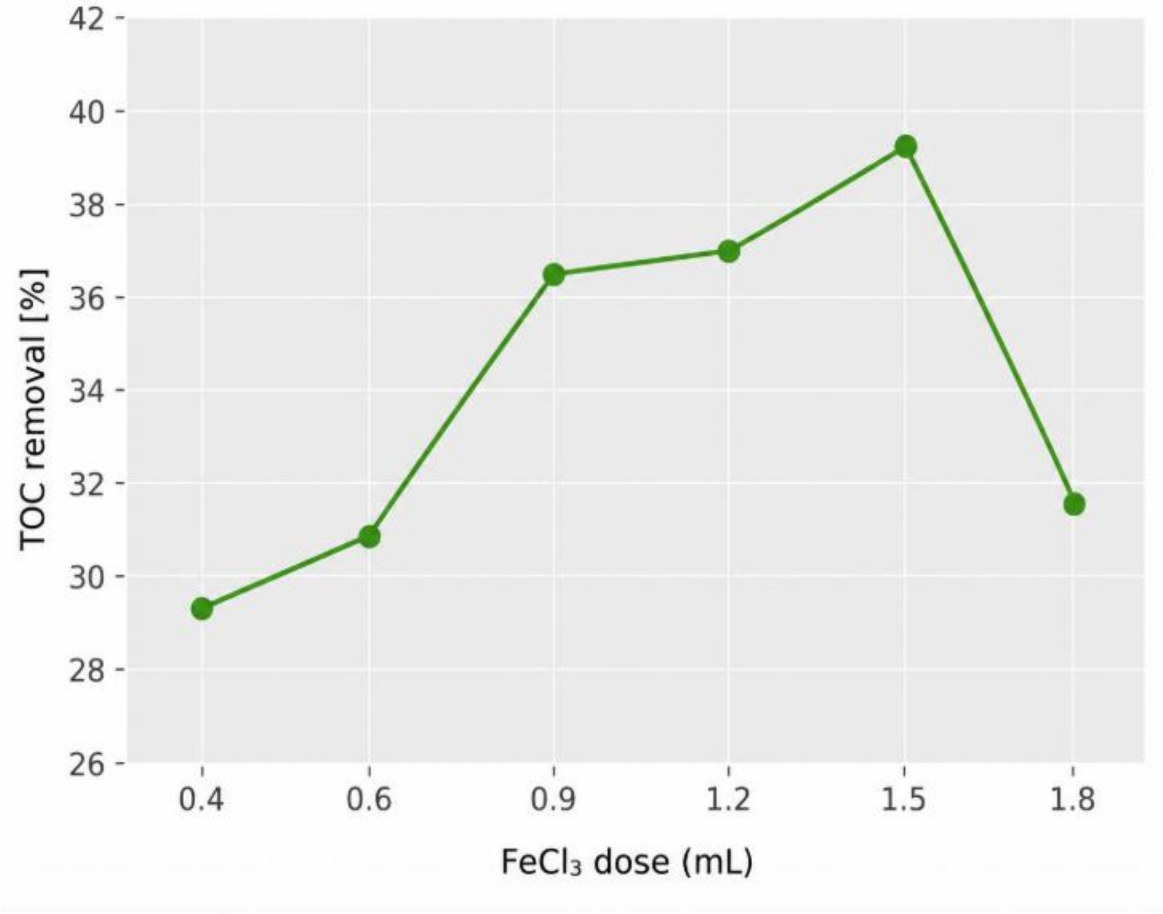

Figure 12. Effect of $FeCl_3$ dosage on TOC removal.

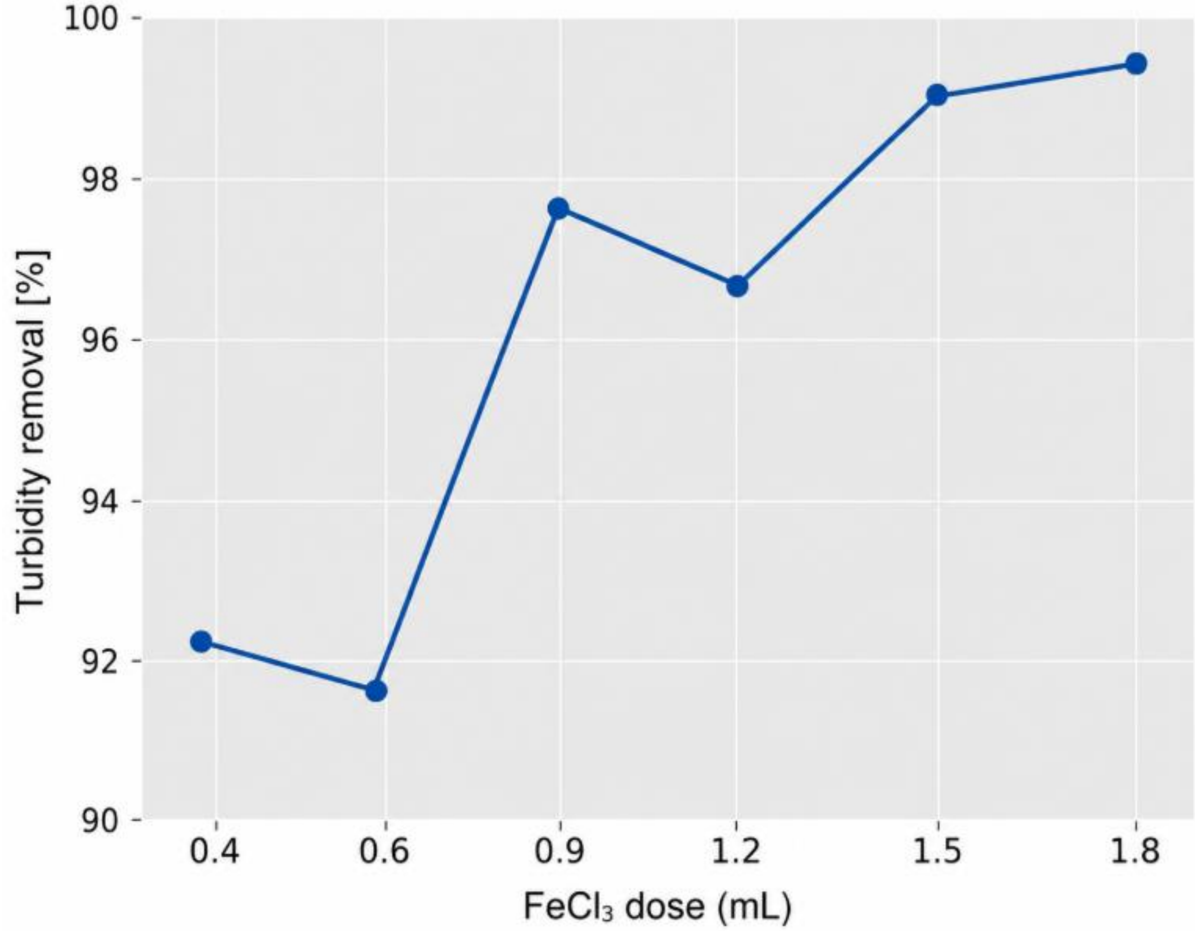

Figure 13. Effect of $FeCl_3$ dosage on turbidity removal.

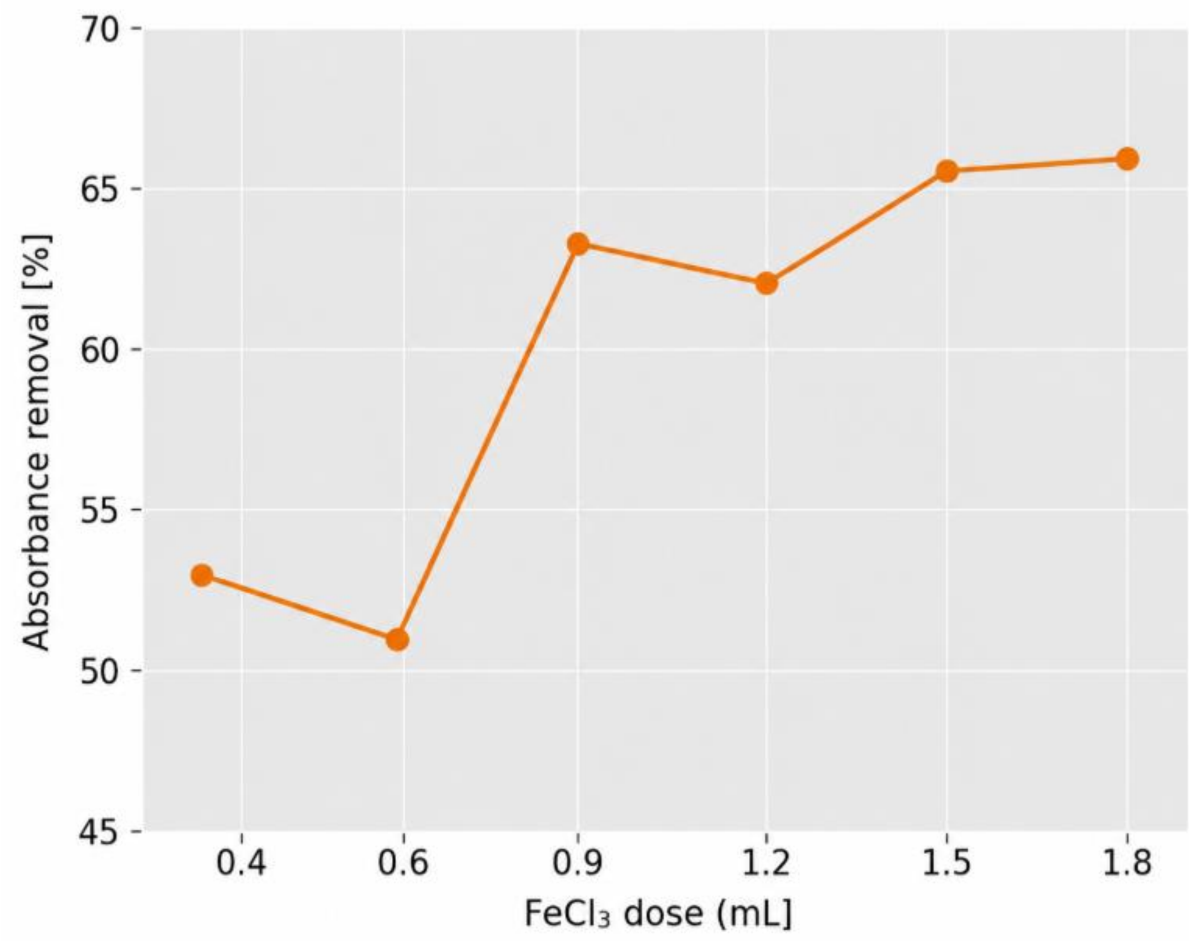

Figure 14. Effect of $FeCl_3$ dosage on UV254 absorbance removal.

4.7 Correlations Between Raw Water Parameters

When plotting the relationships between TOC/absorbance, TOC/turbidity, and absorbance/turbidity, R^2 values slightly above 0.5 were obtained, indicating moderate trends but not strong linear correlations (Figures 15, 16 & 18). In contrast, the relationships between TOC/conductivity, absorbance/conductivity, and turbidity/conductivity showed weak or no clear linear trends. The R^2 values for these parameter combinations did not exceed 0.35, indicating poor linear correlations (Figures 17, 19 & 20). This suggests that conductivity has limited influence on the relationships between the measured parameters.

Overall, the R^2 values and linearity of the graphs were not strong enough to provide reliable input data for the predictive Python model. Nevertheless, some moderate relationships between specific parameters could still be observed, particularly for TOC, absorbance, and turbidity.

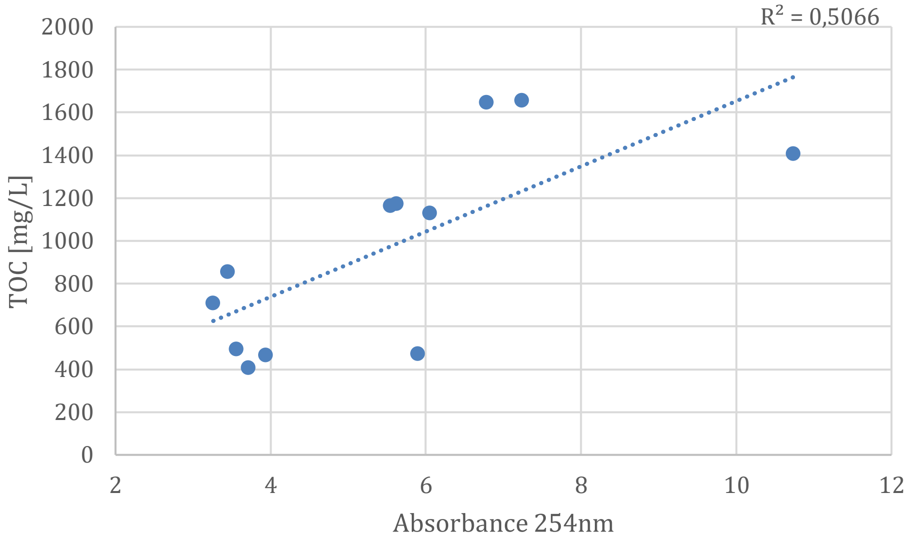

Figure 15. Correlation between TOC and UV254 absorbance.

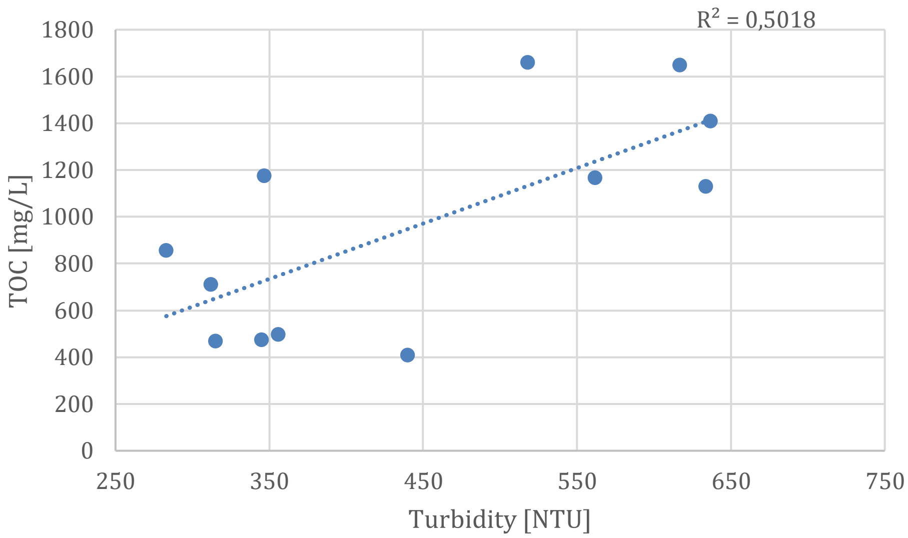

Figure 16. Correlation between TOC and turbidity.

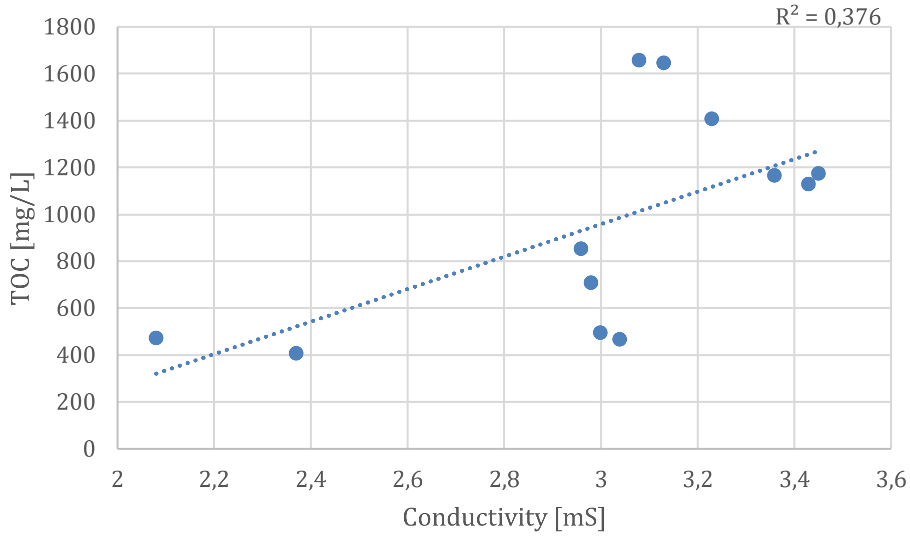

Figure 17. Correlation between TOC and conductivity.

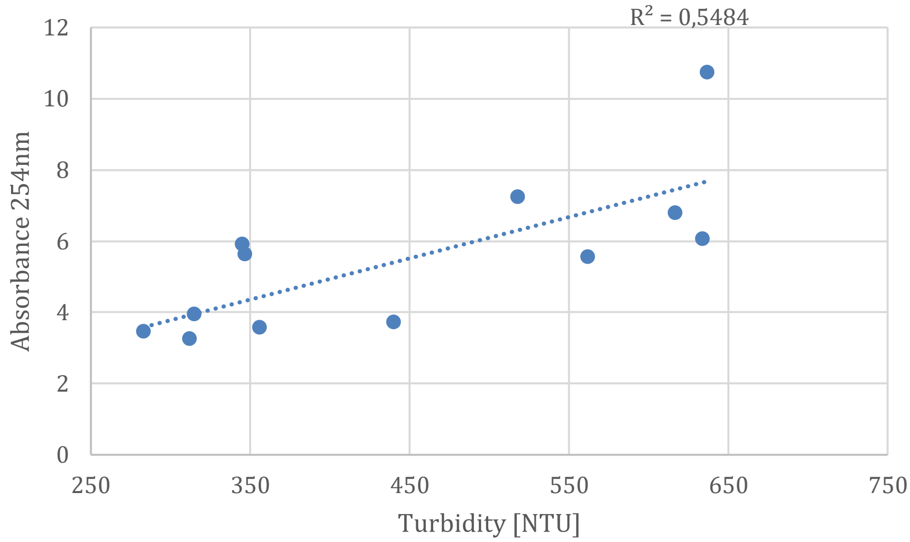

Figure 18. Correlation between UV254 absorbance and turbidity.

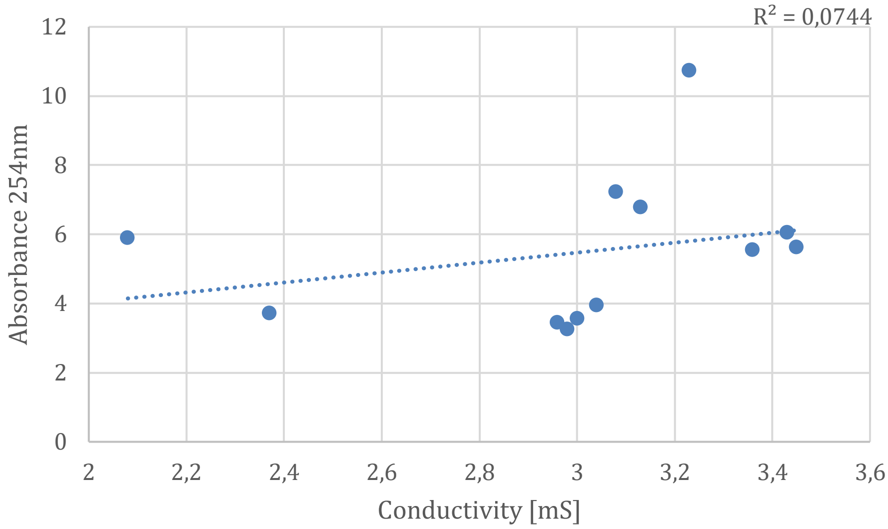

Figure 19. Correlation between UV254 absorbance and conductivity.

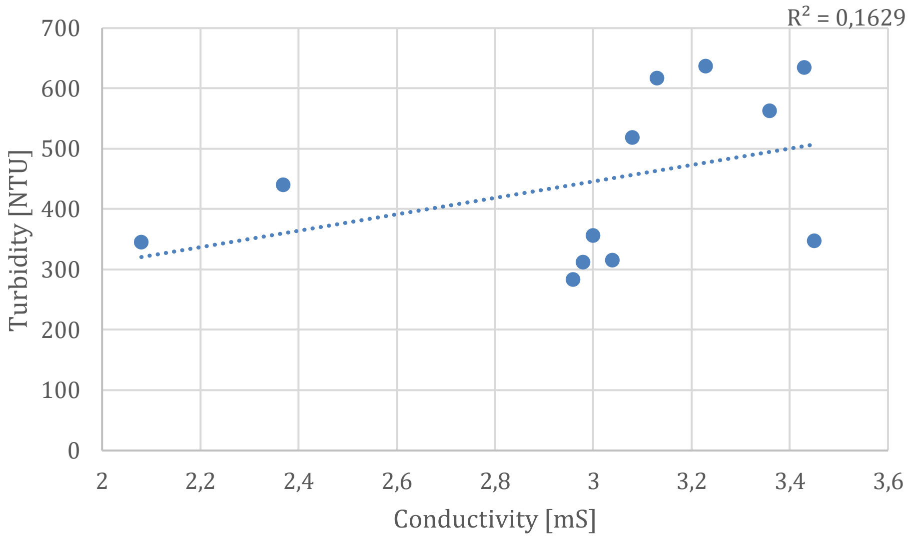

Figure 20. Correlation between turbidity and conductivity.

4.8 SUVA as a Predictor

Initially, in relation to coagulation outcome, ferric chloride dosage and raw water parameters such as TOC, absorbance, turbidity and conductivity were evaluated. No clear linear relationships were observed between these parameters and treatment performance, and these results were therefore not considered suitable for the predictive model considering a low R^2 value. The corresponding figures are presented in Appendix A34 – A57.

When SUVA was evaluated instead of TOC concentration alone, clearer trends could be observed for TOC removal at several ferric chloride dosages. As shown in Figure 21, higher SUVA values were generally associated with increased TOC removal at 0.3 mL/L $FeCl_3$. Similar trends were observed for several additional ferric chloride dosages in Appendix A34 – A57.

In contrast, the relationships between SUVA and UV254 absorbance removal (Figure 22) as well as turbidity removal (figure 23) were weaker and less consistent. The results therefore indicate that SUVA may be more useful for predicting TOC removal than for predicting turbidity or absorbance removal. Based on these results, SUVA was included as an input parameter in the predictive Python model.

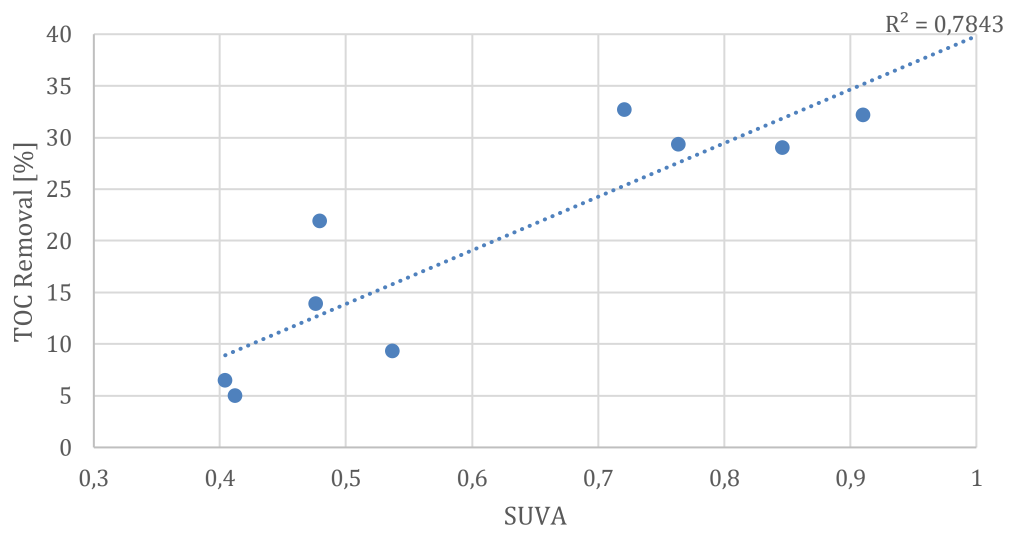

Figure 21. SUVA and TOC removal at 0.3 mL/L $FeCl_3$.

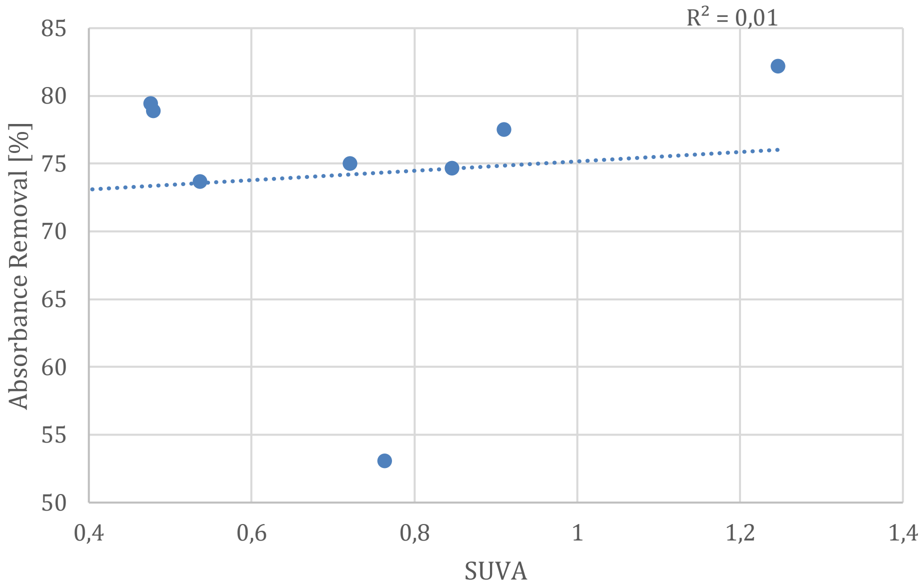

Figure 22. SUVA and UV254 absorbance removal at 0.3 mL/L $FeCl_3$.

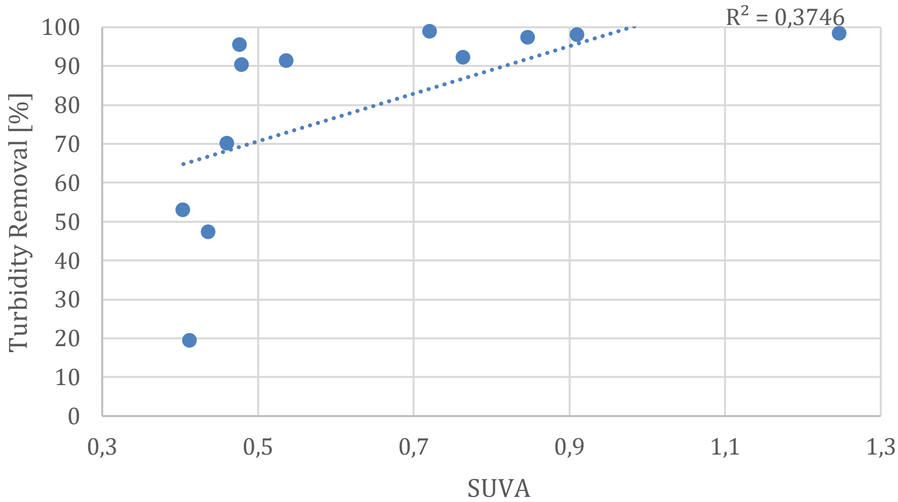

Figure 23. SUVA and turbidity removal at 0.3 /L $FeCl_3$.

4.9 Predictive Models Developed in Python

To complement the jar testing, Python was used to develop simplified predictive models for ferric chloride coagulation performance based on measurable raw water characteristics. The purpose was to investigate whether treatment performance could be estimated using incoming water quality parameters and thereby support more adaptive dosing strategies.

Separate linear regression models were developed for different ferric chloride dosages using SUVA as the predictor variable and TOC removal as the response variable. The results indicated that SUVA showed clearer trends and stronger linear relationships to TOC removal compared to raw TOC concentration alone, suggesting that the composition of organic matter may be important when estimating coagulation performance.

The predictive models generally indicated that higher SUVA values corresponded to higher TOC removal efficiencies. This suggests that wastewater containing larger fractions of aromatic and hydrophobic organic matter may be easier to treat using ferric chloride coagulation.

The Python model was further combined with a simplified chemical minimization strategy. Instead of only maximizing TOC removal, the model prioritized lower ferric chloride dosages when the predicted treatment efficiency remained within 4% of the highest predicted removal. This approach allowed the model to identify dosing strategies with lower estimated chemical consumption while maintaining similar predicted treatment performance.

The model also estimated final TOC concentrations after treatment and compared relative chemical cost indices between dosage levels. The results indicated that lower ferric chloride dosages could, in several cases, achieve similar predicted removal efficiencies compared to higher dosages while reducing estimated chemical consumption, operational cost and environmental impact. However, the predictive capability of the model was limited by the relatively small dataset and the simplified linear regression approach. Therefore, the model should primarily be considered an exploratory decision support tool rather than a fully validated predictive model. Nevertheless, the results indicate potential for using measurable raw water parameters to support adaptive coagulation control strategies under varying wastewater conditions.

4.10 Carbon Footprint

When calculating the current chemical consumption, costs and total specific chemical emissions per year based on the present dosing strategy, Table 3 shows that the primary contributor to greenhouse gas (GHG) emissions is the consumption of NaOH. Further discussion regarding the potential reduction of NaOH and H_2SO_4 consumption is presented in Section 5. The results indicate that NaOH has the highest environmental impact, followed by ferric chloride and lastly H_2SO_4. All data and calculations are presented in Appendix A.58.

Table 3. Annual chemical consumption, cost and CO2 emissions.

	Consumption/ year [kg]	Cost/ year [SEK]	Emission factor (kg CO_2-e/kg)	Total kg CO_2e/year
NaOH	40600	216720	0.915	37260.128
H_2SO_4	12240	58644	0.122	1590.996
$FeCl_3$	23415	101939.25	0.803	18909.062

5 Discussion

This section considers the current coagulation and flocculation process in the context of the experimental results highlighting all conditions which were tested and how they affect the treatment process.

This study aimed to provide information regarding how variations in incoming raw water quality affect the performance of the coagulation and flocculation process, and how the process at the facility can be improved using both data driven and experimental approaches. To summarize the findings, the results indicate that the current process is not sufficiently stable considering the variability of the incoming industrial wastewater, and that the current dosing strategies are not adequately adapted to these variations. This is demonstrated in Section 4.5, Baseline Performance and Variability

The results presented in Section 4 clearly demonstrate that the current treatment performance varies depending on the raw water conditions. The baseline results show substantial variations in TOC removal, ranging from high removal efficiencies to cases where the removal was very low or even negative. This strongly indicates that the current dosing strategy is neither consistently effective nor always optimal for the incoming wastewater and its corresponding treatment demand. However, turbidity removal remained relatively high and stable throughout most experiments, suggesting that Particulate Organic Carbon (POC) removal is less sensitive to process variations than Dissolved Organic Carbon (DOC) removal. This highlights that DOC removal is more complex and more dependent on coagulant and polymer dosage. These observations are consistent with general wastewater treatment principles described by Tchobanoglous et al. (2014).

One important finding throughout all experiments was the strong influence of pH on treatment performance depending on the coagulant applied. The pH-based experiments demonstrated that the highest TOC and absorbance removal occurred within a pH range between 4 and 5, with an optimal peak around pH 4.5. This confirms that pH is a critical control parameter in coagulation processes.

The results from the pH experiments are consistent with expectations based on previous literature, which describes ferric chloride coagulation as strongly pH dependent due to the formation of hydrolyzed iron species that control particle destabilization and adsorption mechanisms (Bratby, 2016). In practical terms, this indicates that pH adjustment represents one of the most effective strategies for improving coagulation efficiency while reducing unnecessary chemical consumption. However, this also represents one of the most complex aspects of the system due to variations in the incoming water, which possesses different acid and base buffering capacities. A positive finding is that the effective coagulation range extended between pH 4 and 5 rather than consisting of only one optimal value. Consequently, increasing chemical dosage without controlling pH conditions will not result in optimal treatment performance.

At the facility, the current operational strategy involves reducing the pH to approximately 4 prior to ferric chloride addition. Since ferric chloride itself is acidic, its addition further decreases the pH, often below the optimal coagulation range identified in this study. This may result in less efficient coagulation conditions and unnecessary chemical consumption. The results therefore indicate that pH control should not only focus on the initial pH adjustment but should also account for the additional pH reduction caused by ferric chloride dosing. Increasing chemical dosage without controlling the resulting pH will therefore not lead to optimal performance.

The mixing experiments demonstrated that optimized mixing conditions, consisting of rapid mixing followed by slower mixing and subsequent settling, significantly improved TOC removal. When simulating conditions similar to the current process, where chemicals are added from the side of the tank, a mixing speed of 200 rpm was used, resulting in vortex formation. The slower rapid- and slow mixing strategies also produced results similar to those obtained using the vortex mixing scheme.

These observations are consistent with findings in the literature stating that proper mixing is essential for effective coagulation (Bratby, 2016), where rapid chemical dispersion followed by controlled floc growth is required to achieve optimal treatment performance. Insufficient mixing is likely to result in uneven chemical distribution and weaker floc formation.

Polymer experiments demonstrated that polymers could improve the treatment process. However, the effect was relatively limited compared to the influence of pH and mixing conditions. The polymer dosage showed no theoretical upper limit for TOC removal (Bolto & Gregory, 2007), but as the polymer dosage increased beyond optimal levels, the turbidity removal decreased. This may result in residual polymers entering the subsequent biological treatment stage, potentially affecting the bacteria on which the process depends. According to previous research, polymers can enhance floc formation, but overdosing may not only reduce turbidity removal efficiency but also increase unnecessary operational costs, as discussed in Section 2.7 (Polymers as a Coagulation Aid). This highlights that polymer addition should primarily be considered a supporting measure rather than the main treatment solution. The second polymer experiment further supports this observation, as it resulted in significantly lower TOC, absorbance and turbidity removal compared to the experiments where polymers were applied as a coagulation aid (Section 4.3).

Another important observation was the role of SUVA in treatment performance. The results demonstrated that SUVA exhibited a stronger relationship with TOC and turbidity removal than TOC concentration alone. This suggests that coagulation performance was influenced not only by the quantity of organic matter present in the wastewater but also by its composition. The findings further indicate that treatment performance cannot be reliably predicted using only a single parameter such as TOC.

The Python modelling approach is supported by these findings, as the model links raw water parameters such as TOC, pH, conductivity, absorbance and SUVA to treatment performance. Although the number of data points was limited, the model demonstrates that it is possible to identify treatment trends and estimate coagulant dosage based on these input conditions. According to these results, the facility could improve its process performance by implementing data driven strategies that adapt to variations in raw water quality. Instead of applying fixed dosing conditions, an adaptive strategy could be adjusted continuously depending on the characteristics of the incoming wastewater. This could improve process stability while simultaneously reducing unnecessary chemical consumption (Zamfir et al., 2025).

The results further demonstrated that higher ferric chloride dosages often resulted in slightly improved removal efficiencies, although the differences compared to lower dosages were relatively small. This implies, and is implemented within the Python model, that similar treatment performance can often be achieved using lower coagulant dosages. The results also showed that turbidity increased during overdosing conditions, resulting in orange colored water containing higher amounts of unused ferric chloride.

When evaluating the cost and carbon footprint associated with ferric chloride consumption, the results indicate that the environmental impact may either increase or decrease depending on the selected dosage. However, the current full-scale process applies a fixed dosage of 1.2 mL/800 mL for relatively “easy-to-treat” wastewater, while this dosage is often doubled for more difficult wastewater streams. This suggests that all evaluated optimization cases have the potential to reduce both carbon footprint and operational costs when applying predictive Python modelling. Furthermore, by targeting a pH value of 4.5 after ferric chloride addition, the consumption of sulfuric acid could be significantly reduced for many wastewater types and, in some cases, potentially eliminated entirely when the desired pH is achieved using ferric chloride alone. This remains dependent on the incoming wastewater characteristics but is expected to result in an overall reduction in sulfuric acid usage. Similarly, lower amounts of sodium hydroxide may be required to increase the pH back to 7 due to the higher initial pH values applied, although this also depends strongly on the incoming water quality.

These findings are highly relevant from both economic and environmental perspectives, since reducing coagulant consumption also lowers operational costs. In addition, reduced sludge production may indirectly decrease environmental impacts associated with sludge management. This is consistent with sustainable treatment strategies and circular approaches, including the reuse of treatment residuals (Ahman et al., 2016).

Overall, the results indicate that the primary limitations of the current process are not only related to the quantity of chemicals used but also to the system's limited ability to adapt to changing raw water conditions. This results in unstable treatment performance and inefficient chemical consumption. The study demonstrates that coagulation and flocculation performance can be improved by combining dosing at appropriate pH conditions, optimized mixing strategies, selective polymer usage and adaptive, data driven dosing based on incoming raw water quality. These improvements have the potential to increase process stability while reducing chemical consumption and improving cost efficiency, thereby lowering environmental impact without compromising treatment performance.

6 Outlook

During the project, several opportunities for further development were identified. These improvements could increase treatment efficiency and strengthen the reliability of the results.

One important area for future improvement is the implementation of adjustable mechanical mixing systems within the existing treatment process. The current setup relies primarily on turbulence generated during chemical addition, which limits the control of coagulation and flocculation conditions. Future studies should therefore investigate optimized mixing systems where both rotational speed and mixing duration can be controlled in order to improve process stability and treatment efficiency. According to Edzwald (2011), controlled mixing conditions are essential for achieving stable coagulation performance.

Another potential improvement could involve connecting the treatment steps in series, similar to conventional drinking water treatment plants. Instead of evaluating coagulation as a single batch process, the treatment system should be investigated together with sedimentation, filtration and final polishing stages. Many modern treatment plants combine several treatment operations in order to maximize the removal of turbidity, dissolved organic matter and suspended solids (CDC, 2024).

Conducting additional experiments under varying raw water conditions would improve the reliability of the predictive models developed in Python. Furthermore, closer collaboration with industrial partners would allow the process to be evaluated under more realistic operating conditions, including varying flow rates, storage limitations, sludge handling capacity and target water quality requirements.

Another promising approach is the use of polymer as coagulation aid. Many treatment plants apply polymers together with ferric chloride or aluminuim in order to improve floc formation, increase settling velocity and reduce the required coagulant dosage. According to Bolto and Gregory (2007), polymer additives can significantly improve separation efficiency and sludge dewatering. Future experiments could therefore investigate whether polymer addition can reduce ferric chloride consumption while maintaining effective TOC and turbidity removal.

A more circular solution would involve reusing sludge from drinking water treatment plants as a coagulation or flocculation aid. Residual sludge from water treatment facilities often contains aluminium or iron hydroxides that still possess adsorption and coagulation properties. Several studies have demonstrated the reuse of such sludge for phosphorus removal, turbidity reduction and wastewater treatment applications (Ahmad et al., 2016). Reusing these residual materials could reduce the demand for virgin chemicals and support more circular resource management strategies.

Overall, these improvements could transform the current process from a relatively simple settling system into a more efficient, scalable and sustainable treatment solution.

Finally, the implementation of real time monitoring and automated dosing systems represents an important future development opportunity. By combining online sensors with predictive models, the treatment process could continuously adapt to changing wastewater conditions.

7 Conclusion

Here we describe how the coagulation and flocculation process at the facility is affected by variations in the raw water quality. Possible improvements to the current system and answers to the research questions are provided with the aim of increasing treatment cost efficiency, stability and sustainability.

The aim of this thesis was to investigate how variations in incoming raw water quality affect coagulation and flocculation performance, and how the process can be improved to reduce chemical consumption, increase cost efficiency and lower environmental impact without compromising treatment performance.

Regarding Research question 1, the study identified several operational parameters that influenced treatment performance under varying wastewater conditions. pH was found to be the most influential factor, where the optimal treatment performance for TOC, turbidity and absorbance removal was observed between pH 4 and 5, with the highest overall removal around pH 4.5. Optimized mixing conditions, consisting of rapid mixing followed by slow mixing, improved TOC removal compared to the current full-scale process. Polymer addition also improved treatment performance, although higher polymer dosages only resulted in limited additional improvements and indications of reduced turbidity removal during overdosing conditions.

Regarding RQ2, the baseline evaluation demonstrated that the current coagulation and flocculation process is highly influenced by variations in incoming raw water quality. Large variations in TOC removal were observed, including several negative TOC removal values during periods with high incoming TOC concentrations. In contrast, turbidity removal remained relatively stable throughout most sampling days, suggesting that the current process performs more consistently for particle removal than for dissolved organic matter removal. The results also showed that SUVA had stronger relationships with treatment performance than TOC concentration alone, indicating that the composition of the organic matter influenced coagulation efficiency.

Regarding RQ3, the results indicate that the facility could improve its process by implementing more adaptive and data driven operational strategies. Parameters such as TOC, pH, UV254 absorbance and especially SUVA showed potential for supporting operational decision making regarding chemical dosing. Improved pH control, optimized mixing conditions and selective polymer use could reduce chemical consumption while maintaining relatively high treatment performance. Lower ferric chloride dosages frequently achieved similar removal efficiencies compared to higher dosages, indicating potential for reducing operational costs and environmental impact.

In summary, the study demonstrates that the current process at the facility can be improved by moving from static fixed chemical dosing towards a more adaptive treatment strategy based on variations in incoming wastewater quality. By combining optimized pH conditions, improved mixing strategies and data driven process management, the facility has strong potential to improve treatment stability, reduce chemical consumption and lower environmental impact without significantly compromising treatment performance.

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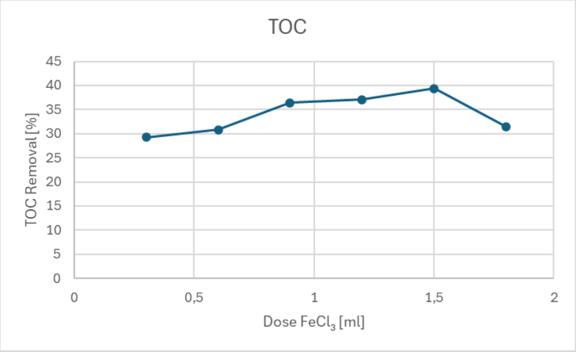
Appendix

- A1-A33 Effect of ferric chloride on removal efficiency
- A34-A57 SUVA as a predictor
- A58 Carbon footprint
- A59-A62 Baseline performance and variability

Effect of ferric chloride on removal efficiency (Test 1)



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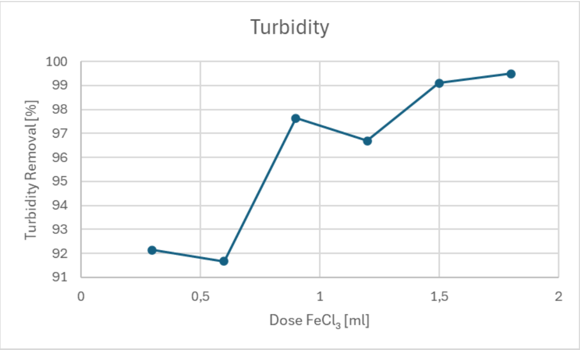

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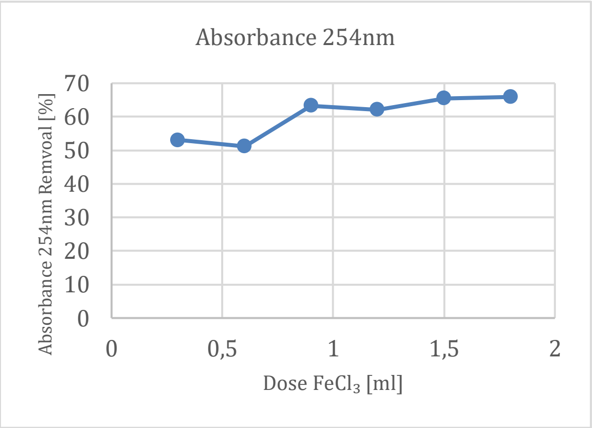

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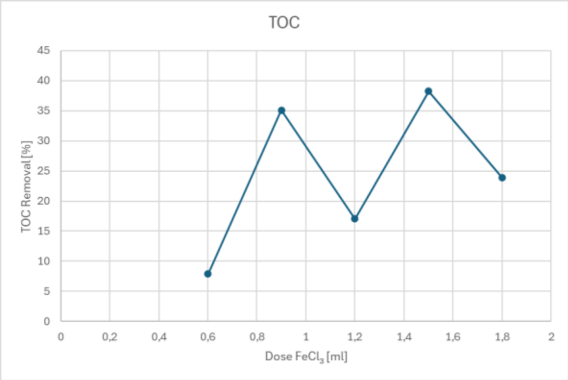

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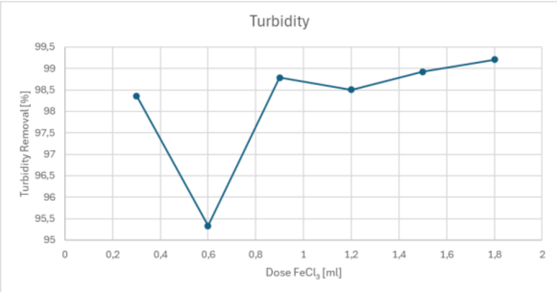

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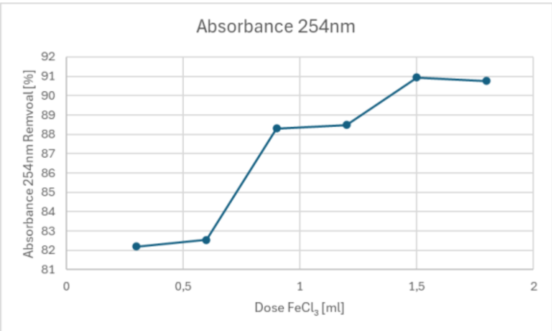

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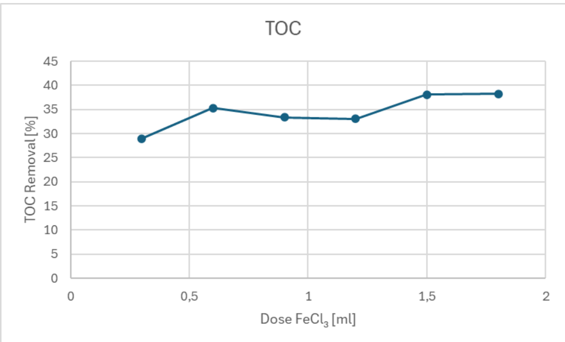

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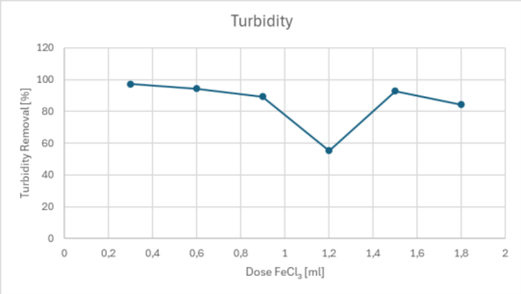

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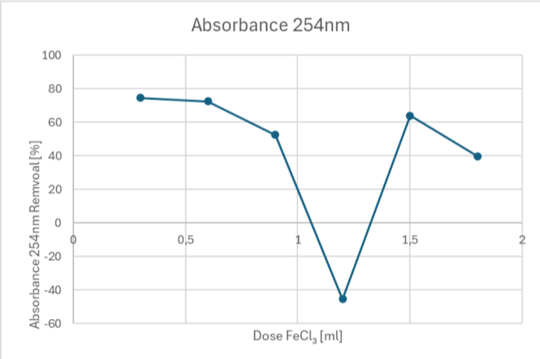

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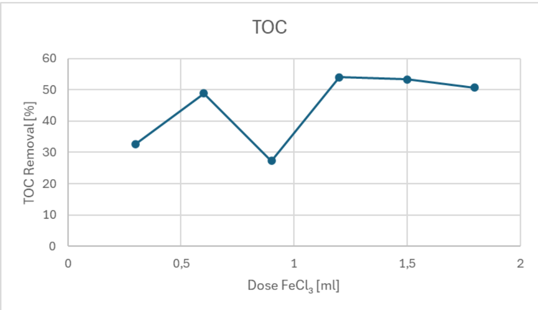

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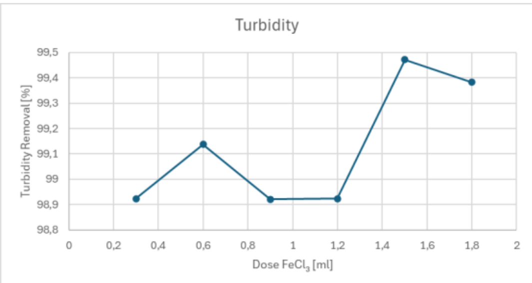

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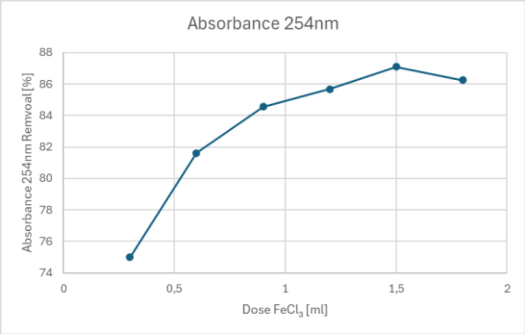

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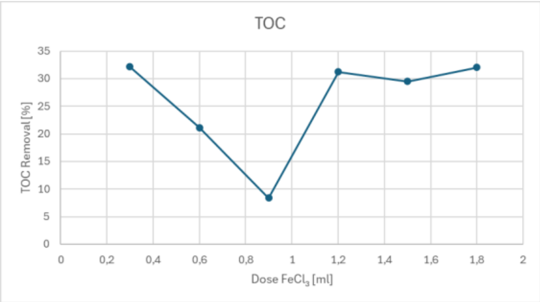

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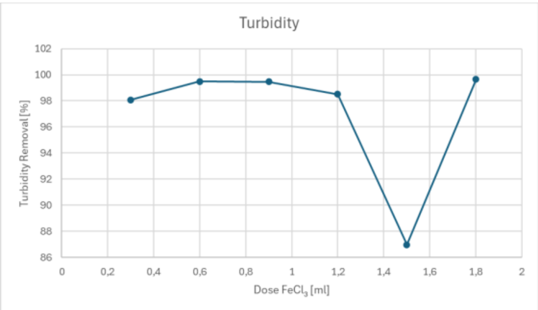

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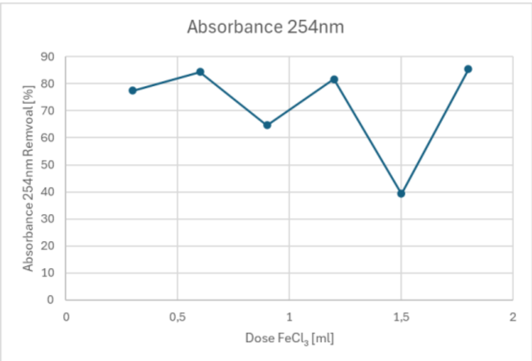

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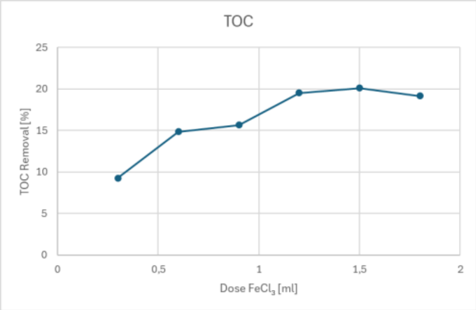

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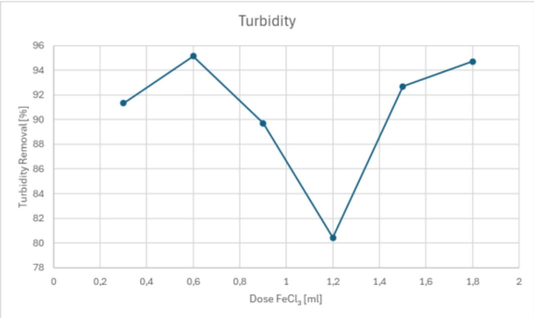

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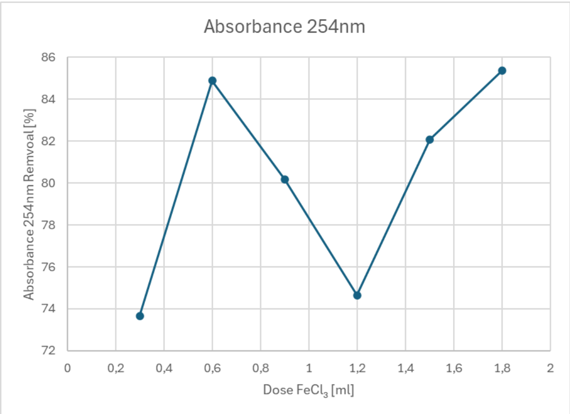

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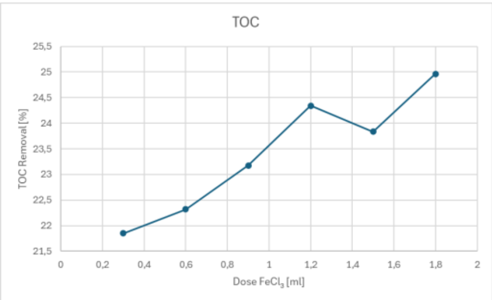
Effect of ferric chloride on removal efficiency (Test 7)



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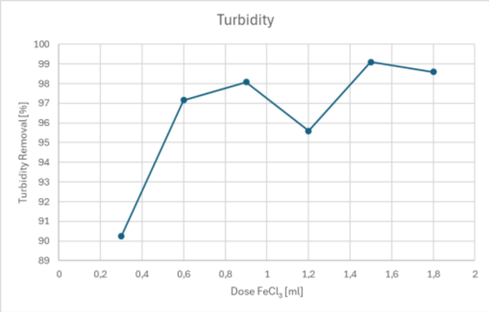

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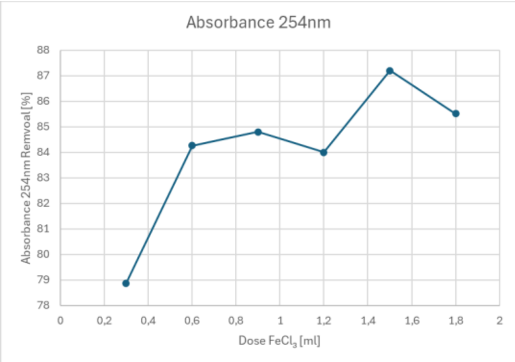

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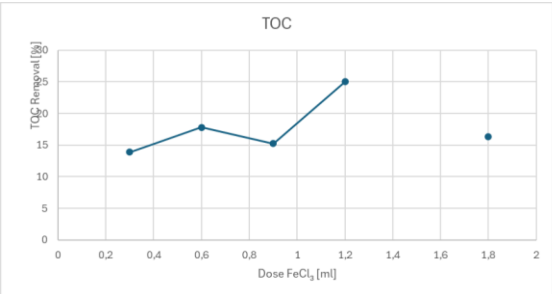
Effect of ferric chloride on removal efficiency (Test 8)



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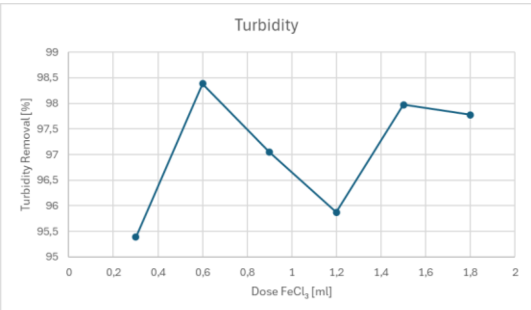

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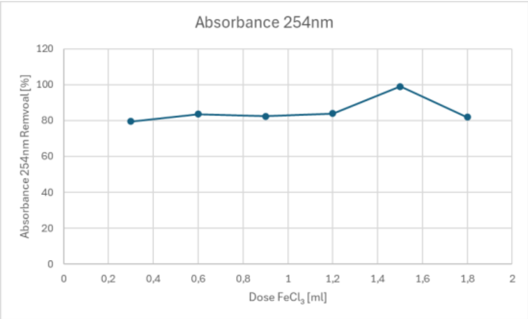

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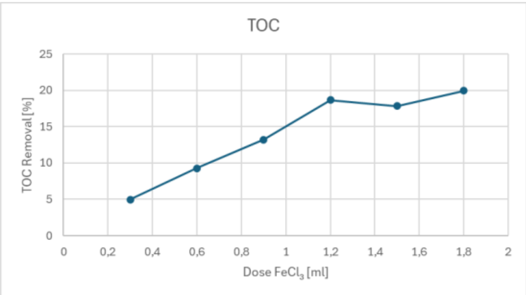
Effect of ferric chloride on removal efficiency (Test 9)



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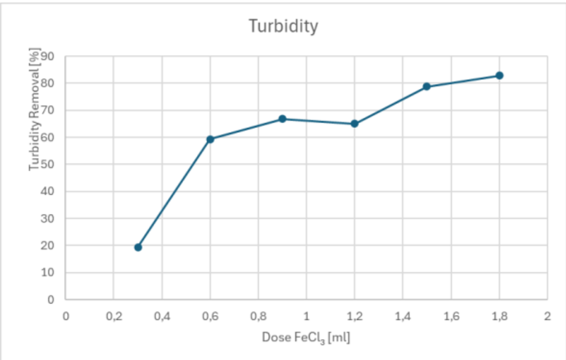

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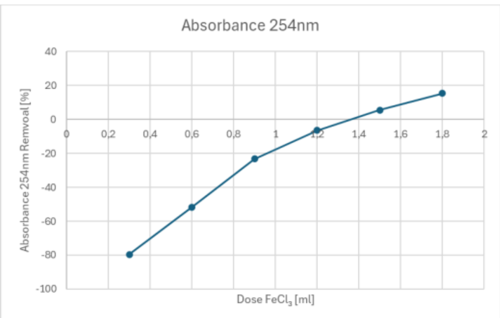

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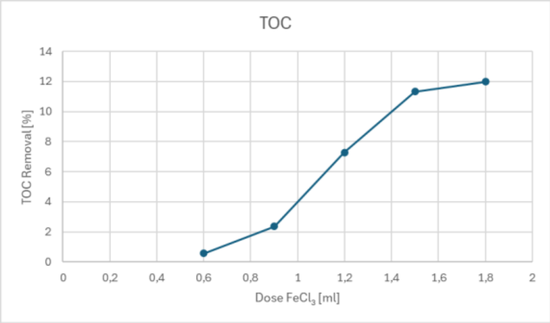
Effect of ferric chloride on removal efficiency (Test 10)



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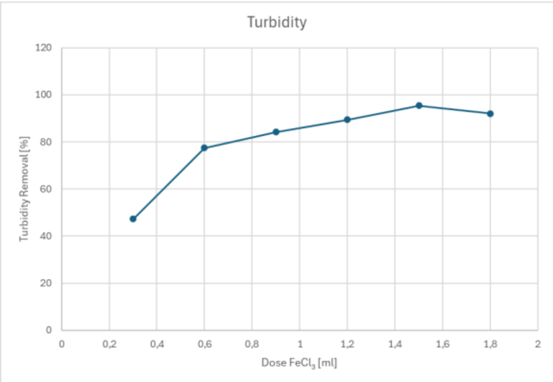

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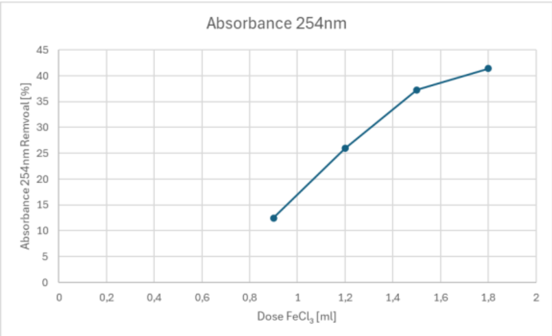

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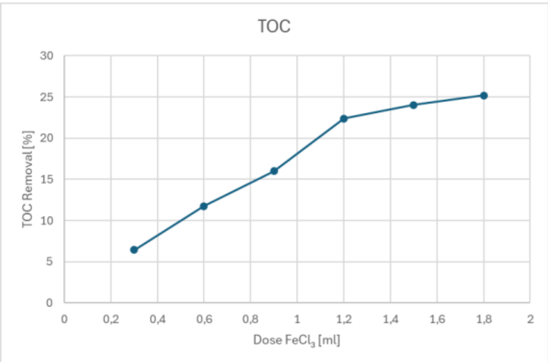
Effect of ferric chloride on removal efficiency (Test 11)



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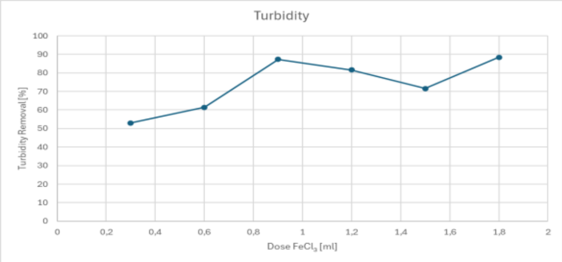

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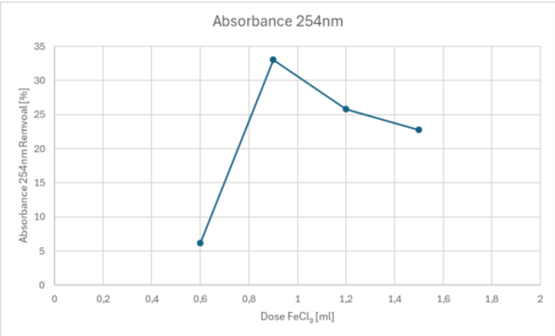
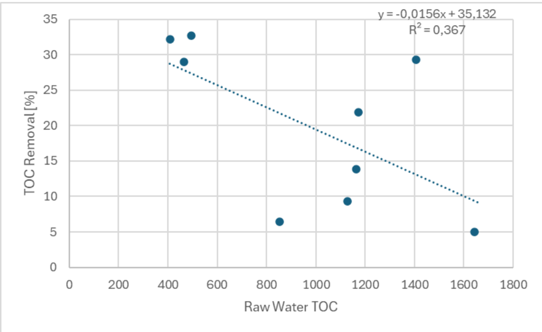


A 33

SUVA as a predictor (0.3mL)



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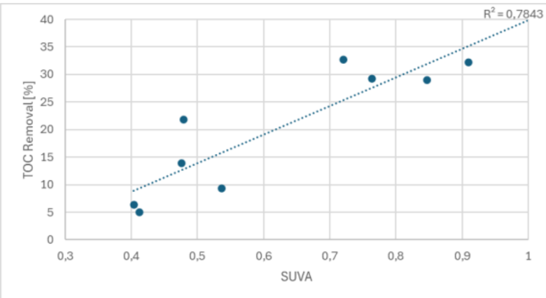

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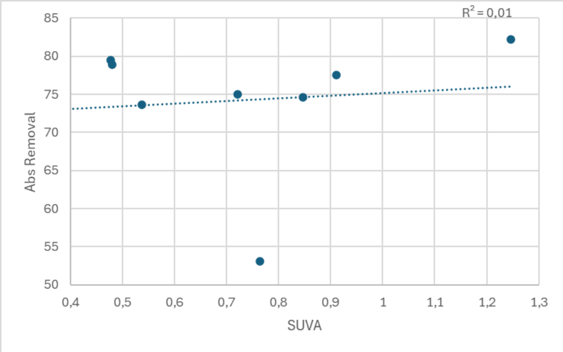
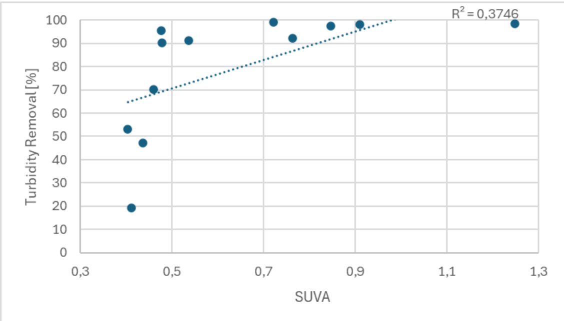
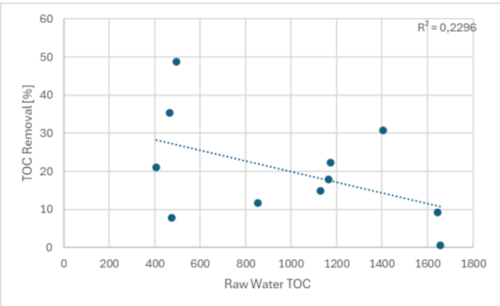


A 36

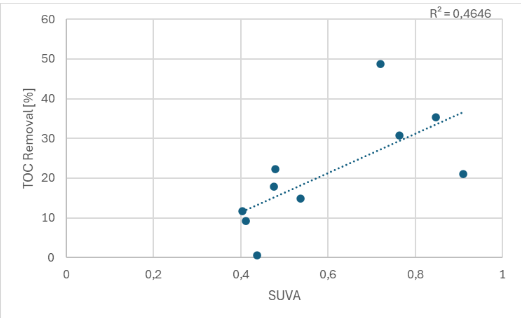


A 37

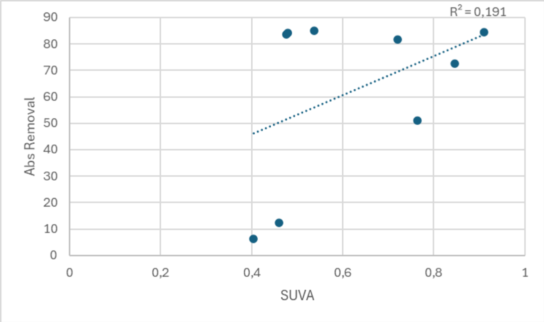
SUVA as a predictor (0.6mL)



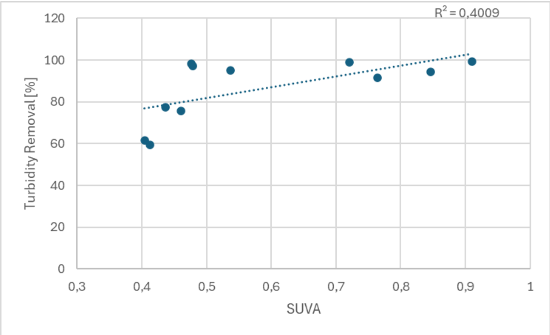
A 38



A 39

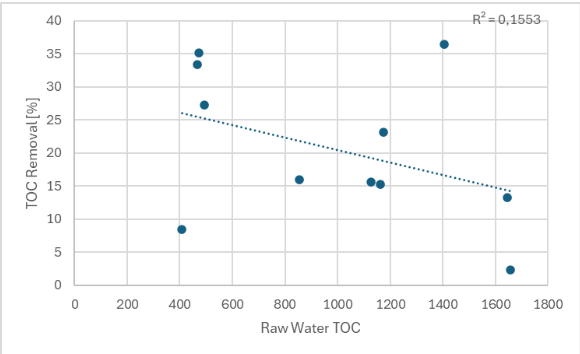


A 40

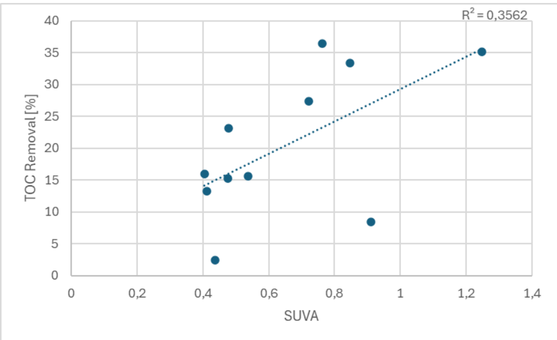


A 41

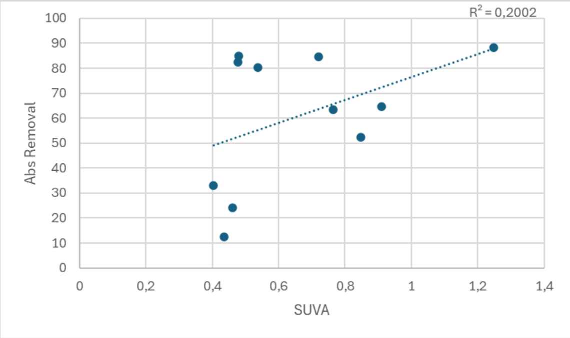
SUVA as a predictor (0.9mL)



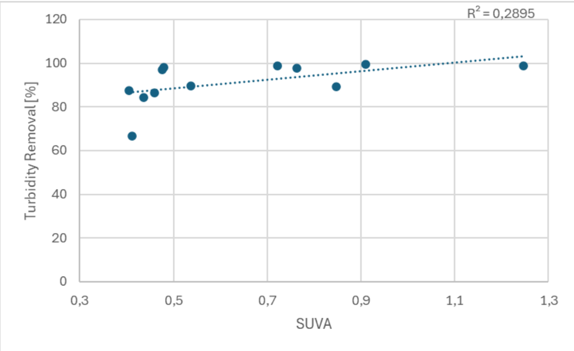
A 42



A 43

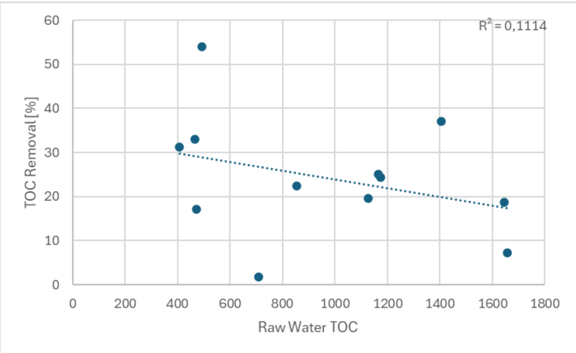


A 44

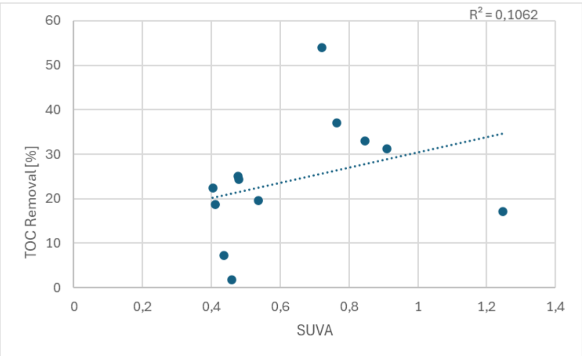


A 45

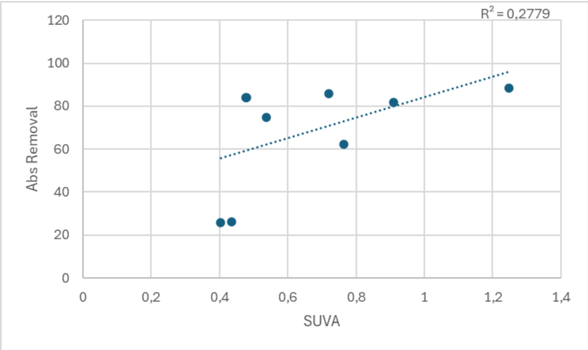
SUVA as a predictor (1.2mL)



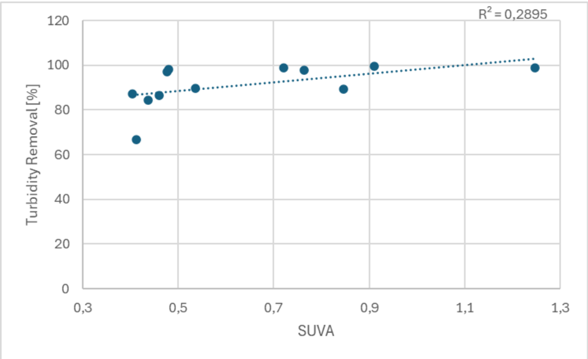
A 46



A 47

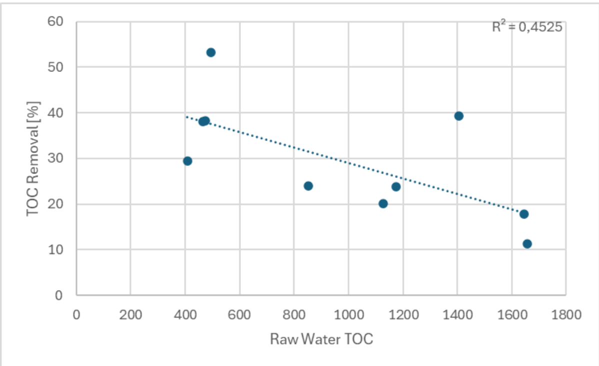


A 48

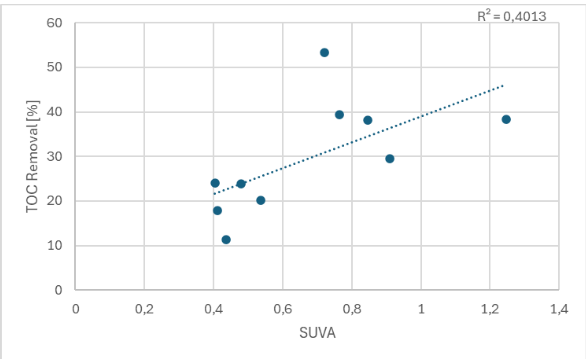


A 49

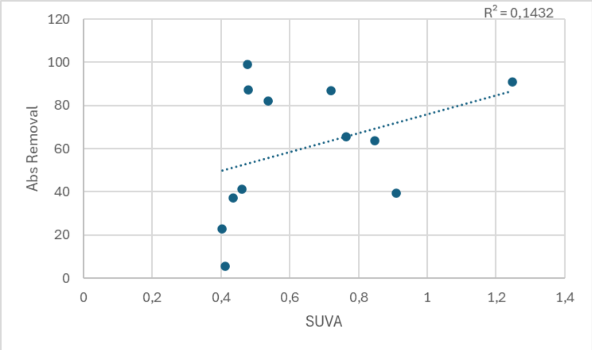
SUVA as a predictor (1.5mL)



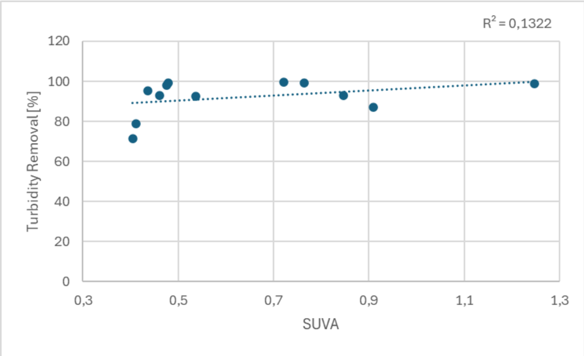
A 50



A 51

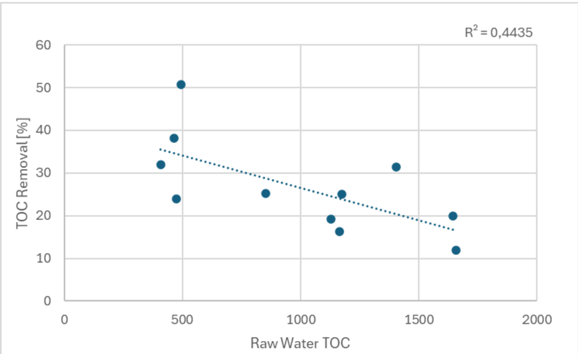


A 52

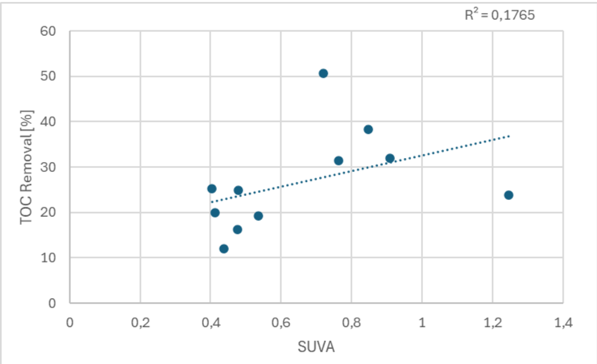


A 53

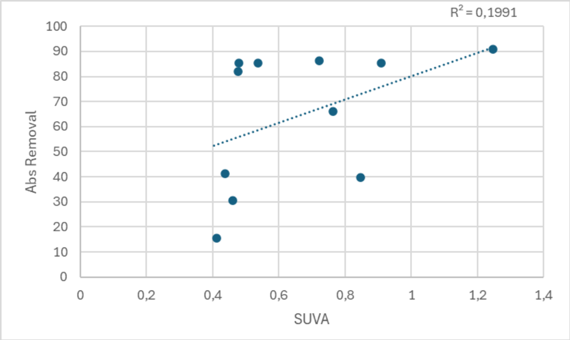
SUVA as a predictor (1.8mL)



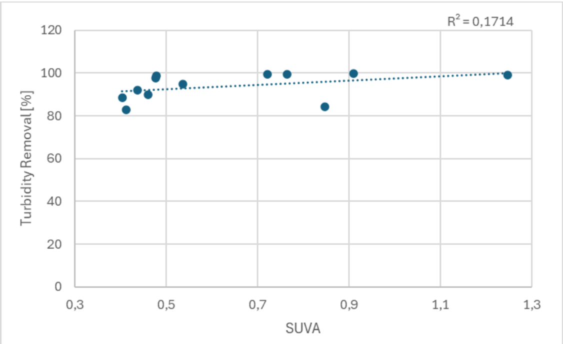
A 54



A 55



A 56



A 57

Carbon Footprint

Carbon Footprint

Current dosing (1,2ml/800ml)											
Soduim Hydroxide (IBC)	Price Soduim Hydroxide	NAOH Weight/IBC	Yearly Consumption Soduim Hydroxide	Yearly Cost Sodium Hydroxide	CO2e factor	Transport Factor	Production kg CO2e/year	Transport kg CO2e/year	Total kg CO2e/year		
35	6192	1160	40600	216720	0,915	0,0958	37149	111	37260		
Sulfuric Acid (IBC)	Price Sulfuric Acid	Sulfuric Acid Weight/IBC	Yearly Consumption Sulfuric Acid	Yearly Cost Sulfuric Acid	CO2e factor	Transport Factor	Production kg CO2e/year	Transport kg CO2e/year	Total kg CO2e/year		
12	4887	1020	12240	58644	0,122	0,0958	1493	98	1591		
FeCl3 (IBC)	Price FeCl3	FeCl3 Weight	Yearly Consumption FeCl3	Yearly Cost FeCl3	CO2e factor	Transport Factor	Production kg CO2e/year	Transport kg CO2e/year	Total kg CO2e/year		
21	4854,25	1115	23415	101939	0,803	0,0958	18802	107	18909		
Using predictive model (0,3ml/800ml)											
FeCl3 (IBC)	Price FeCl3	FeCl3 Weight	Yearly Consumption FeCl3	Yearly Cost FeCl3	CO2e factor	Transport Factor	Production kg CO2e/year	Transport kg CO2e/year	Total kg CO2e/year	Reduction CO2e FeCl3 [%]	Reduction Cost FeCl3 [%]
5,25	4854,25	1115	5854	25485	0,803	0,0958	4701	107	4807	75,00	75
Using predictive model (0,6ml/800ml)											
FeCl3 (IBC)	Price FeCl3	FeCl3 Weight	Yearly Consumption FeCl3	Yearly Cost FeCl3	CO2e factor	Transport Factor	Production kg CO2e/year	Transport kg CO2e/year	Total kg CO2e/year	Reduction CO2e FeCl3 [%]	Reduction Cost FeCl3 [%]
10,5	4854,25	1115	11708	50970	0,803	0,0958	9401	107	9508	50,00	50
Using predictive model (0,9ml/800ml)											
FeCl3 (IBC)	Price FeCl3	FeCl3 Weight	Yearly Consumption FeCl3	Yearly Cost FeCl3	CO2e factor	Transport Factor	Production kg CO2e/year	Transport kg CO2e/year	Total kg CO2e/year	Reduction CO2e FeCl3 [%]	Reduction Cost FeCl3 [%]
15,75	4854,25	1115	17561	76454	0,803	0,0958	14102	107	14209	25,00	25
Using predictive model (1,5ml/800ml)											
FeCl3 (IBC)	Price FeCl3	FeCl3 Weight	Yearly Consumption FeCl3	Yearly Cost FeCl3	CO2e factor	Transport Factor	Production kg CO2e/year	Transport kg CO2e/year	Total kg CO2e/year	Reduction CO2e FeCl3 [%]	Reduction Cost FeCl3 [%]
26,25	4854,25	1115	29269	127424	0,803	0,0958	23503	107	23610	-25,00	-25
Using predictive model (1,8ml/800ml)											
FeCl3 (IBC)	Price FeCl3	FeCl3 Weight	Yearly Consumption FeCl3	Yearly Cost FeCl3	CO2e factor	Transport Factor	Production kg CO2e/year	Transport kg CO2e/year	Total kg CO2e/year	Reduction CO2e FeCl3 [%]	Reduction Cost FeCl3 [%]
31,5	4854,25	1115	35123	152909	0,803	0,0958	28203	107	28310	-50,00	-50

A 58

Baseline performance and variability

FF2 IN										
Date	Conductivity	pH	Turbidity	Abs	TOC.1	TOC.1 after claculations	TOC.2	TOC.2 after claculations	TOC Average	% TOC Removal
09-feb	7,66	5,08	394	6,4	9,951	995,1	11,32	1132	1063,55	x
10-feb	7,87	6,35	13,3	6,378	5,517	551,7	6,836	683,6	617,65	x
11-feb	8,08	6,83	20,2	7,8	7,959	795,9	10,4	1040	917,95	x
12-feb	7,99	6,14	23,2	7,86	8,02	802	8,028	802,8	802,4	x
19-feb	8,12	6,18	30,1	5,06	9,136	913,6	10,03	1003	958,3	x
20-feb	8,71	8,27	27,6	4,2	8,39	839	8,398	839,8	839,4	x
21-feb	6,73	8,51	107	4,34	12,41	1241	13,47	1347	1294	x
FF2 OUT										
Date	Conductivity	pH	Turbidity	Abs	TOC 1	TOC 1 after claculations	TOC.2	TOC.2 after claculations	TOC Average	% TOC Removal
10-feb	5,72	6,36	128	2,34	7,158	715,8	7,519	751,9	733,85	30,99995299
11-feb	6,08	6,34	163	2,84	7,121	712,1	7,386	738,6	725,35	-17,43705982
12-feb	4,61	6,85	327	3,48	7,622	762,2	7,826	782,6	772,4	15,85598344
13-feb	6,54	5,76	117	3,44	7,914	791,4	8,477	847,7	819,55	-2,137337986
17-feb	7,79	6,55	33,7	2,94	7,982	798,2	7,829	782,9	790,55	x
18-feb	6,71	6,76	35,7	2,5	7,641	764,1	7,61	761	762,55	x
19-feb	4,79	7,52	307	2,72	8,012	801,2	8,392	839,2	820,2	x
20-feb	4,69	7,22	108	2,5	11,17	1117	11,25	1125	1121	-16,97798184
21-feb	4,49	7,36	132	4,8	11,49	1149	12,25	1225	1187	x

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FF2 IN											
Date	Conductivity	Turbidity	Turb. Removal	Abs	Abs. Removal	TOC.1	TOC.1 after claculations	TOC.2	TOC.2 after claculations	TOC Average	% TOC Removal
24-feb	6,61	96,6	x	11,02	x	46,95	2347,5	45,13	2256,5	2302	x
25-feb	5,75	80,2	x	4,015	x	26,72	1336	26,99	1349,5	1342,75	x
26-feb	4,74	67,6	x	7,42	x	25,95	1297,5	26,23	1311,5	1304,5	x
27-feb	3,67	408	x	7,415	x	23,27	1163,5	23,22	1161	1162,25	x
28-feb	3,89	126	x	2,705	x	10,79	539,5	10,84	542	540,75	x
01-mar	3,39	96,9	x	2,655	x	10,12	506	9,673	483,65	494,825	x
02-mar	3,54	607	x	7,325	x	21,05	1052,5	21,56	1078	1065,25	x
03-mar	3,41	284	x	4,475	x	13,03	651,5	12,96	648	649,75	x
04-mar	2,41	249	x	2,65	x	8,676	433,8	8,651	432,55	433,175	x
05-mar	4,51	482	x	6,555	x	24,28	1214	25,07	1253,5	1233,75	x
FF2 OUT											
Date	Conductivity	Turbidity	Turb. Removal	Abs	Abs. Removal	TOC 1	TOC 1 after claculations	TOC.2	TOC.2 after claculations	TOC Average	% TOC Removal
24-feb	9,74	44,5	x	3,955	x	38,63	1931,5	38,45	1922,5	1927	x
25-feb	6,58	41,4	0,571428571	3,41	0,690562613	19,95	997,5	20,1	1005	1001,25	56,50521286
26-feb	7,36	35,2	0,561097257	2,935	0,268991283	25,71	1285,5	26,29	1314,5	1300	3,183764662
27-feb	6,45	65,9	0,025147929	2,49	0,664420485	17,84	892	17,7	885	888,5	31,88961288
28-feb	6,74	16,6	0,959313725	1,855	0,749831423	13,82	691	14,24	712	701,5	39,64293396
01-mar	6,96	14	0,888888889	1,495	0,447319778	10,66	533	10,8	540	536,5	0,785945446
02-mar	5,77	38,4	0,60371517	2,455	0,075329567	12,94	647	12,89	644,5	645,75	-30,50068206
03-mar	6,96	28,9	0,952388797	3,17	0,567235495	15	750	15,51	775,5	762,75	28,39708989
04-mar	7,16	28,9	0,898239437	1,46	0,673743017	8,278	413,9	8,204	410,2	412,05	36,58330127
05-mar	6,27	41	0,835341365	3,375	-0,273584906	20,36	1018	20,68	1034	1026	-136,8557742

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FF2 IN												
Date	Conductivity	pH	Turbidity	Turb. Removal	Abs	Abs. Removal	TOC.1	TOC.1 after claculations	TOC.2	TOC.2 after claculations	TOC Average	% TOC Removal
06-mar	3,58	6,2	457	x	6,07	x	19,8	990	20,27	1013,5	1001,75	x
09-mar	3,65	6,58	1200	x	7,085	x	22.30	1115	22,4	1120	1117,5	x
10-mar	4	6,77	1085	x	6,87	x	21,25	1062,5	22,06	1103	1082,75	x
11-mar	1,515	7,42	463	x	2,76	x	9,85	492,5	9,937	496,85	494,675	x
12-mar	3,25	8,65	275	x	3,175	x	7,91	395,5	8,093	404,65	400,075	x
13-mar	4,26	7,79	45,8	x	1,46	x	7,975	398,75	8,22	411	404,875	x
16-mar	2,82	8,83	333	x	3,195	x						x
FF2 OUT												
Date	Conductivity	pH	Turbidity	Turb. Removal	Abs	Abs. Removal	TOC 1	TOC 1 after claculations	TOC.2	TOC.2 after claculations	TOC Average	% TOC Removal
06-mar	6,6	6,83	46,5	0,903526971	2,65	0,595728452	20,11	1005,5	20,37	1018,5	1012	17,97365755
10-mar	6,93	7,15	36,9	0,96925	3,04	0,570924488	17,67	883,5	17,8	890	886,75	20,64876957
11-mar	4,77	7,38	35,3	0,967465438	1,425	0,792576419	8,772	438,6	8,841	442,05	440,325	59,33271762
12-mar	5,06	7,97	30	0,935205184	1,5	0,456521739	9,174	458,7	9,008	450,4	454,55	8,111386264
13-mar	5,49	8,99	29,1	0,894181818	1,11	0,650393701						
16-mar	4,3	6,02	53,3	x	0,895	x						
17-mar	4,98	6,76	28,7	0,913813814	1,04	0,674491393						

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FF2 IN													
Date	Conductivity	pH	Turbidity	Turb. Removal	Abs	Abs. Removal	TOC.1	TOC.1 after claculations	TOC.2	TOC.2 after claculations	TOC Average	% TOC Removal
18-mar	2,94	7,1	164	x	1,785	x	6,937	346,85	7,444	372,2	359,525	x
20-mar	3,26	6,54	790	x	4,735	x	76,77	3838,5	74,98	3749	3793,75	x
23-mar	4,08	6,9	705	x	4,86	x	77	3850	77,65	3882,5	3866,25	x
25-mar	4,15	6,79	235	x	2,435	x	97,51	4875,5	96,52	4826	4850,75	x
26-mar	3,15	6,75	510	x	6,165	x	29,14	1457	29,27	1463,5	1460,25	x
27-mar	3,3	6,75	476	x	5,6	x	31	1550	31,7	1585	1567,5	x
30-mar	3,66	6,88	264	x	5,66	x	36,74	1837	37,25	1862,5	1849,75	x
31-mar	3,55	7,1	227	x	5,355	x	21,62	1081	22,12	1106	1093,5	x
01-apr	2,92	6,98	299	x	3,59	x	17,49	874,5	16,59	829,5	852	x
02-apr	3,08	7,49	217	x	2,995	x	16,01	800,5	15,11	755,5	778	x
FF2 OUT												
Date	Conductivity	pH	Turbidity	Turb. Removal	Abs	Abs. Removal	TOC 1	TOC 1 after claculations	TOC.2	TOC.2 after claculations	TOC Average	% TOC Removal
18-mar	4,48	6,9	67,5	-1,351916376	0,745	0,283653846	7,28	364	7,501	375,05	369,525	x
20-mar	5,45	6,11	31.3	x	1,66	x	24,2	1210	24,37	1218,5	1214,25	x
23-mar	6,53	6,64	850	x	4,18	x	115,9	5795	114,2	5710	5752,5	-51,63097199
25-mar	5,83	6,83	56,3	x	1,275	x	22,6	1130	22,39	1119,5	1124,75	x
26-mar	5,48	7,04	275	-0,170212766	5,27	-1,164271047	26,31	1315,5	26,59	1329,5	1322,5	72,73617482
27-mar	5,35	7,49	109	0,78627451	5,075	0,176804542	29,33	1466,5	30,14	1507	1486,75	-1,814757747
30-mar	5,26	7,5	124	x	5,715	x	33,21	1660,5	32,63	1631,5	1646	-5,007974482
01-apr	5,85	7,38	133	0,496212121	5,39	-0,006535948	28,32	1416	27,56	1378	1397	-27,75491541
02-apr	5,89	8,96	43	0,856187291	3,49	0,027855153	27,99	1399,5	28,63	1431,5	1415,5	-66,13849765
7?	5,5	7,3	73	?	1,165	?	22,92	1146	22,36	1118	1132	?

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