A socio-technical network analysis on the industrial symbiotic performance of water within chemical parks

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accenture

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Thesis report

by

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Preface

This thesis marks the end of my 6-year journey as a TPM student and also the conclusion of my time in Delft. I still vividly remember the first day I set foot in Delft, filled with excitement about the new city and the people I would meet, but also with doubts about my choice of study. Would the program I selected truly align with my interests? Would I be able to meet the requirements? Looking back, I can confidently say that I am very grateful for making this decision to pursue a Bachelor's degree in Technology, Policy and Management and a master's degree in Engineering and Policy and Analysis. I am proud of the end result, finishing my master's with this thesis. In this preface, I would like to express my gratitude to those who have played a crucial role in shaping this thesis and take a moment for reflection.

First and foremost, I would like to thank my supervisor, Petra, for your valuable time, genuine interest, and unwavering support. Because I knew you would want me to do my best and were always interested in my progress, it stimulated me to perform better. Moreover, your straightforward feedback stimulated me as well, as it did leave me with no space but accept it and improve it. The nature of working on a thesis is often solitary, which I did not enjoy. Although you have probably not realized this to such an extent, my graduation experience would have been very different without your kindness and support. Therefore, thank you for providing a cheerful ending to my master's.

I would also like to express my appreciation to Martijn. Although we did not have extensive interactions, you made me feel comfortable and assured that I could always turn to you for guidance. Your constructive criticism was helpful, especially for a thesis student uncertain about her progress. I am grateful for the smooth cooperation between you and Petra, as your aligned perspectives made our meetings productive and ensured a well-structured approach. During the kick-off meeting, you provided an extra boost by highlighting the significance of my research topic, which encouraged me when I was unsure about its scope.

Furthermore, I want to thank Rik, my supervisor from Accenture. From the very beginning, we established a good connection, and although we didn't delve extensively into the thesis content, I always found our weekly meetings enjoyable and valuable in guiding me towards a more structured approach.

Most importantly, I would like to express my gratitude to my parents and my sister. Your support and encouragement have been instrumental throughout my studies and my time in Delft. You were always available when I needed you. I am also thankful for all the friends I have made in Delft, who have made my time here unforgettable and have added joy to my studies. And last but not least, I would like to thank Pien for letting me borrow her laptop. Without her laptop, most of the computational intensive runs, necessary for this thesis research, would not have been performed.

As a now fully-fledged graduate, I would like to reflect briefly on my time as a student. Scientifically, I have experienced personal growth and am proud of the model I have built from scratch for this thesis. However, I have also realized that while unstructured thinking and jotting down ideas may work well for me personally, when it comes to writing a 100-page thesis, both I and those who read my work may have a different perspective (; Although I have gained knowledge in the field of academia during this thesis research, the most significant lesson I have learned is how to structure my thoughts and effectively convey them in writing. Hopefully, you, who will read (parts of) my thesis, agree with me (; Enjoy!

Josse Wiss
Delft, May 2023

Executive Summary

Research background and main research questions
The depletion of the earth's freshwater resources has been significantly impacted by the exceptional rise in human activity in recent decades (Oturan & Aaron, 2014). Should this trend persist, it could potentially endanger the survival of humans on earth (Tiu & Cruz, 2017). After the agricultural sector, the industrial sector is the second largest freshwater user in the world (Ritchie Roser, 2017). The rising environmental concerns have prompted a need for the creation and execution of sustainable measures. Within the industrial sector, sustainable measures have been taken that belong to the concept of industrial ecology. Industrial Symbiosis (IS) expands this concept by taking an approach that emphasizes the efficient use of resources. Specifically for water, this involves one company utilizing the residual wastewater of another company based on the differences in water quality requirements (Lawal et al., 2021).

The chemical industry is one of the largest water consumers and the biggest producer of wastewater within the industrial sector. The chemical industry encompasses a broad economic sector that produces chemicals from pharmaceuticals to polymers such as food petrochemicals, polymers, and dyes. However, industrial symbiosis of water does not happen enough within the chemical parks while the potential is high. Much water is being recycled, and technologies within treatment facilities are improved, but reducing the external water sources is not part of the mitigating measures (Zeng et al., 2013). Two important reasons cause this trend. Firstly, it is technically challenging to recycle water because of all the different water qualities used and produced in chemical parks. And secondly, the industrial symbiosis initiatives have to start with the stakeholders involved in the chemical park themselves in bottom-up regulated countries, while currently, many stakeholders decide not to join an IS water network.

Until now, most studies have focused on finding an economically and environmentally optimal design for an industrial symbiosis water network within a chemical park. Still, many studies neglect the aspect of the stakeholders deciding to take part in this IS water network or not. This is why this research presents a methodology taking different stakeholder behaviour into account and determining if an IS water network design can still operate effectively, meaning enough water is recycled and costs are not too high. The main research question which will be answered is formulated as:
To what extent is industrial symbiosis of water within chemical parks possible, taking into account stakeholder behaviour?

Involved actors and influential decision criteria
The owners of the chemical factories and the treatment facilities are the most important stakeholders within the chemical parks. They can decide to join or not to join an industrial symbiosis network. They will base their decision on different criteria, like how feasible connection to the network is, whether they can expect revenue growth or decline from it, whether they will get a fine for non-compliance, how progressive their internal sustainability policy is regarding water circularity, whether they trust other stakeholders located on the chemical park and how aware they are that within the chemical park more water can be recycled.

Designed model to measure the optimal industrial symbiotic performance of a chemical park
A model is designed that measures the industrial symbiotic performance of an IS water network within a chemical park. The industrial symbiotic performance is defined according to how much the additional infrastructure to create IS connections will cost, how much extra water will be recycled and how robust the water network will be against certain stakeholders not joining. The model consists of two parts, the technical optimization part and the social behaviour part. The technical optimization part finds the optimal combination of water pipes with water flows and stakeholders within a specific chemical park based on maximizing the amount of water that can be recycled and the least amount of additional costs. The

stakeholder behaviour part of the model considers different scenarios in which different decision criteria impact the stakeholders' decisions. In every scenario, specific stakeholders do not join the IS water network, according to which a new optimal structure of the chemical park is sought with new outcomes for the amount of recycled water and costs.

The different outcomes of chemical parks in which all stakeholders join, and after several stakeholders have decided on not joining, are compared with each other. This is how the robustness to stakeholder behaviour of the IS water network is defined.

Results

The findings of this research show that the potential for industrial symbiosis within chemical parks greatly depends on the existing treatment facilities within the chemical park and the number of involved stakeholders and their preferences. When more stakeholders choose not to participate in the IS water network, the possibilities for symbiotic relationships decrease rapidly.

There is a significant difference in performance between two common treatment facility structures in chemical parks: the in-house or separate structure. In the in-house treatment facility structure, it is assumed that each chemical factory located in a chemical park has its own pre-treatment facility in-house. While in the separate treatment facility structure, it is assumed that several separate treatment facilities exist in a chemical park that treats wastewater of multiple chemical factories.

The costs for recycling the same amount of water are higher in chemical parks with separate treatment facilities, ranging from 1 billion to 500 million euros for recycling 25% or 30% of the water. Chemical parks with in-house treatment facilities also have lower possibilities for water recycling compared to parks with separate treatment facilities. With fewer stakeholders joining, the chance of recycling water already does not surpass the 12%.

The most important decision criteria for stakeholders deciding on whether to join or not to join an IS water network are whether they can expect revenue growth or decline from it, whether they will get a fine for non-compliance, or how much they trust the other stakeholders within the chemical park. Efforts to increase the amount of participating stakeholders can improve the overall performance of IS water networks in chemical parks, however, only to a small extent.

Recommendations

To improve the possibilities for industrial symbiosis when certain stakeholders choose not to join, certain technical adjustments and construction efforts can be made within the chemical park. For example, the number of water qualities the IS water network is designed for can be optimized, and treatment technologies within the facilities can be upgraded towards consisting of a membrane bioreactor. However, these measures would only lead to a 3% decrease in costs and a 12% increase in water recycling.

In situations where there is low economic motivation for joining the IS water network and no strict regulations exist, few chemical companies will join the IS water network. By focusing on creating IS connections for a smaller number of water qualities, it is still possible to recycle 10% of the water within a chemical park.

In situations where trust among stakeholders is low and awareness of the IS water possibilities is lacking, upgrading the treatment technologies of separate treatment facilities can still enable recycling of 14% of the water. However, in chemical parks with in-house treatment facilities, the possibilities for water recycling become negligible.

Efforts should also be made to convince stakeholders to participate in the IS water network. This could decrease the costs for the IS water network with 5% and increase the amount of recycled water with 20%. This can be achieved through policies that address stakeholders' concerns. First of all, the decision criteria of stakeholders to comply to regulations could be addressed by setting more strict limits for the water intake, wastewater disposal or concentration connected to the license to operate. The license to operate is a license given by the chemical park owner to the chemical factories located on the chemical park.

Secondly, the decision criteria of revenue growth can be addressed by introducing different economic-related policies: a carefully distributed subsidy for the construction of water pipes above 20% and a water tax of a high increase of 1000%.

Lastly, a policy for organizing a monthly park meeting relevant to creating trust among the stakeholders on a chemical park could be introduced.

Contributions

Integrating the technical optimization part and the stakeholder behaviour part into one model is a suitable way of approaching the design of an IS water network in a socio-technical environment of a chemical park for two reasons. Firstly, by including different stakeholder behaviour within the model, a more realistic analysis can be performed of the possibilities and effectiveness of IS water networks within a chemical park. Within a socio-technical system, there will always be conflicting interests. Secondly, optimizing the different structures of IS water networks, containing inhouse or separate treatment facilities, is interesting because it shows that there are different possible optimal designs concerning combinations of technical components and involved stakeholders between the two types of chemical parks. By engaging with stakeholders and analyzing the present structure of the chemical park, the most feasible design can be found. The model can facilitate learning among decision-makers instead of imposing decisions on them.

This research is a first step in including socially oriented objectives in an optimal industrial symbiosis water design. Two main contributions to the field are made. Firstly, this study has bridged the gap between economic and environmental wastewater network optimization studies and social optimal designs regarding stakeholder relations within chemical parks. Secondly, this study has given more insight in which decision criteria should be addressed first and how they should be addressed to enable more industrial symbiosis in specific chemical parks and to see in which situations it will be more difficult to create industrial symbiosis possibilities.

Contents

Nomenclature

List of Abbreviations

AOP	Advanced oxidation processes
EIP	Eco-industrial Park
IS	Industrial Symbiosis
MCDA	Multi Criteria Decision Analysis
WN	Water Network
WSM	Weighted Sum Method

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δ	TD-error

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1

Introduction

The extraordinary increase in human activity over the last few decades has had a significant impact on the depletion of the earth's freshwater resources. Only about 0.65% of the total water mass can be directly utilized by humans, while the rest is constituted by resources such as salted oceans and glaciers (Oturan & Aaron, 2014). If this trend continues, it may pose a serious threat to human survival on earth (Tiu & Cruz, 2017). The rising environmental concerns have prompted a need for the creation and execution of sustainable measures. When referred to the definition of the United Nations, the term "sustainable development" is: *"the developmental ability to meet the present generation's needs without comprising the future generations' ability to meet their own needs"* (Nations, 2020). The most recent trends in establishing sustainable development are now tailored toward reducing pollution at the source. Such approaches promote cleaner production more efficiently than end-of-the-pipe approaches (Aviso et al., 2010).

After the agricultural sector, the industrial sector is the second largest freshwater user in the world (Ritchie & Roser, 2017). Europe, the industrial sector accounts for 40% of total water abstractions and 60% of the total water pollution (Förster, 2014). To increase sustainability within the industrial sector, the topic of industrial ecology (IE) has been introduced. The main goal of industrial ecology is to preserve the environment while increasing business success (El-Haggar, 2007). By taking an approach that emphasizes the efficient use of resources, Industrial Symbiosis (IS) expands the concept of industrial ecology to encompass the industrial sector. This involves one company utilizing the unused or residual resources - such as materials, energy, water, assets, logistics, and expertise - of another company. The goal is to enhance environmentally friendly, sustainable, and cleaner production by reducing waste generation and greenhouse gas emissions (Lawal et al., 2021). The potential benefits of a symbiosis can be economic, environmental, and societal (Hein et al., 2015, Hellweg and Canals, 2014). Water symbiosis is considered a special type of material symbiosis. Based on the difference in water quality requirements of different production processes, water resources are reused to the maximum extent to achieve water-saving purposes.

To date, the most widespread embodiments of Industrial Symbiosis are Eco-Industrial Parks (EIPs). An EIP can be defined as *"an industrial system of planned material and energy exchanges that seeks to minimize waste and build sustainable economic, ecological, and social relationships"* (Alexander et al., 2000). An example is shown in Figure 1.1. Despite significant efforts, many industrial parks around the world do not meet the environmental standards to be classified as eco-parks, due to a lack of symbiotic relationships of water among industries and a failure to address environmental issues comprehensively within those parks (Genc et al., 2019).

Figure 1.1: Example of an operating Eco-industrial park

1.1. Chemical industry and reducing pollution at the source

The amount of wastewater produced in the chemical industry can vary depending on the specific processes and technologies used, as well as the size and location of the chemical plant. However, in general, the chemical industry is one of the largest water consumers and the biggest producer of wastewater within the industrial sector (Shatalov, 2018). Substantiated by chemical production processes often requiring more water, the resulting wastewater can contain higher levels of pollutants and contaminants.

Within Europe, 62 chemical parks exist. Chemical parks typically consist of a cluster of businesses engaged in both heavy and light manufacturing and chemical processing, with the goal of maximizing production output. By grouping businesses in a dedicated colocation, they can offer important efficiency and collaborative opportunities (Gao et al., 2011). A special website has been dedicated to enlisting facts and figures about these chemical parks in Europe (ECSPP, 2020). However, no facts or figures can be found on reduced water usage or industrial symbiosis of water. Chemical players do have the desire to reduce their freshwater usage and pollutant wastewater flows as the water stress becomes higher, but only by internal changes. They invest a lot and their investors expect a certain level of sustainability. In the annual report of DSM, one of the top 10 biggest chemical companies in Europe, they discussed how they coped with the accompanied short-term risks of water stress. They took mitigating measures, of which 97% were implemented by 2021 (DSM, 2020). In the annual report regarding water usage of Akzo Nobel, another chemical company producing paint, the same mitigating measures were performed (AkzoNobel, 2021). However, as this shows, all the chemical players are still reluctant to reduce freshwater income by reusing other chemical companies' wastewater (Zeng et al., 2013).

So, the chemical industry is not only a crucial pillar of the industrial sector but also one that consumes the most water of the resources and produces the most waste and pollutants (K. Liu et al., 2022). Moreover, this industry is also at the forefront of developing novel technologies and advanced solutions for sustainable resource management (Unicef, 2018). The chemical industry encompasses a broad economic sector that produces ”commodity chemicals” from pharmaceuticals to polymers such as food petrochemicals, polymers, and dyes. To achieve sustainable water management, it is imperative for the chemical industry to move beyond an individualistic approach and adopt a holistic perspective that fosters symbiotic interactions with other sectors or industries of the same nature. Implementing industrial symbiosis within chemical parks can yield strategic benefits such as reduced exposure to resource and licensing risks, increased competitiveness, business development, and better stakeholder reputation (Unicef, 2018). However, in reality, there are only very few examples of chemical parks that have implemented industrial symbiosis of water. Moreover, within the plants, a lot of water is being recycled and technologies within treatment facilities are improved, but reducing the external water sources is not part of the mitigating measures. Why is the urgency so high but very less real-life cases of inter-plant industrial symbiosis of water exist?

1.2. Designing an industrial symbiotic wastewater network for the chemical industry: a socio-technical challenge

From the previous sections, it is clear that more inter-plant IS water implementations in chemical parks are necessary, but in reality, generating such connections is more difficult than expected (Aviso et al., 2010). To be able to analyze if IS connections will create more advantages than in the current situation,

	Challenge
Technological	Find a way in which all the different water quality demands and supplies and different treatment technologies could be represented and analyzed Be able to define the industrial symbiotic performance of an IS water network
Social	Find out what factors influence stakeholder behaviour within chemical parks and what is their influence

Table 1.1: Summary of the technical and social challenges relevant to this research

technical designs, often mathematical optimal water networks, are made in most studies. But, especially, within the chemical industry, the quality of water plays a prominent role, causing extra complexity in the web of influencing aspects to the technical IS water designs (Lawal et al., 2021). Although there are technological challenges, just looking at the technological side of the IS network implementations does not fully explain the failing implementations shown in Table 1.1: already certain multi-contaminant inter-plant network methods exist according to which IS water networks have been implemented in practice. To understand the failing implementations, a socio-technical perspective is necessary. Behind the material flows occurring in the industrial chemical system there is a complex web of actors, with differing and sometimes opposing interests, who interact with each other. As a result, the actual physical flows are determined by these actors, as noted by Vahidzadeh et al. (2021) in their study of the regional aspects of this system. IS within chemical parks is a socio-technical system that has both a technological and a social side which are strongly interconnected (Song et al., 2018).

Essentially, understanding the dynamics of IS chemical system networks requires a grasp of the social factors underlying water exchanges, as well as the circumstances that increase the likelihood of cooperation among chemical companies (Doménech & Davies, 2009). Stakeholders within the chemical park will keep conflicting ideas about how the IS water network should be implemented and what their role in this process should be (Song et al., 2018). Hence, the complexity of a problem is influenced by the number of actors involved and the degree to which their interests diverge from one another.

In designing an IS water network, while costs are undoubtedly a crucial factor to consider, relying solely on finding a technically cost-optimized design may be a limited approach. It is also essential to consider the potential behaviour of the various stakeholders involved (Yao et al., 2017). In many projects, stakeholder management is an important aspect. It means keeping the stakeholders informed and satisfied, so they will not opt out of the project (Lawal et al., 2021). However, could this approach also be turned around? Is it possible to design a project in a way it is most resilient to stakeholders opting out? This study intends to include quantitative measures to be able to measure the effect of the behaviour of stakeholders taking part in IS networks, which is underrepresented in other studies. This section will discuss some critical challenges to the generation of IS water networks from the socio-technical perspective. Both technological and social challenges will be discussed in the following paragraphs.

1.2.1. Technological challenge to the IS of water possibilities within chemical parks: technical designs that incorporate all the different water qualities, involved plants and could measure the resilience

As already shortly explained above, challenges exist in the designs to research if IS connections are possible and beneficial within certain chemical parks. Much research has been conducted to optimal designs of wastewater networks for industrial parks. However, two main challenges remain in designing such networks. These challenges are described in the following paragraph.

The variety of water qualities and treatment technologies within the chemical industry

Several chemical parks exist that recycle wastewater for cleaning tasks within the chemical park or for irrigation of nearby wetlands, however, not a lot of examples exist where wastewater is actually recycled for use in new industrial processes. In the first ever designed EIP, the Kalundbourg Industrial Park in Denmark, wastewater from the Novo Nordisk pharmaceutical plant was treated and then reused for irrigation of nearby fields (Grann, 1997). One of the few EIP's in which wastewater is actually used within the factory process is in the Zhangjiang High-Tech Park in Shanghai, China (Lü et al., 2012). There are several technical reasons that explain why it is harder to recycle wastewater for actual factory processes. First of all, the composition of wastewater streams from the chemical industry can be highly complex and can contain a wide variety of contaminants. Treating this wastewater to a high standard for reuse in industrial processes can be technically challenging and requires significant expertise and investment in designing the right combination of treatment facilities (J. Liu & Tang, 2018). Secondly, there is often a lack of the right infrastructure, building the infrastructure required for the industrial symbiosis of water within an EIP requires a good overview of all different water demands and supplies. According to Tiu and Cruz (2017), this overview often lacks, as well as monitoring and evaluation systems. This particularly requires the right network design method that could evaluate if certain IS connections are possible regarding water quality and efficiency.

Define the performance of an IS water network
Industrial symbiosis consists of an economic, environmental, and social aspect (Zheng et al., 2012). While environmental and economic indicators are relatively straightforward to quantify, social indicators involve more subjectivity and complexity, and collecting data on them can be challenging. As a result, the social component of industrial symbiosis is often the least researched. Nonetheless, it can be crucial for the success of industrial symbiosis, as if the local community and regional authorities are aware of the benefits of these synergies, they may actively support the development of industrial symbiosis. So, it is important a technological network design also incorporates the social aspect, in most terms, the impacts on society derived from this practice, to be able to fully measure the impact of possible IS connections (Neves et al., 2020).

1.2.2. Social challenge of IS of water in chemical parks: the need of collaboration of stakeholders

Many studies have been conducted to focus on optimizing material and energy flows within industrial parks, but less attention is paid to social aspects, leading to that many industrial symbiosis opportunities disappearing. However there are many failed attempts, there are examples of EIP´s in practice. The notable thing is that these EIPs are mostly located in China and Korea (Tian et al., 2014). These are top-down regulated countries, meaning most of the decisions relevant to a high amount of inhabitants, are taken by the government, and the inhabitants do not have an influence on these decisions. Figure 1.2, shows this disparity between EIP cases in each country. Apart from the imbalance in the volume of published research, the number of industrial symbiosis cases in each country is also depicted through the varying subdivisions within each bar (Neves et al., 2020). China, where there is a higher prevalence of industrial symbiosis, is justified by the implementation of public policies. The findings indicate that industrial symbiosis can bring about significant environmental advantages, and highlight that economic incentives - such as tax preferences, financial subsidies, and the benefits derived from material substitution - resulting from stricter environmental regulations, are the primary motivators for stakeholders to engage in industrial symbiosis.

Researchers suggest in other parts of the world where EIP's should be created bottom-up, it is harder to generate a practical EIP (Huang et al., 2019). Within the US, many EIP projects failed to come to fruition or have transformed and fallen back on traditional industrial practices (Perrucci et al., 2022). This is because the stakeholders themselves are often reluctant and hard to convince to use other stakeholders' wastewater. They play a crucial role in the prevention of full implementation of an EIP (Valenzuela-Venegas et al., 2018). Other factors play a role than only wanting to become more sustainable. Researchers suggest that especially industry participants are hard to convince to take part in industrial symbiosis with the resource water. It intensifies important social dilemmas of trust and security if economic viability is questionable (Gibbs & Deutz, 2005). More connections could mean more failures as this is propagated through a network (Zeng et al., 2013). But it is not specifically known and researched in literature, what specific decision aspects influence (and to what extent) the decision-making process for stakeholders within a chemical park to prevent industrial symbiosis of water from happening.

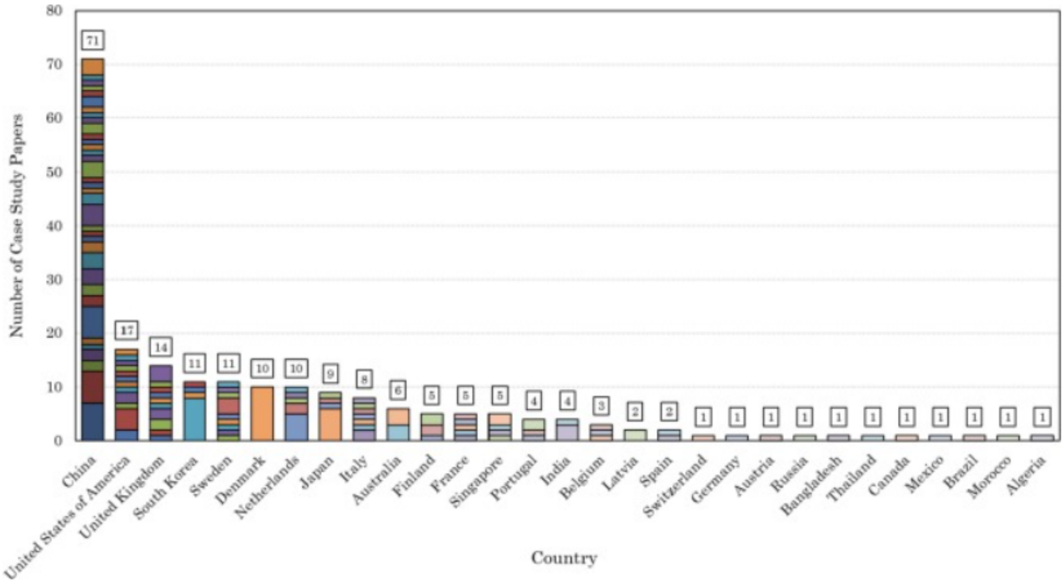

Figure 1.2: The number of studies conducted on the practical workings of EIPs globally, source (Neves et al., 2020)

To be implemented effectively, IS water network design requires a combination of technical and social factors (Cagno et al., 2023). This research will present an innovative approach to IS water network design that includes the influence of some decision criteria on the stakeholder's behaviour in determining the optimal design, regarding costs, recycled water, and resilience. The next section will further introduce the problem statement and this research.

1.3. This research: problem statement, research objective and relevance to the EPA program

This section aims to provide a comprehensive overview of the research presented in this thesis. The discussion begins with an introduction to the research problem. Subsequently, the research questions are formulated and the thesis structure is presented.

1.3.1. Problem statement

Combining the findings from the literature review, it becomes clear that the urgency for less fresh water usage and wastewater generation for stakeholders within the chemical sector is high. Their next step is to reuse more water between chemical plants, called industrial symbiosis. But in practice, when analysing EIP's this does not happen, especially in bottom-up regulated regions, as other factors than technical factors play a role. Social aspects like trust and resilience could be impacting factors on the behaviour of stakeholders in deciding to take part in an IS water network within an EIP. The behaviour of these stakeholders should be incorporated into the current IS water networks to see if optimization could still be applied within these parks. However, it is not known which social aspects specifically influence, and to what extent, the behaviour of the stakeholders and therefore the performance of these wastewater networks. Therefore, the following research question has been identified.

Research Question

To what extent is industrial symbiosis of water within chemical parks possible, taking into account stakeholder behaviour?

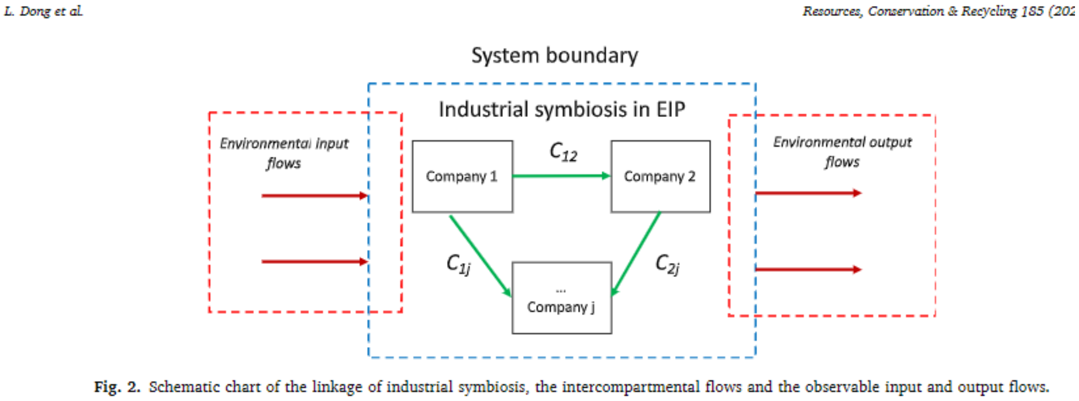
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Fig. 2. Schematic chart of the linkage of industrial symbiosis, the intercompartmental flows and the observable input and output flows.

Figure 1.3: Schematic chart of the system boundary of IS water network, the involved stakeholders and the observable water flow.

1.3.2. Goal of thesis

According to Song et al. (2018), stakeholders may have varying opinions about joining IS water networks, which could affect the effectiveness of the network. This thesis aims to research from a technological perspective whether IS water network designs can still have an industrial symbiotic performance even if certain stakeholders choose not to participate. The system boundary of the IS water network is visualized in Figre 1.3. Specifically, the study will explore the impact of decision criteria and stakeholder decisions on the technological system. The research will examine whether a particular network design, containing a specific set of components, such as one with a central treatment facility or more decentralized water treatment facilities, is more resilient to the decisions of stakeholders.

To measure the resilience of different network designs, the study will analyze the trade-offs between technological network components and decision criteria. If an IS water network design can still operate effectively, meaning enough water is recycled, even when certain stakeholders are not participating, it will be deemed sufficiently resilient. By exploring the relationship between technological components and decision criteria, this study aims to provide insights into the development of more effective and sustainable IS water networks.

1.3.3. Sub questions

To be able to answer this main research question, some other questions also need to be answered. The sub-questions in this research are:

1. How is water currently used within chemical parks and which aspects are relevant for industrial symbiosis?
2. What are important criteria to assess industrial symbiotic performance within a chemical park and how can these be measured?
3. Which stakeholders should be involved in industrial symbiotic wastewater networks and what are their decision criteria for joining such a network?
4. How could the impact of stakeholder behaviour on the industrial symbiotic performance of a water network within a chemical park be tested?
5. What is the effect of the different decision criteria on the industrial symbiotic performance of wastewater within chemical parks?
6. Which trade-offs between different technical components and decision criteria can be identified from analyzing the industrial symbiotic performance metrics?
7. When is the industrial symbiotic performance within chemical parks the highest?
8. What are the most important implications for policy-makers from this research?

1.3.4. Link to EPA master programme

This thesis was written to obtain the MSc. degree for the Engineering and Policy Analysis (EPA) programme at the Delft University of Technology. The EPA program is dedicated to addressing major global challenges by taking a multi-stakeholder approach to socio-technical systems. One of the key objectives of the EPA program is to provide policymakers with valuable insights using modelling techniques and to facilitate the integration of technology and society. This research aims to make a contribution to the grand challenge of water scarcity and aims to bridge the gap between the technological optimisation networking models and the more social studies focusing on the influence of stakeholders and the potential of IS. Advanced modelling techniques are applied to be able to design a system that incorporates all important aspects to measure industrial symbiotic performance. A multi-actor perspective is taken to learn more about the preferences of the involved stakeholders. Eventually, a piece of advice will be given on how to design an IS water network in a way the chance of a successful implementation is higher than currently.

1.4. Structure of the Report

This report includes a comprehensive analysis of the research conducted. The research methodology and report structure are illustrated in Figure 1.4. This introduction provides a background to the research topic, introduces the concept of Industrial Symbiosis as a socio-technical system, and outlines the research questions. Chapter 2 investigates the exact water usage and wastewater flows in chemical parks, the system criteria to measure industrial symbiotic performance and the most relevant literature for existing optimal IS water network designs. Chapter 3 gives an overview of the involved stakeholders and their decision criteria for joining an IS water network. Based on the findings, the report identifies the most significant decision criteria that should be considered when designing an Industrial Symbiosis water network. Additionally, the report identifies a significant research gap, which will serve as the foundation for the subsequent chapter. In Chapter 4, the model used in the research is introduced. The model consists of two parts: the design of the technical optimization model and the design for the social interaction model. Chapter 4 will provide the high-over design. Chapter 5 defines all the steps of which the technical optimization model exists and explains the linked simplifications made in the model. Moreover, the method for the optimal water network design will be presented and explained. In Chapter 6, the method for the social interaction part of the model will be presented and explained. Moreover, the different social scenarios that are used in the model are introduced. The model that has been created is generic: it can be used to find an optimal IS water network design for any chemical park. In Chapter 7 the data input for the model is discussed, the experimental setup is given and the model is verified. The results of the model are presented in Chapter 8 and the impact of several incentives are given. In Chapter 9, the report presents the validation of the results obtained for the various Industrial Symbiosis water networks. This validation is achieved by comparing the results with those of previous research and actual data obtained from an interview, and by testing the results for sensitivity. Following the validation, Chapter 10 discusses the implications of the research results for chemical park owners and policy-makers and highlights any limitations of the research. Lastly, Chapter 11 presents the answers to the research questions and provides recommendations for future research.

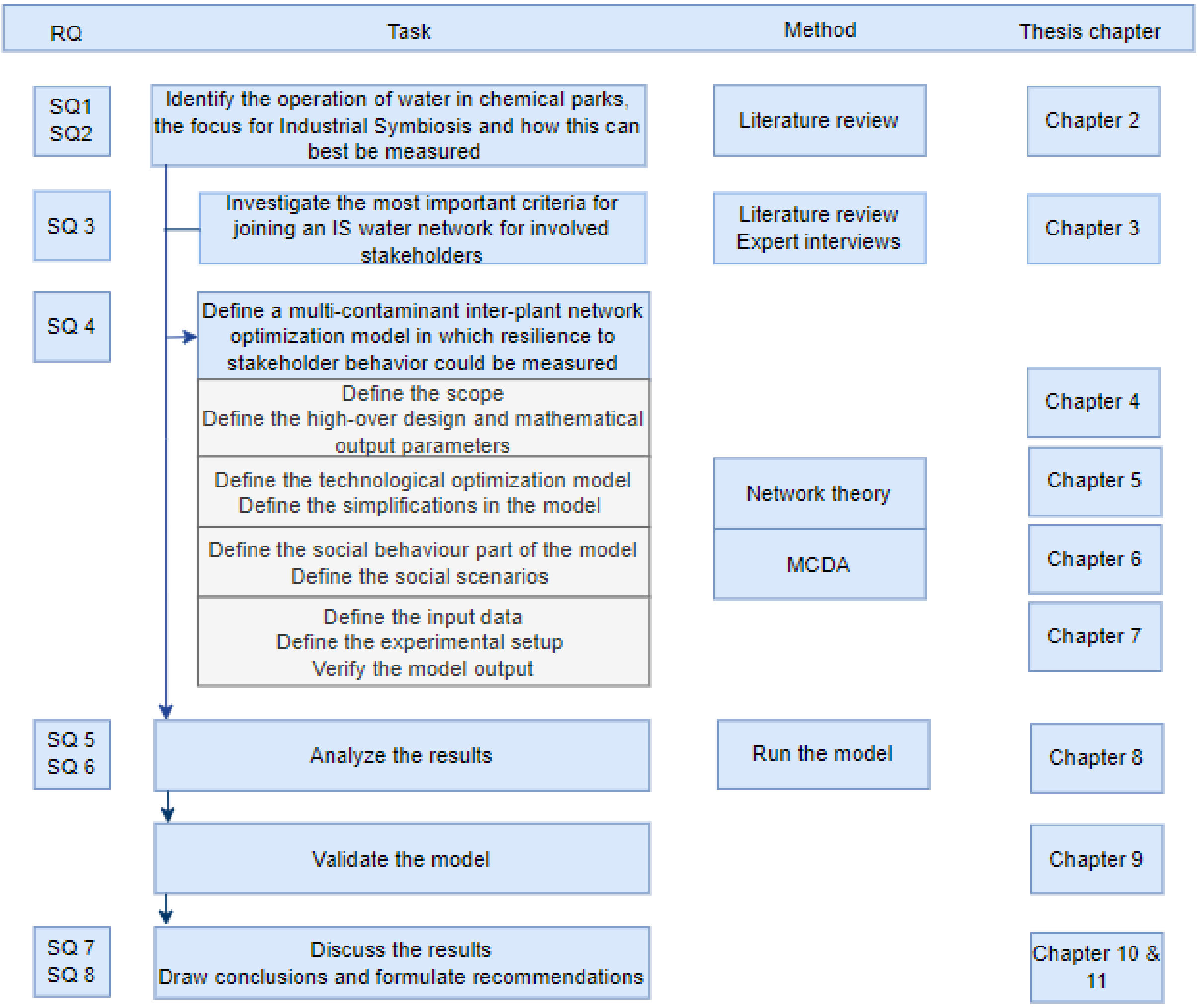


Figure 1.4: Schematic overview of the structure of this thesis report

2

Literature Study: water usage in chemical parks and methods for measuring the industrial symbiotic performance

To gain insight into the optimal design of an IS water network of a chemical park, and into the resilience towards stakeholder behaviour of this design, a model needs to be constructed that could perform network analysis, as explained in Chapter 1. Multiple objectives need to be analyzed and the number of parameters to consider in this analysis is too large to find an optimum by hand. This model should represent the most characteristics possible from a water network in a chemical park in reality. To obtain this model design, the working of a water network in a chemical park will have to be elaborately analyzed. Moreover, the model should represent an optimal design of a water network. Multiple studies have already researched possible optimal designs for (waste) water networks in industrial parks. This research can therefore use previous research to build an optimal design. To decide what the standards are for an optimal design, performance metrics need to be defined. This chapter sets out to identify the most important concepts and components of water networks in chemical parks first. Secondly, the most important performance metrics of an IS water network are defined. Lastly, the most relevant developments in the field of optimal IS water network designs are discussed and afterwards discussed in more detail according to an overview.

2.1. Water usage and wastewater flow in chemical parks

This research will focus on the industrial symbiotic performance of water within chemical parks. Therefore, it is needed to study in the literature what factors are important considering the usage of water in chemical parks, how water is used within chemical factories, what happens with the wastewater and what are possibilities to reuse wastewater. This information forms the basis of the research.

2.1.1. Quality standards of water for a chemical factory

The most important factor considering the usage of water in chemical parks is the quality of the water. As such, the use of possibly polluted water that contains heavy metals or other contaminants in this manufacturing process could lead to the production of imprecise and faulty end products. If the products produced are for human use, it could pose a risk on the health of the human. So, controlling and maintaining the quality of the water to a certain quality is crucial.

Quality standards for water used at chemical factories are set by regulatory agencies. Such as the Environmental Protection Agency (EPA) in the United States or the European Union's Water Framework Directive. These standards are based on scientific research and are intended to protect public health and the environment from potential contaminants in water used for industrial purposes (EuropeanCommission, 2000). The quality standards for water used at chemical factories can vary depending on the intended use of the water. For example, water used for cooling or washing may have different quality standards

Parameter	**Factory that manufactures paint**	**Factory that manufactures vitamin A**
pH	Between 6.0 and 9.0	Between 6.5 and 8.5
Total suspended solids (TSS)	50 mg/L	20 mg/L
Chemical Oxygen Demand (COD)	250 mg/L	300 mg/L
Heavy metals	Not contain lead, cadmium and mercury	Not contain lead, cadmium and mercury
Nutrients	Limited level of e.g. nitrogen and phosphorus	Limited level of e.g. nitrogen and phosphorus
Organic solvents	-	Limited amount of solvents in the water

Table 2.1: Differences in quality standards of specific parameters for water for chemical factories

than water used for manufacturing processes (K. Liu et al., 2022). The quality standards for water used at chemical factories typically include limits for specific parameters such as:

- Physical parameters: These include pH, temperature, turbidity, and total suspended solids (TSS), which can affect the efficiency of chemical reactions or cause fouling of equipment.
- Chemical parameters: These include limits for specific chemicals such as heavy metals, organic chemicals, and nutrients like nitrogen and phosphorus, which can be harmful to human health and the environment.
- Microbial parameters: These include limits for harmful bacteria, viruses, and other microorganisms that can cause waterborne illnesses.

The water quality standards for a specific chemical factory will depend on the specific chemicals used in the manufacturing process, as well as the local and national regulations that apply (Lyu et al., 2020). The purpose of the factory defines which certificates are given containing the quality standards of the water. For example, the water quality standards for a chemical factory manufacturing paint are less strict than water quality standards for a chemical factory manufacturing substances for vitamin A, which is used in food (AkzoNobel, 2021). Table 2.1 shows the differences in requirements.

Chemical plants have installed several monitoring technologies to ensure the water that enters the factory always meets the requirements (K. Liu et al., 2022).

2.1.2. Wastewater generation within chemical parks

In the context of chemical factories, it is observed that all the water utilized within their operations becomes contaminated, resulting in a continuous degradation of its quality. This contaminated water also referred to as wastewater, is defined as any water that has been polluted or altered due to human activities. In the context of industrial parks, it is generated at any given time as a byproduct of various industrial processes (Long et al., 2018).

In comparison to other industrial sectors, such as food and beverage manufacturing or electronics manufacturing, the chemical industry tends to generate a higher volume of wastewater (Abdel Wahaab & Alseroury, 2019), (Valta et al., 2015). This can be attributed by the fact that within chemical factories for each product manufactured, chemicals need to be added. Examples of these chemicals are nitrate, methanol, ammonia, and barium. According to a research from The United States Environmental Protection Agency, did the chemicals within the water released by chemical companies in 2021 consist for 90% out of nitrate compounds (Gadipelly et al., 2014). Nitrate compounds are a class of chemicals that are relatively low in toxicity to humans. However, in waters where nitrogen is scarce, nitrates can contribute to the growth of algae, ultimately leading to eutrophication of the aquatic environment. Most of the other chemicals form risks for the environment or humans if they exist in the water in high quantities. This is why the quality of the water downgrades containing a selection of these chemicals. However, it does differ per chemical process what quantity of the chemicals are added to the water (K. Liu et al., 2022).

2.1.3. Wastewater treatment by treatment facilities within chemical parks

The proper treatment of wastewater in a chemical park plays a crucial role in mitigating pollution and safeguarding the environment. Effective treatment processes can eliminate hazardous pollutants and contaminants from the wastewater, rendering it safe for either disposal, reuse, or other end-use (J. Liu & Tang, 2018).

To get the water a certain quality, it is processed by treatment facilities. It is restricted by law in multiple countries globally to have at least one central wastewater treatment facility located on a chemical park, to assure the level of contaminants does not exceed the regulatory limits (Navarro Martínez et al., 2020). In China, it was requested as an indispensable and mandatory infrastructure in Chinese national industrial parks (NIPs) since 2015 for example. Two main wastewater treatment models exist for chemical parks, shown in Figure 2.1.

The first model, the upper network in Figure 2.1, which is widely employed in Chinese industrial parks, requests the individual enterprise to treat its wastewater in a plant with at least secondary treatment technology (explained in next paragraph) to commit to the requested emission limits, and then discharge it into the central wastewater treatment facility, in the park for further treatment to meet national environmental discharge standards (Yao et al., 2017). In these cases, it is necessary to subject-specific wastewater streams originating from particular factories to pre-treatment before they can be discharged into the pipes that transport them to the central treatment facility, as the wastewater is too polluted (Yao et al., 2017). These factories often construct dedicated wastewater transmission pipelines to facilitate the grouping of diverse types of wastewater before connecting to a common wastewater gathering pool (J. Liu & Tang, 2018).

The second model, the bottom model in Figure 2.1, the individual enterprise sorts its wastewater and does not necessarily treat the wastewater. Then it transports the wastewater in separate pipes towards wastewater treatment facilities located in the park. The central wastewater treatment facility will intentionally mix the wastewater from different enterprises and treat with tailored technologies according to the pollutant's characteristics (Lyu et al., 2020).

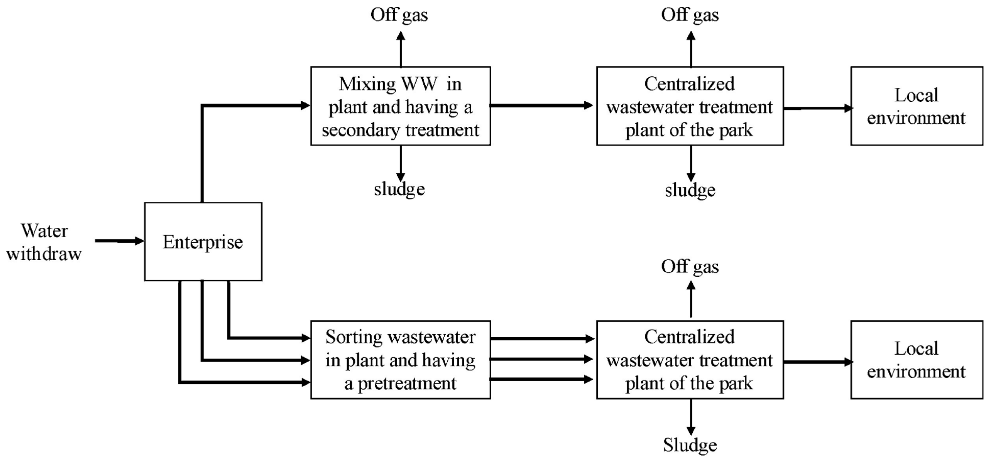


Figure 2.1: Generalization of the two typical wastewater treatment models in industrial parks, source: Lyu et al., 2020

The selection of wastewater treatment systems is contingent on a number of factors. It depends on the requirements for the quality of the wastewater of that certain government and the quality of the water after it has been used by the chemical factory on which treatment technologies are installed (O'Dwyer et al., 2020). As reported by both Sousa et al. (2002) and Lyu et al. (2020), the wastewater treatment methods utilized in chemical parks around the world vary widely. Some chemical plants treat their wastewater individually, while others send all the wastewater produced in the area to a single treatment plant.

Navarro Martínez et al. (2020) argues the model with multiple separate treatment facilities, shared by different companies in the park, combining wastewater stream, works best. EPSC (2005) states one of the main advantages of a chemical park is that wastewater can be treated in shared treatment facilities. However, the study of Hu et al. (2019) states that in China the model with all inhouse treatment facilities works fine.

Since the input of the various companies into the shared wastewater treatment facility has a major influence on the performance of this facility and thus on the quality of the treated wastewater, it is very important to check that the correct licenses have been obtained from the authorities and that the contractual relationships between the companies generating the wastewater and those treating it are appropriate (Sousa et al., 2002).

A difference exists in the advancement of the treatment facilities. Primary, secondary and tertiary treatment can be distinguished. Primary and secondary treatment typically get wastewater only clean enough to discharge safely into the environment. In contrast, tertiary treatment has the capability to achieve high levels of water purification that render the water safe for reuse in water-intensive processes or even as potable water, as noted by Kaviya (2022). These treatment levels are defined by the treatment technologies it consists of.

Over more than 110 treatment technologies exist. Treatment technologies are often combined within one treatment facility to filter as many contaminants (suspended solids and COD) out of the water. The removal efficiencies differ per technology. Filtration, fermentation and bioreactors are examples of treatment technologies (Topare et al., 2011). The most efficient treatment technology is anaerobic-anoxic-oxic membrane bioreactor. This is a technology that is part of the advanced oxidation processes (AOP's), and filters almost 100% of the suspended solids out of the water and 100% of the COD out of the water. AOPs are significant, promising, efficient, and environmentally friendly technologies for removing persistent organic pollutants (POPs) from waterways and wastewaters (Oturan & Aaron, 2014). So, it is possible to generate treated wastewater out of a treatment facility that is almost clean for 100%, however, this treatment technology is very expensive. Aerobic biological treatment is the most popular (86%) and relatively cost-effective technology employed by wastewater treatment facilities, according to an assessment of 51 industrial parks in China. The removal efficiencies of these aerobic biological treatment facilities are on average above 90% (Lyu et al., 2020). Appendix A consists of all information of the three different treatment technologies that will be considered in this research.

2.1.4. Wastewater flow after treatment

After wastewater is treated by a treatment facility at a chemical park, the treated water can be reused for certain non-potable purposes or discharged into receiving water bodies such as rivers, lakes, or oceans. The specific method of disposal will depend on the quality of the treated water and the local environmental regulations. In some cases, the treated water may be suitable for reuse within the chemical park. For example, it may be used for cooling water or in manufacturing processes that do not require high-quality water. Reusing treated wastewater within the chemical park can help reduce the demand for freshwater resources and lower overall water consumption (Agrawal & Verma, 2022).

In recent years, more focus is given towards the reuse of resources in industrial parks, of which water is part as well. As has already been introduced in Chapter 1, this solution is industrial symbiosis in eco-industrial parks. According to Navarro Martínez et al. (2020) and Tiu and Cruz (2017), the actual reuse of treated wastewater for other chemical companies, could be possible. Neves et al. (2020) constructed a new design for IS in a chemical park, shown in Figure 2.2. In this figure is shown that the wastewater is treated, and the water is reused again by a chemical factory. In Chemelot, Brightsite, the research company for sustainability in Chemelot is also researching the option for reusing the effluent from the central treatment facility. However, as also stated by Brightside (2021) and Navarro Martínez et al. (2020), the actual effluent reuse does not happen yet.

This can be substantiated by the fact that it is technically difficult to treat the highly complex wastewater stemming from the chemical factories to a quality it can be used again by chemical factories. Most treatment facilities that are located in chemical parks nowadays are equipped for treating the water to a level it can be discharged into nature. Requiring less advanced treatment technologies (J. Liu & Tang, 2018). Moreover, additions to the existing infrastructure of the park have to be made as currently the right infrastructure often lacks (Tiu & Cruz, 2017).

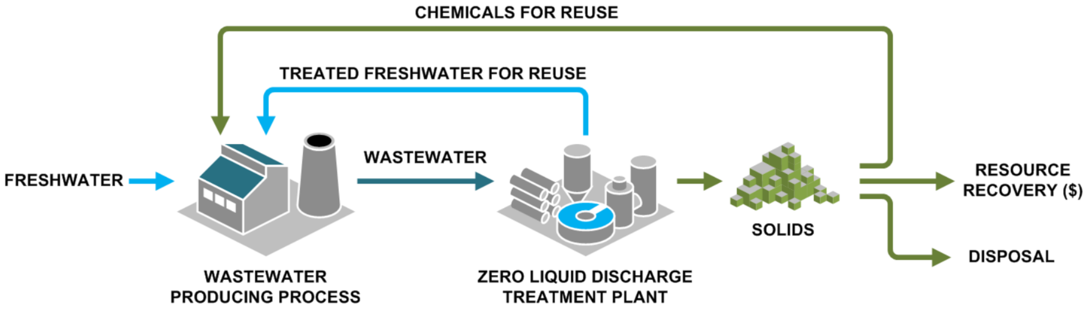


Figure 2.2: Water flow within an Eco-Industrial Park, source: Neves et al., 2020

2.1.5. Conclusion from section 2.1

What can be concluded from section 2.1 is that the quality of the water is the most important factor in the water usage within chemical parks. The quality of the water always downgrades in chemical factories as different chemicals (all having different effects on the environment and human) are added to the water. This water needs to be treated within the chemical park by a treatment facility before it gets disposed into nature again. The chemical park can be structured in different ways according to the treatment facilities. No consensus exists on which model, with inhouse treatment facilities or separate treatment facilities, works most efficient in chemical parks. Multiple different kinds of treatment technologies exist, all treating different parts in the water. Sets of treatment technologies exist that treat the water up to a 100% quality again, however, these technologies are very expensive. In recent years, more focus is given to reusing the treated water from treatment facilities not only for cleaning or cooling purposes within chemical parks, but also for the actual chemical processes. Possibilities exists for this, however often no additional components are implemented yet enabling this reuse within chemical parks.

2.2. Designing Eco-Industrial Parks and Industrial Symbiotic Performance of water

The introduction has provided an explanation of Eco-Industrial Parks (EIPs) and the potential benefits of increased wastewater recycling in chemical parks. Furthermore, it has been argued that designing an effective EIP represents a socio-technical challenge. However, in order to construct a model for researching whether industrial symbiotic (IS) performance can be improved, it is necessary to identify the key elements of EIP design. In the previous paragraph, the key elements and components of a water network of a chemical park have been identified. This paragraph will focus more on the identification of additional crucial factors in designing a wastewater network for an EIP and to determine the most significant criteria for assessing IS performance in EIPs based on the existing literature.

2.2.1. Important aspects in the design of Eco-Industrial Parks regarding water reuse

In paragraph 2.1, several reasons are given that explain why it is technically challenging to recycle wastewater in industrial parks. However, if in the design of an EIP in which wastewater is reused, several steps are incorporated that are carried out precisely, the technical challenges can be addressed (Tiu & Cruz, 2017).

Roberts (2004) argues the first phase of designing an IS water connection is understanding the water needs of the different plants located on a park. This involves identifying the quantity and quality of water required by each factory, as well as the types of contaminants and by-products that are generated.

The second phase, explained by Rubio-Castro et al. (2012) and Tiu and Cruz (2017) is designing the water reuse system. This involves identifying potential uses for these water streams in other factories within the park and analyzing the locations. A crucial element for IS of water is geographical proximity. The design of an eco-industrial park should consider the water needs of different industries and aim to integrate water-using industries in close proximity to one another to facilitate the sharing of water resources. Moreover, within the optimal design, treatment facilities should be incorporated (O'Dwyer et al., 2020).

The third phase, after the optimal designs have been created, involves creating trust and collaboration between different industries within the park. For an effective IS design, the development of strong relationships and collaborative partnerships between park stakeholders should be prioritized as their collaboration is very important (Ashton, 2011), (Hein et al., 2017).

Lastly, effective monitoring and evaluation are essential for ensuring that the water reuse system is operating efficiently and that water quality standards are being met. The first step in designing monitoring and evaluation systems in establishing performance indicators for EIP's according to which the EIP's can be analyzed (Roberts, 2004), (Tudor et al., 2007).

Overall, the design of industrial symbiosis of water within industrial parks should prioritize understanding the water needs of different industries, identifying opportunities for water reuse, designing an efficient water reuse system including locations, establishing trust and collaboration, and implementing effective monitoring and evaluation indicators and systems. Effective design can help to optimize the efficient use of water resources and promote sustainable industrial development.

2.2.2. Criteria defining the Industrial Symbiotic Performance of a chemical park

As highlighted in the preceding paragraph, the establishment of distinct performance indicators for water symbiosis in EIPs is crucial in enabling effective monitoring. However, the measurement of performance appears to be essential for encouraging the execution of better activities, benchmarking outcomes, and successfully communicating them to various stakeholders. Despite the growing interest in this area, a robust performance measurement system pertaining to the ecological and ethical transition is yet to be established (Cagno et al., 2023). According to Agarwal and Strachan (2006), the growth of industrial symbiosis is hampered by a lack of thorough assessment methodologies. Park and Behera (2014) support this claim by discovering that there is no commonly acknowledged approach for evaluating the success of industrial symbiosis networks. However, Neves et al. (2020), Fraccascia and Giannoccaro (2020), Yu et al. (2015) all argue that the performance of industrial symbiosis of water will always be related to the economic, environmental, and social topics. As the initial goal of IS in industrial parks is to minimize waste, and build sustainable economic, ecological, and social relationships (Alexander et al., 2000). Moreover, Chopra and Khanna (2014) stated "*IS studies the interaction of industrial development with environmental, social, and economic systems of different scales and aims at increasing business success, preserving environment and taking into account the life of local community*". The World Bank Group, defined together with the United Nations Industrial Development Organization, an international framework to assess the performance of Eco-Industrial Parks. In this framework, the three criteria on which the performance is based, are again economic, environmental and social indicators (Organization et al., 2017). So, the criteria for defining the Industrial Symbiotic Performance of water in a chemical park will always be related to economic, environmental and social performance topics.

Environmental performance
This criterion measures the environmental impacts of the water-related IS exchanges within the park. This involves assessing the ability to reduce water intake of high-quality water, also known as water efficiency (Jacobsen, 2006). Also, measures relating to the efficacy of the water reuse system in recovering resources from wastewater streams. This included determining the quantity and quality of recovered resources, such as nutrients, energy, and materials (Yu et al., 2015). Moreover, the potential environmental risks associated with wastewater treatment and disposal of these exchanges within the park could potentially be assessed (Jacobsen, 2006).

Economic performance
This criterion measures the economic benefits and expenses of water-related IS exchanges within the park. This involves assessing the cost-effectiveness of the water reuse system and the financial benefits

of resource recovery. This is measured and discussed as a mix of investments at the time of initiation, and direct and indirect economic savings resulting from upstream or downstream water-related concerns (Jacobsen, 2006). Moreover, studies typically attempt to evaluate the investment and operational costs and savings for each of the participants that partake in IS activities (Ashton, 2011).

Social performance
This criterion measures the social benefits and impacts of the water-related IS exchanges within the park. This involves assessing the social benefits of reduced water consumption and resource recovery, as well as the potential social impacts of wastewater treatment and disposal on local communities, measured as job creation and retention (Domenech et al., 2019). Secondly, the effectiveness of collaboration and governance structures in supporting water-related IS exchanges within the park is part of the social criterion. This includes evaluating the quality of stakeholder participation, decision-making processes, and conflict resolution systems. In the research of Fraccascia and Giannoccaro (2020), in which 638 research papers have been analysed related to the performance of IS, only in two papers has the social performance actually been addressed.

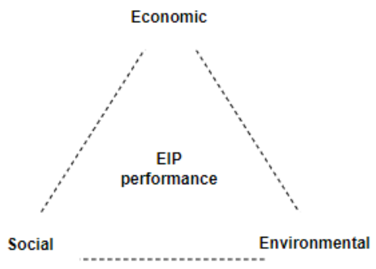


Figure 2.3: Visualization of the factors of which EIP performance exists

2.2.3. Conclusion from section 2.2

In summary, different aspects are important in the design of an Eco-industrial park. Besides understanding the water needs, optimal allocation of IS water connections with treatment facilities and chemical factories in close proximity, creating trust between the different stakeholders in the park, defining performance indicators for water symbiosis in Eco-Industrial Parks are crucial for effective monitoring and communication. The criteria for defining Industrial Symbiotic Performance of water in chemical parks are economically, environmentally, and socially related, shown in Figure 2.3. Environmental criteria involve reducing water intake and assessing resource recovery. Economic criteria measure cost-effectiveness and financial benefits. Social criteria evaluate job creation and retention, collaboration effectiveness, and governance structures. A robust performance measurement system for the ecological and ethical transition is yet to be established.

2.3. Measuring the Industrial Symbiotic Performance of water in chemical plants

In the previous sections, the water usage within chemical parks is described and the according wastewater streams and treatment of the wastewater are defined. Possibilities and examples are given on how wastewater could be reused again after it has been treated. Moreover, the most important aspects for designing and eco-industrial park have been defined and the criteria for defining the IS performance are derived. In this section, an analysis will be pursued of what technical methods there are to research a change in the industrial symbiotic performance of a chemical park and which suits this research the best. Moreover, the last paragraph identifies existing studies using this method.

2.3.1. Categorization of Industrial Symbiotic Performance measure models of water: relevant methods

As argued in the previous paragraph, the methods for measuring the IS performance should be able to analyze the economic, environmental, and social performance of an IS water network/EIP. Azapagic and Perdan (2000), Lütje and Wohlgemuth (2020), and Cagno et al., (2023) argue that to measure the performance of IS it is crucial to measure the difference between the input and output of the system.The system requires inputs of financial, human, and environmental resources, while simultaneously producing outputs in the form of economic, social, and environmental impacts. This makes it possible to assess the effectiveness of an IS water network within a chemical park in a quantitative manner. This quantitative assessment of an EIP is required to help identify comparisons between different configurations and to support decisions on its design (Lütje & Wohlgemuth, 2020).

According to the comprehensive research of Fraccascia and Giannoccaro (2020), in which 638 publications are analyzed that use specific research methods to measure the industrial symbiotic performance, can the methods to measure the industrial symbiotic performance of networks, be divided into four main methods. In particular, Life Cycle Assessment (LCA), Material Flow Analysis (MFA), emergy and exergy analysis and network analysis (Fraccascia and Giannoccaro, 2020).

Life Cycle Assessment (LCA) is a method used to evaluate the environmental impacts of a product, service, or technology throughout its entire life cycle, from raw material extraction to disposal. Finkbeiner (2014) define it as a methodology that assesses the (potential) environmental impacts of a product, service, or technology from ”cradle to grave”. In a study by Daddi et al. (2017), two scenarios were compared using LCA with average data: one where industrial symbiosis initiatives are implemented and another where they are less developed, in order to determine the impact category results.

Further, Material Flow Analysis (MFA) is regarded as the fundamental approach for mapping physical material flows and stocks across a particular system. This approach is effective for determining the environmental load on the system and determining how economic activities affect the environmental performance of the system under consideration (Brunner & Rechberger, 2016). In their study, Sendra et al. (2007) applied the indicators obtained from Material Flow Analysis (MFA) to assess the efficiency and materialization ranks of an industrial area situated in Catalonia, Spain. Although the area had a diverse range of industries, the researchers were able to use basic data to identify companies with high consumption and inefficiency by utilizing these indicators. Specific to water, the MFA method can be executed in the form of hydraulic modelling (Sendra et al., 2007).

Borgatti et al. (2009) stated: *’Network analysis is a methodology that uses quantitative methods to analyze physical and social interactions among entities belonging to a system*. The system is conceptualized as a network, consisting of nodes and links. In this context, each node represents a specific entity, and the relationship between two entities is represented by a link between the corresponding nodes. Network analysis can model various types of links, including material and energy flows, information, financial transactions, and even social interactions (Fraccascia & Giannoccaro, 2020). Faria et al. (2022) included a network analysis in the research to identify water reuse opportunities and optimize the network design. The methodology was tested in a Brazilian industrial park, and it was discovered that water reuse might cut freshwater usage by up to 60%.

The four categories mostly supply complimentary information and need the computation of distinct abilities. However, they differ in terms of data and information required and computational effort. Most importantly, it becomes clear that network analysis is the only method that incorporates the social aspect, as social interactions between stakeholders in the IS water network. The social aspect is an important criterion to measure the industrial symbiotic performance, mentioned in paragraph 2.2.2. But, contrary to environmental and economic criteria, social criteria are more complex to incorporate into the method as data for their quantification is more difficult to obtain. The review of Fraccascia and Giannoccaro (2020) also emphasized that the method network analysis used to quantify the impacts and to analyze the network of industrial symbiosis was the most used in the analysis of the case studies. So, network analysis is the only method in which the social aspect can be analysed, besides the environmental and economic aspects, and it is the most used method for quantifying the impact of IS.

2.3.2. Relevant information regarding network analysis of industrial symbiosis of water within chemical parks

In the previous section, it was concluded that the method of network analysis suits best to measure all aspects of the industrial symbiotic performance. This section aims to provide a more comprehensive understanding of the potential applications of network analysis in the context of IS water networks within chemical parks. Network analysis is an effective method to evaluate the complex wastewater distribution network within a chemical park, identifying the locations and flows of wastewater streams. By analyzing this network, researchers can identify potential opportunities for wastewater recycling and determine the most effective locations for treatment and reuse (Galán & Grossmann, 2011). To enhance the efficiency of an industrial plant, it is essential to incorporate not only advanced treatment technologies and a robust process control system but also a layout that guarantees the most efficient route for each waste stream. This challenge requires the optimal design of a wastewater treatment network (WWTN) (Ahmetović & Grossmann, 2011). Many papers have been written proposing new optimal designs for wastewater networks. However, not yet specifically for chemical parks, while the potential for more effective allocation and treatment of wastewater in chemical parks is high.

Lyu et al. (2020) researched that because of all the different water qualities in chemical parks, individual chemical factories and treatment facilities tend to look only at their relevant water streams.

H. Liu et al. (2019) analyzed the treatment performance of a plant in a comprehensive industrial park with that of a chemical industrial park considering the entire park as a whole. The former received significantly higher scores compared to the latter. Due to the lower evaluation scores, the treatment issues at the chemical industrial park were identified, and corrective measures were implemented for the optimal allocation of treatment facilities regarding the different water streams. Following the implementation of these measures, the chemical park was reassessed as a whole, and its scores on the primary indicator for process improvement and the dependent performance regarding the downstream environment showed a significant increase.

Besides using network analysis for the optimal design of a wastewater network regarding costs and the amount of recycled water, social network analysis can also be applied. Social network analysis focuses on the structural relationships among actors. The network approach to policy-making is distinct from state-centric views, as it recognizes the importance of informal decision-making arrangements and the participation of non-state actors (Adam and Kriesi, 2007). Social network analysis can be used to identify the structural patterns of actors involved in planning processes, including those outside formal institutional settings (Scholz and Wang, 2006). This is particularly relevant for assessing natural resource and water management, which often involves decentralized decision-making and implementation structures, rather than top-down approaches (Lienert et al., 2013).

Nevertheless, some limitations have been detected when utilizing the network analysis approach. In designing an optimized network through network analysis, the extent of the scope may have a significant impact. The involved actors or instances may significantly alter the network's efficiency, and this choice of scope must be made at the outset of the analysis. Moreover, when using social network analysis, data is needed to identify the social relations. However, this data is often absent, as it are qualitative relations, or this data is often biased (Doménech & Davies, 2009).

2.3.3. Relevant studies in the field of wastewater network optimization algorithms

In the previous paragraph, the opportunity of designing optimal wastewater networks with network analysis for chemical parks has been discussed. The industrial symbiotic performance of a wastewater network will be valued according to the economic, environmental and social aspects. In this paragraph, existing studies will be analysed to see what kind of optimal wastewater networks have already been designed and how the industrial symbiotic performance of these networks could be measured.

For a long time, optimization-based water network designs have been kept simple. No water loss, one water source, only two water contaminants, a single water treatment technology and most importantly, all within one industrial plant (Cheng & Li, 2020). Karuppiah and Grossmann (2006) was the first who designed a superstructure for a water network specifically for a chemical plant, including the parameters of different treatment processes and according to different removal rates. In 2012, the first optimal water network was designed to focus on EIP's, connections between different plants (Rubio-Castro et al., 2012). The model proposed in this study is based on a superstructure and considers both modifications within a plant and between plants. This includes relocating or reassigning existing treatment units, increasing the capacity or efficiency of existing units, installing new treatment units within participating plants or in a shared facility, and re-routing streams associated with these modifications. The model also allows for monitoring of changes in process performance resulting from these modifications. Inter-plant studies are typically solved as water allocation problems, where water must be distributed, treated, and discharged optimally between process units in each factory within the park and treatment facilities (Dong et al., 2022). K. Zhang et al. (2018) made a comparison between intra- and inter-plant optimal water networks within the steel industry. The results showed that improving the water efficiency at plant scale helps obtain optimal results. The freshwater consumption and total network cost have been reduced by 22% and 21% respectively via an optimal network integration strategy.

In 2017, the first water optimization network algorithm has been developed taking into consideration different water qualities (contaminants) and focused on EIP's, and connections between different plants (Tiu & Cruz, 2017). This study proposes a model that simultaneously minimizes the economic and environmental objective functions of an EIP through goal programming. This network represents the first attempt in the direction of how water networks would look within EIP's, especially within the chemical sector, in which water contaminants are an important factor, see Figure 2.4 (Tiu & Cruz, 2017). Cheng and Li (2020) made an extra addition to the multi-contaminant inter-plant wastewater network, namely the multi-commodity flow. Meaning, multiple contaminants flow through the same pipe, however, this method is computationally very intensive.

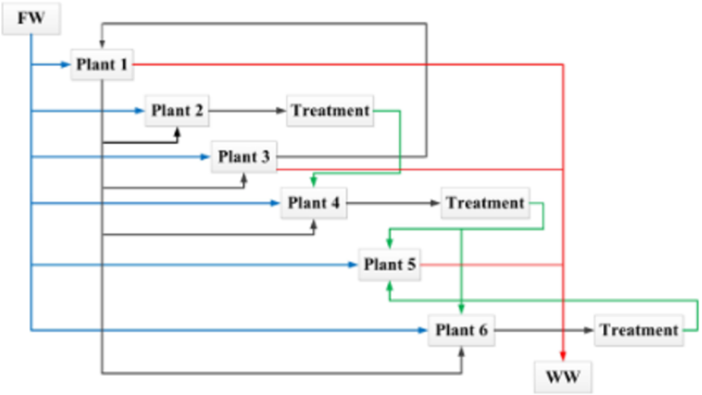


Figure 2.4: Waste water network containing multiple contaminants and multiple plants, source Tiu and Cruz, 2017

In most of these studies, the optimization network model has been constructed in a few steps. Initially, the study identifies all unit-scale water systems present in the industrial park and develops simplified unit models that serve as the fundamental element for the superstructure. Subsequently, the inter-plant superstructures are established to depict possible water network arrangements at both plant-scale and park-scale. Finally, using the unit models and superstructures as a foundation, a Mixed Integer Non-Linear Programming model is constructed. The total annual costs and total volume of recycled water are used as objectives to explore the potential for optimizing the water network within an industrial park.

Many studies have been conducted to focus on optimizing water flows and reducing costs for EIP's, summarized in Table 2.2. However, there is a lack of focus on social acceptance and site layout considerations (Dong et al., 2022). The first industrial symbiotic system that has been designed globally, Kalundbourg in Norway, already stated the social aspects of such a system are very important (Grann, 1997). The social aspect poses the greatest challenge in terms of mathematical formulation since it encompasses concepts that cannot be expressed numerically. According to Doménech and Davies (2009), there is a need for further empirical research to gain a better understanding of the exchange conditions and social control mechanisms that may impact the development of IS networks and the structural dynamics of successful IS networks.

Currently, no consensus exists on how social performance should be measured (Boix et al., 2015). In a literature review from Boix et al. (2015), different methods are enlisted. El-korchi and Millet (2011) conducted a study on the design of logistic channels that was not specifically focused on eco-parks, but included a social assessment based on the number of local labour hours generated through remanufacturing. In a more recent study, Hipolito-Valencia et al. (2014) put forth an optimization approach for designing interplant trigeneration systems that consider the social impact of their optimal solution in terms of job creation. Aviso et al. (2011) and K. Zhang et al. (2018) stated that within an industrial symbiosis design, if it is technically and economically an optimal design, the trigger will always be the willingness of the individual plants to participate. They considered the social impact as quantifying the satisfaction of the stakeholders and including their participation in the optimization model, researching the different influences of these stakeholders. If one plant is satisfied, it will be included in the overall model and the influences of stakeholders within the overall model could change. However, Boix et al. (2015) states it is not really an indicator of social effects, it could not guarantee any local social benefit.

As stated in paragraph 2.3.1 does the method of network analysis suit best for this research. The last method mentioned to quantify the social aspect within optimization methods is the only method that could be performed with network analysis. The inclusion or exclusion of certain stakeholders and the effect on their influence can be measured with social network analysis.

After 2012, more studies conducted research on the influence of stakeholders within IS water networks, using social network analysis. Social network analysis offers a more quantitative approach to investigate collaborative processes (Lienert et al., 2013). The social relations between the different stakeholders partaking in IS water networks were analyzed. Chopra and Khanna (2014) was the first to understand the social aspect, in terms of the influence of certain stakeholders in the Kaloundburg IS network. They identified the different relations between the factories, shown in 2.5. Zheng et al. (2012) and X. Zhang and Chai (2019) saw information sharing about their resource usage also as a condition for a link between stakeholders in a network. In 2018 Valenzuela-Venegas et al. (2018) analyzed the resilience of an EIP network. The research analyzed how social network metrics change if certain stakeholders fall out of the network. The study emphasized the possibility that stakeholders would not want to take part in an IS network, because their dependence would become too high. They measured the performance of the new structure of the network model according to different metrics, such as the stress centrality, betweenness centrality and network efficiency. X. Zhang and Chai (2019) executed a social network analysis on two separate industrial parks, analyzing the difference in resilience of the networks towards different stakeholder satisfactions. They compared the change in different social network metrics, such as the small-world effect and the network efficiency, with each other.

However, these papers did not research the links between the technical factors of a network and the social aspects. Moreover, not any paper has focused on the specific industrial symbiosis of water within chemical parks. Aviso et al. (2022) researched how stakeholder goals in industrial symbiosis could best be modelled. He concluded optimization-based techniques are the best suitable. Agent-based modelling is also an option, but the effect of IS performance can not be measured as good as the first method. This statement fits in well with the optimal network studies of wastewater networks. It proofs that linking stakeholder behaviour within optimal wastewater designs is possible. Moreover,Doménech and Davies (2009) claims that social network analysis should always be combined with an analytical tool that could analyze the 'material' conditions of IS. Social network analysis is a method of analysis but a prescriptive dimension can only be attained when complemented with other theories.

2.3.4. Conclusion from section 2.3

What can be concluded from this section is that network analysis is the best method for measuring all aspects of industrial symbiotic performance. With using this method, an optimal design can be created for a chemical park in which opportunities for wastewater recycling can be determined and the most effective locations for treatment and reuse. Especially within the chemical industry, the application of optimal water network designs is high. However, the current optimal water network design mostly incorporates the environmental and economic aspects, excluding the social aspect. This can be substantiated by the fact that it is difficult to quantify the social aspect. Different methods exist to quantify the social aspect within

Research	Objective	Method	Industry	Resource	Plant/inter-plant	Contaminants	Parameters	Economic metrics	Environmental measures	Social metrics
Cheng and Li (2020)	Design of a superstructure for multi-commodity flow formulation for the optimal design of wastewater treatment networks	Optimal network	All	Water	Plant	Multi-commodity flow	Source,sink,splitter,mixer,treatmentcenter,pipes	NA	Exact estimation of how much and which contaminants flow where	Different treatment centers/technologies
Tiu and Cruz (2017)	Design of an optimal water network in an eco-industrial park considering water quality	Optimal network	All	Water	Inter-plant	Multi contaminant	Source,sink,pipes, plants,treatment centers	Piping, operating, freshwater, wastewater and treatment costs	Volume and quality of water	NA
Dong et al (2022)	Combine ecological network method, and environmental and economic analysis to dynamically monitor and evaluate the EIP performance	Optimal network	All	Water and energy	Inter-plant	Single	Sources,sinks,pipes, plants	Product value of Eip - costs for resource, energy, waste treatment and operation	Water pollutants, waste pollutants, air pollutants	Network efficiency
Zhang et al (2018)	Mutli-scale water network optimization considering intra- and inter-plant integration	Optimal network	Steel	Water	Plant and Inter-plant	Single	Source, sink, plants, central treatment center, water systems, flow rate	Freshwater, wastewater treatment, desalination, pumping and piping costs	Water concentration	NA
Chopra and Khanna (2014)	Understanding resilience as an emergent property of an IS network via a network-based approach with application to the Kalundborg Industrial Symbiosis (KIS)	Social network analysis	All	Water	Inter-plant	Single	Sources, plants, pipes, demand	NA	NA	Fall out of certain nodes effect on Stress centrality, betweenness, degree centrality, network efficiency
Karuppiah and Grossmann (2006)	Design of a superstructure for optimal system in a chemical process	Optimal network	Chemical	Water	Plant	Single	Source, splitter, mixer, process units, sink, pipes, treatment centers, flow rate, removal ratio treatment centers	Operation costs, investment costs	Discharge load	Network efficiency
Song et al (2018)	Social network analysis on industrial symbiosis: A case of Gujiao eco-industrial park	Social network analysis	Coal	Raw materials, gas, power	Inter-plant	NA	Plants, treatment plants, attributes and pipes	NA	NA	Degree distribution analysis, clique analysis and effect if fall out of certain nodes
Zheng et al (2012)	Evaluation of an Eco-industrial Park Based on a Social Network Analysis	Social network analysis	All	Raw materials, energy, information	Inter-plant	NA	Plants and links	NA	NA	Centrality degree, closeness degree, subgroup relations
Rubio-Castro et al (2012)	Optimal reconfiguration of multi-plant water networks into an eco-industrial park	Optimal network design	All	Water	Inter-plant	Single	Sources, sinks, treatment facilities, plants, pipes, flowrate	Sources, sinks, treatment facilities, plants, pipes, flowrate	Total freshwater intake, total wastewater production	NA
Lechtenberg et al (2020)	Design of an optimal Wastewater network representing main characteristics of multi-contaminants	Optimal network design	All	Water	Inter-plant	Multi-contaminant	Source, sink, three types of treatment facilities, distributor, plants	Generated revenue, operational expenses	Amount treated water	NA
Zheng et al (2016)	Network analysis of eight industrial symbiosis systems	Social Network Analysis	All	Knowledge, raw materials, waste	Inter-plant	NA	Plants and links	NA	Mutualism degree if links of same resources could be linked	Density, connectivity, effect if fall out of certain nodes/links
Zhang and Chai (2019)	Structural features and evolutionary mechanisms of industrial symbiosis networks: Comparable analyses of two different cases	Social Network Analysis	All	Energy flows, information	Inter-plant	NA	Plants and links	NA	NA	Small world effect, scale-free mechanism, network efficiency

Table 2.2: Literature overview of all research that has been conducted to IS water networks using network analysis

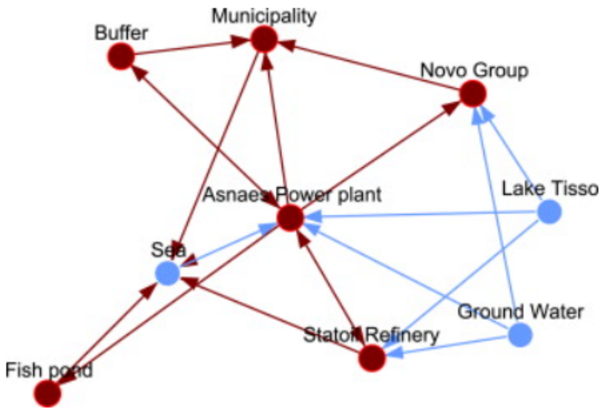


Figure 2.5: Waste water network containing multiple contaminants and multiple plants, source Chopra and Khanna (2014)

industrial symbiosis, however, within network analysis it should be incorporated as the influence of certain stakeholders not partaking, on the entire network. This influence is measured with social network analysis. This specific method has been applied in certain studies. However, these studies have not included the effect on economic and environmental performance as well. This is why an optimal design should be created, combining these two methods.

2.4. Conclusion and knowledge gap

Based on the information of the preceding paragraph 2.1, it can be inferred that water is a crucial resource within chemical parks, a diverse set of wastewater qualities are produced and treatment facilities are an important aspect in chemical parks. Technically, it is feasible to restore the quality of wastewater to a level that permits reuse as inflow for chemical factories (Oturan & Aaron, 2014). In Eco-Industrial Parks, treated wastewater gets reused for cooling or cleaning processes, or as irrigation water for adjacent fields (Agrawal & Verma, 2022). Nevertheless, minimal research has been conducted to the potential for reusing treated wastewater for actual chemical factories (Neves et al., 2020).

In order to investigate the possibility of reusing more wastewater in chemical parks, it is imperative to design Eco-Industrial Parks. An essential aspect of the designing process is understanding the water requirements of each factory part of the chemical park. Furthermore, the measurement of the performance of an EIP is critical, as otherwise no conclusions can be drawn if the design of an EIP for water in the chemical industry is effective and has certain opportunities. Therefore, performance metrics for the industrial symbiotic performance must be defined. According to Neves et al. (2020), (Fraccascia & Giannoccaro, 2020), and Yu et al. (2015), the performance of IS should always be measured according to the economic, environmental and social aspects. Moreover, a quantitative comparison of the input and output of different factories is the most effective way to measure performance (Azapagic & Perdan, 2000), (Azapagic & Perdan, 2000), (Cagno et al., 2023) (Lütje & Wohlgemuth, 2020). Although different research methods exist in literature that measure the industrial symbiotic performance, network analysis is the only method that could incorporate the social aspect within the design (Fraccascia & Giannoccaro, 2020). Specifically in chemical parks in which a wide variety of wastewater streams containing different water contaminants, the potential is high with network analysis to find reusing opportunities with optimal designs (Ahmetović & Grossmann, 2011). Significant research has been conducted to designing optimal wastewater networks, but most of these designs are geared towards economic and environmental optimization (K. Zhang et al., 2018), (Tiu & Cruz, 2017). On the other hand, social network analysis, which analyzes the IS water network in terms of positions and resilience of certain stakeholders in these networks, do not include water efficiency measures or cost-efficient measures (X. Zhang & Chai, 2019), (Valenzuela-Venegas et al., 2018). These two methods should be combined into an optimal IS water network design.

3

Literature Study: Stakeholders and their decision criteria

As indicated in the introduction, a lot of EIP's have to be created in bottom-up regulated countries, meaning the stakeholders have to collaborate with each other to create IS networks (Eslamizadeh et al., 2022). The initiative should come from the firms themselves (Tudor et al., 2007). This means that getting to know the stakeholder considerations for collaborating to generate an IS water network is very important for this research. Moreover, in the previous chapter, it becomes clear that the analysis of the behaviour of stakeholders is not linked yet to the studies in which optimal wastewater networks are designed regarding economical and environmental performance. The analysis of the behaviour of stakeholders is currently performed according to analyzing the resilience of the networks if certain stakeholders fall out. But, to know in reality which stakeholders would potentially fall out of the network (they do not want to join the IS water network in a chemical park), first, the involved stakeholders and their influence need to be identified. Afterwards, a method needs to be identified in which the behaviour and influence could be quantified. Lastly, the most important criteria on which the stakeholders base their decision (behaviour) to join an IS water network will be identified.

3.1. Stakeholders and social behaviour analysis

In this section, the stakeholders that physically take part in the water network of a chemical park will be identified. According to Hein et al. (2017), the formation and sustainability of an industrial symbiosis relies on the involvement of multiple stakeholders. These stakeholders are individuals or groups who have an interest in the symbiosis and the ability to impact it. According to the report of Organization et al. (2017), in which an international framework to assess the performance of Eco-Industrial Parks is given, are stakeholders on national, regional, and local levels involved in IS networks. Examples of stakeholders involved on a national level are the government, NGO's and scientific research institutions. On a regional level, municipalities, and funding agencies could be involved. Lastly, on a local level, industrial park operators and management, and firms located in the industrial park are actors that are involved (Organization et al., 2017).

According to Ashton (2011) and Hein et al. (2017), there are two forms of collaboration in industrial symbiosis. The first form involves actors who are directly involved or intend to be involved in a resource exchange, and these actors are referred to as "symbiosis partners." The second form of collaboration involves actors who are not symbiosis partners, such as business associations, anchor tenants, governmental agencies, and stakeholders at the regional and national levels. In most countries, EIP's need to be created bottom-up, starting with the local symbiosis partners that want to work together. Therefore, this research will focus on the first form of collaboration in IS networks, namely the local symbiosis partners.

The goal of the stakeholder scan is to identify the most relevant local symbiosis partners in creating a physical IS water network of a chemical park and their possible influence on this network. The stakeholders have been identified according to the literature and the interview with Lianne van Oord, attached in Appendix D.

Stakeholder	Interest	Objective	Resource
Chemical factory	Generate profit for stakeholders	Minimize production costs	Financial investment
	Generate profit	Maximize return on investment	Choose to share resources
	Adjust to global trends	Comply to regulations	
		Reduce wastewater in manufacturing processes	
		Reduce freshwater intake in water-intensive sites	
Treatment facility	Sustainable and stable water treatment	Reduce water pollution	Financial investment
		Deliver cleaner and environmentally friendlier effluent	Provide technical know-how
		Comply to regulations	

Table 3.1: Overview of interests, objectives and resources of the two relevant stakeholders

3.1.1. Stakeholders that take part in water networks of chemical parks

In Figure 2.2, an overview is given of how wastewater could be reused within a chemical park. As can be seen, a wastewater-producing process and a treatment plant are involved. Moreover, in the studies in which SNA had been applied to research IS of water networks and in the studies in which an optimal wastewater network is searched, all include plants and treatment plants as parameters, shown in Table 2.2 of Chapter 2. Industrial Symbiosis is a collaboration between different plants where one plant's waste or byproducts become another plant's raw materials. Companies that participate in by-product synergies often create formal agreements to establish the terms and conditions of their relationship, including the cost, amount, frequency, and quality of residual materials that will be exchanged over a specific period of time (Ashton & Bain, 2012). So, the owners of these chemical companies and treatment plants, managing the decisions and contracts, are the actual stakeholders. These studies all include a source and a sink as well as parameters. However, mostly the source represents an actual water source, such as a river or a lake, and the sink represents an actual water discharge location as, both are not managed by a stakeholder (van Oord, 2023, Cruz-Avilés et al. (2021)). What can be concluded from these two statements, is that the stakeholders managing the chemical plants and the stakeholders managing the treatment plants are the local industrial symbiosis partners, relevant for the initial symbiosis connections in the chemical parks.

Table 3.1 shows a summary of the most important interests, objectives and resources of the relevant stakeholders. The interests of the stakeholders describe the issues that matter most to the stakeholders regarding water usage and industrial symbiosis. The objectives of these stakeholders will be explained, which describe the concrete goals that the stakeholders have regarding water usage and industrial symbiosis. The resources of the stakeholders enlist the means available to the stakeholders to reach their objectives. However, this is a simplification of the real-world situation, in which the local industrial symbiosis partners could have more varying interests and objectives. In addition to this summary, the stakeholders are discussed in more detail below.

Owners of chemical factories

Chemical factories are part of chemical companies that produce industrial chemicals by converting raw materials. globally, a lot of chemical companies exist, with international operations and plants in numerous countries. In The Netherlands, big companies such as DSM and Akzo Nobel are the producers of chemicals, having multiple factories that produce chemicals within the Netherlands. Their interests are mainly to maximize profits and increase value for their shareholders. They want to reach this by minimizing the price of production chemicals and maximizing the returns on their investments (van Oord, 2023, DSM (2020)). Chemical companies are subject to strict safety protocols due to the hazardous nature of their materials and processes. Therefore, they must adhere to a multitude of strict national, regional, and local regulations. Compliance with these regulations is important, as non-compliance may result in costly fines. This serves as a significant incentive for chemical companies to comply with the regulations (Bahadorestani et al., 2020).

Chemical companies can have a significant impact on the environment, including air and water pollution, greenhouse gas emissions, and waste disposal. The regulatory instances are intensifying the regulations for waste disposal of chemical companies. This is one of the reasons why lately chemical companies are paying more attention to current trends in reinventing themselves as champions of the circular economy (Tonelli & Cristoni, 2018). Therefore, the focus shifts to being more sustainable and circular and their goals incorporate more often the reduction of wastewater in manufacturing processes and the reduction of freshwater intake (AkzoNobel, 2021), (DSM, 2020).

The factories can influence the network's performance by being willing to share their resources (wastewater), and by investing in sustainable practices that minimize their freshwater intake or wastewater generation.

Management team of treatment facilities

A wastewater treatment facility receives and treats industrial wastewater. the treatment facilities play a critical role in the performance of industrial symbiotic water networks as they provide the treatment services that provide the reuse of water (Bahadorestani et al., 2020). The main interest of wastewater treatment facilities is to remove pathogens, nutrients, organics, and other pollutants from wastewater in a stable manner. This means that always all these contaminants are treated from the water in percentages that the discharge complies with all national regulations. Ensuring that nature or humans will not be affected by the wastewater discharged from the treatment facility. Moreover, recent trends ensured that treatment facilities want to use more sustainable treatment technologies.

The ownership of a treatment facility can vary depending on the ownership structure of the chemical park. The chemical park can be managed by a public entity. The public entity can be a ministry, agency, or authority, or it can take the form of a commercially-oriented State-Owned Enterprise (SOE) or Special Purpose Vehicle (SPV). In the latter scenarios, the government is the owner, funder, and investor of the company, granting it strong control over the park's day-to-day operations, including the management of the treatment facility (UNIDO, 2019). In contrast, if a chemical park is managed by a private entity, the park operator (a private company) is typically contracted by the park's owner or investors, who may also be resident firms that own plots and buildings within the park. This approach is usually used when private investors have made substantial investments in or own the industrial park. Private management contracts are also frequently established with specialized facilities management companies in government/state-owned industrial parks. In this ownership structure, the treatment facility is privately owned (UNIDO, 2019).

The difference in ownership structure has an impact on some decision-making processes in relation to project implementation (design and construction) and to operational aspects with respect to the profit-oriented perspective of the private sector related to the perspective of the public sector. This does apply to decisions on resource allocation, like financing and technical solutions. The public-managed treatment facility will invest more likely in expensive sustainable treatment technologies with less return on investment than privately-owned treatment facilities.

On the other hand, core objectives in wastewater treatment should stay the same for both management structures, even with 'far-reaching' privatisation models. Such core objectives are all efforts geared to sustainable wastewater treatment as reducing water pollution, delivering cleaner and environmentally friendlier effluent and complying with national regulations as contributions to the protection of health and the environment (Grünebaum & Bode, 2004).

Recently, there has been a movement towards privatization of the water sector, driven by several factors. These include the desire to gain access to external expertise and funding, as well as the potential for synergies to be realized through the integration of wastewater treatment with other tasks that are similar in nature (Grünebaum & Bode, 2004).

3.1.2. The influence stakeholders could have on IS water networks

In the preceding paragraph, the general interests, objectives and resources of stakeholders that would take part in IS water connections within chemical parks have been enlisted. However, the degree to which the stakeholders want to reach their objectives could differ, because of differing cultures, work ethics, and internal policies for example. Certain stakeholders could be more profit-focused, only wanting to make investments with a high return. While other companies could be more sustainability or future-focused, wanting to make more investments to reduce their wastewater production. This has an impact on the view towards the generation of IS water connections resulting in stakeholders deciding on taking part or not taking part in IS water networks. These firms involved in the synergies can have a significant influence on the performance of Industrial Symbiosis water networks. The aim of IS is to create a closed-loop system that reduces waste and promotes resource efficiency. If certain stakeholders do not take part in the IS network, it often negatively impacts the expected performance of the project (Bahadorestani et al., 2020).

3.1.3. On what grounds is stakeholder behaviour influenced

As it is very important for the performance of the IS project that stakeholders take part in the IS water network, it is necessary to know on what grounds the stakeholder's behaviour is influenced for deciding whether or not to take part in the IS network. Many studies have researched stakeholder behaviour towards sustainability-related topics. According to Park et al. (2008) and Ghorbani et al. (2020), the stakeholder decision-making process specifically related to sustainability-related choices is dependent on the following factors: personal beliefs and desires, informal institutions (norms), contextual factors, and formal institutions, shown in Figure 3.1.

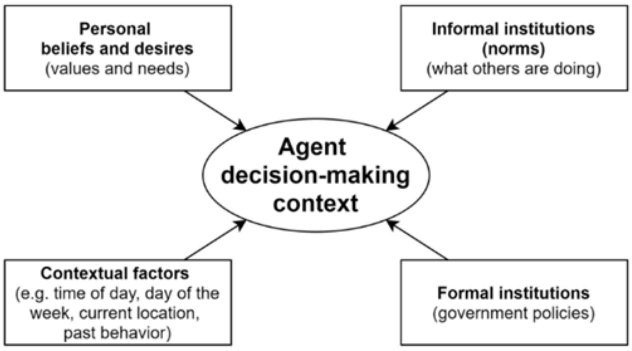


Figure 3.1: Illustration of the factors that impact agents decision-making

However, this research focuses on a water network in a single chemical park. This means that for the stakeholders within the chemical park, the informal institutions, contextual factors and formal institutions are all the same. So their decisions (behaviour) can only differ because of their personal beliefs. Personal beliefs applying to an entire company are formed by culture, level of expertise, knowledge, authority and internal policies (Lienert et al., 2013).

3.1.4. Conclusion from section 3.1

It becomes clear that to create the initial IS water network, the local industrial symbiosis partners within a chemical park need to collaborate. The relevant local industrial symbiosis stakeholders are the owners of chemical factories and the owners of treatment facilities. However, the owners of the treatment facilities differ according to the management structure of the chemical park, namely public or private. Chemical factories can choose to make the investment in IS connections and share their resources. For treatment facilities, it differs according to the management structure how they allocate resources, like in what they invest and how they provide their technical know-how within the chemical park for creating IS water connections. Because of different beliefs and internal policies stakeholder behaviour is influenced, meaning it could differ per stakeholder if they take part in IS water networks. This has a big influence on the performance of these networks.

3.2. Methods for quantifying stakeholder behaviour

The previous section identified the relevant stakeholders for water networks within chemical parks and their possible influence according to their behaviour on these water networks. The specific aim of this section is to investigate what the best method is to research what could possibly cause the different behaviour of stakeholders on deciding differently regarding taking part or not in IS water networks. Quantifying the influence of stakeholders on IS networks allows for the development of an engagement plan that takes into consideration stakeholders' personal beliefs and desires (Lienert et al., 2013). This is why a method for quantifying stakeholder behaviour will be searched.

According to J.-J. Wang et al. (2009) and Jamwal et al. (2021) is the evaluation and calculation in sustainable decision-making usually obtained by the method Multi-Criteria Decision Analysis (MCDA). They analyzed the role and applications of MCDA in the sustainability-related decision processes, according to a literature analysis of respectively 139 and 85 articles. It showed that the results obtained by this method are more rational than other aggregation methods. Moreover, they found that recently this method is used more often in sustainable decision-making.

Another method for quantifying stakeholder behaviour is quantifying the degree of influence of stakeholders in a network. The degree of influence is calculated by combining the rankings of several attributes the stakeholders contain in a network, that affect their influence on a specific subject. This method is specifically designed for network analysis. However, with this method, the degree of influence is quantified, but not the actual decisions of stakeholders are analyzed (Turner, 2009), (Zedan & Miller, 2018). So, MCDA results to be the most used and well-known method for quantifying sustainable related decision processes. However, this method has some important considerations to keep in mind. In practical decision-making situations, traditional multi-criteria evaluation methods may encounter significant practical challenges due to imprecision or vagueness present in the information. Factors such as the availability and uncertainty of information, as well as the subjective and fuzzy nature of human emotions and perceptions, can make it difficult to assign precise numerical values to criteria (Jamwal et al., 2021).

MCDA consists of different stages, namely criteria selection, criteria weighing, evaluation, and final aggregations. The first stage, criteria selection, is the most important stage. This defines the criteria on which the entire analysis is based (J.-J. Wang et al., 2009).

3.3. Criteria that influence stakeholders' behaviour

As explained in the previous section, does MCDA suit best as a method to quantify stakeholder behaviour within this research. The first step in this method is to select the most important criteria of the stakeholders for deciding on joining or not joining the IS water network. Section 3.3.1 will show that six criteria are found to be most important to the involved stakeholders. These criteria will be discussed in more detail in this section.

Table 3.2 displays the criteria that are pertinent to the stakeholders involved in the IS water system. Accordingly, from the literature study in Chapter 2, it is concluded that the performance of IS water networks should always be measured according to the social, economic, and environmental aspects. Logically, the willingness of the industries to participate in an IS network is also based on these three aspects. Moreover, the technological condition, if IS is possible, is a factor that certain stakeholders also take into consideration within chemical IS water networks (Yu et al., 2015). This is why the criteria are categorized into four groups, namely, economic, environmental, social, and technological criteria to provide a structured overview. As there are various criteria involved, only the most crucial ones can be considered, and hence, a selection must be made. The following section will explain this selection process in detail.

3.3.1. Criteria selection of the most important criteria for the stakeholders in IS water networks

To be able to make a selection of the relevant criteria, it is important to first seek all the possible criteria, to be sure that no critical criterion is left out (Jamwal et al., 2021). This is why quite an extensive literature study was performed to evaluate which criteria have been considered in different decision-making processes regarding industrial symbiosis. Several studies, most notably Park et al. (2008), Yu et al. (2015), Tudor et al. (2007), Eslamizadeh et al. (2022), Walls and Paquin (2015), J.-J. Wang et al. (2009) and Jamwal et al. (2021), provide an overview of important criteria to be taken into account, shown in Table 3.2. After all criteria have been gathered, a selection of six important criteria was made. These criteria apply specifically to the willingness of stakeholders on joining an IS water network. The criteria have been selected according to the number of mentions within the literature, and have afterwards been tested according to the selection principles, namely systemic, consistency, independency, measurability and comparability (Jamwal et al., 2021). Other criteria may be relevant to other researchers. Therefore, a discussion of these criteria is provided in Appendix B.

Two economic criteria are most important to the involved stakeholders: increasing revenue and complying to all regulations relevant. These will be discussed in more detail below. Gaining tax is only relevant for stakeholders in certain countries, as the tax regulations differ per country. Reducing costs is an important criteria for stakeholders within the chemical sector, however decisions regarding industrial symbiosis always require investment, which results in stakeholders knowing they will not be able to reduce costs. Therefore, these two criteria are not taken into account.

Reducing water pollution, reducing freshwater intake and internal compliance with sustainability policy are all environmental criteria important to stakeholders when sustainability decisions have to be made about IS of water. However, only the internal compliance to sustainability policy criteria has been incorporated in the selection because of the independency selection principle. Reducing freshwater intake and reducing water pollution could all be included in the internal sustainability policy.

The two social criteria of trust and awareness of IS possibilities are important specifically within the chemical industry. Because of all the different qualities of water, the awareness of IS possibilities is important for stakeholders considering joining an IS water network. Moreover, trusting other companies to use their wastewater or send it to shared treatment facilities is an important criteria. Community spirit, information sharing and dependency are all interrelated criteria, named in different sources. Job creation could also be an important criterion, however, this is mostly applicable for other stakeholders than those considered in this research.

Lastly, technical feasibility is often considered by stakeholders regarding the water quality. Is it technically feasible to upgrade the water quality to a level they can use? This is an important criterion for stakeholders in water networks in chemical parks. Reliability is not considered as important in the found literature.

The following sections will discuss the six most relevant criteria in more detail.

Compliance to regulations

National policies have a large impact on the willingness of stakeholders to participate in IS systems (Park et al., 2008). In the Netherlands, which is a bottom-up regulated country, it has been studied that government regulations are one of the important external stimuli for IS (Park et al., 2008). Stricter regulations on wastewater discharge can increase the need for wastewater treatment, which can make participating in IS networks of water a more attractive option. This need is essentially stimulated by the punishment that comes in combination with these stricter regulations. High fines or cancellations of licenses to operate are consequences of not complying to the regulations, which are crucial for stakeholders operating in chemical parks (AkzoNobel, 2021).

Revenue growth

Another important criterion is the possibility of generating revenue from joining an IS water network. As mentioned in paragraph 3.1, most chemical companies aim to increase profit. Their consideration of joining an IS network will always be related to chances for generating extra revenue. The financial incentives associated with reduced water consumption, lower waste disposal costs, and the possibility of generating revenue from the sale of by-products can motivate stakeholders to join the network. Moreover, the increasing strictness of environmental standards force companies to make high investments. Hence, companies want to recover these costs, and get a return on investment as quickly as possible. By sending byproducts to downstream enterprises, which could increase revenue (Yu et al., 2015).

Internal Sustainability Policy

This criterion is called 'internal sustainability policy', which actually means that the stakeholders want to comply to their internal sustainability policy (Heeres et al., 2004). Every chemical factory owner has its

Aspect	Criteria	Literature	Number mentions
Economic	**Revenue growth**	[2],[3],[4],[5],[6]	5
	Gain tax	[1]	1
	Compliance to regulations	[1],[2],[3],[4],[5],[6]	6
	Reduce costs	[1],[2],[6]	3
Environmental	**Internal compliance to sustainability policy**	[3],[4],[5],[7]	4
	Reduce freshwater intake	[2],[4],[5],[7]	4
	Reduce water pollution	[2],[4],[5],[7]	4
Social	**Trust**	[1],[3],[4],[6],[7]	5
	Community spirit	[3],[4]	2
	Information sharing (security)	[6],[7]	2
	Dependency	[3],[4],[7]	3
	Job creation	[4],[5]	2
	Awareness of IS possibilities	[2],[4],[6],[7]	4
Technical	**Feasibility**	[2],[3],[6],[7]	4
	Reliability	[3]	1

Table 3.2: Enlisting all criteria mentioned in the literature that stakeholders could consider as important for joining an IS water network. The six most important criteria that are used in this research are represented in bold. *(1=Park et al(2008), 2=Yu et al(2015),3=Tudor et al (2007), 4=Eslamizadeh et al(2022), 5=Walls and Panquin(2015), 6=Wang et al (2019), 7=Jamwal et al (2021))*

own internal sustainability policy. This is a trend from recent years, in which more actors dependent on or influential for chemical companies require more insight in the sustainability goals of chemical companies (UNIDO, 2019). As already mentioned in Chapter 1, do Dutch chemical companies, Akzo Nobel and DSM also have their own sustainability policies, specified to different sustainability topics (AkzoNobel (2021), DSM (2020)). The policies have been defined by the companies themselves, meaning differences could exist in the strictness of policies between chemical companies.

Trust

The willingness of stakeholders to participate in IS networks of water can also be influenced by the level of trust and collaboration among participants. According to Hedstrom and Bearman (2009), trust is based on the belief that one party in a relationship has a motive to act in the best interest of the other party, or to prioritize their interests. Trust-building mechanisms, such as transparency and communication, can foster collaboration and improve stakeholders' willingness to participate in the network. Many publications have briefly hinted at "trust" as the potentially very influential factor for a successful IS establishment, (Eslamizadeh et al., 2022). Tudor et al. (2007) stresses the importance that the level of trust needs to be upheld the entire time the stakeholders work together (Tudor et al., 2007). At Chemelot, a few factories are already starting small initiatives to recycle more water between their factories. They hired technological companies to see what possibilities there are. van Oord, L. (2022, December 17th). Personal communication [Personal interview]

Awareness of IS possibilities

For chemical companies to consider the option of joining IS water networks, it is important they know how pollutive water could be and what their own water footprint is. Otherwise, they do not even know they have to take action (van Oosterhout, D. (2022, December 24th) Personal communication [Personal interview]). Education and awareness can also play a critical role in influencing stakeholder behaviour. By increasing stakeholders' understanding of the benefits of IS networks of water, as well as the technical and operational requirements of the network, stakeholders can make informed decisions and participate more effectively. Numerous global studies have demonstrated that attitude, knowledge, and support are the principal factors that affect the acceptance of investments in IS (Eslamizadeh et al., 2022).

	Revenue growth	**Compliance to reg**	**Int sust compl**	**Trust**	**Awareness**	**Feasibility**
Chemical factory	✓	✓	✓	✓	✓	✓
Treatment facility		✓	✓	✓		

Table 3.3: Evaluating the preferences of the stakeholders on the criteria that are included in this research

Technological feasibility
Especially within the chemical industry, could stakeholders' decisions to participate in IS networks of water also be influenced by the technical feasibility of the network. Factors such as water quality, availability, and compatibility of industrial processes can impact the ability to reuse wastewater, which can affect stakeholders' willingness to participate (Rodiguez-Miranda, 2015).

3.4. Aligning most relevant criteria with the involved stakeholders

After identifying the key stakeholders and relevant criteria, the next step involves assessing the significance of each criterion to each stakeholder. Table 3.1 summarizes the interests of the actors, while Table 3.3 provides an overview of the actors' interests concerning the six chosen criteria. The significance has been defined according to all the interviews that have been conducted for this research and literature. The interviews were conducted with different actors within the chemical industry, varying from chemical factory employees, towards employees busy with the circularity goals for the entire Dutch utilities sector.

A finding that should be notified is that in most literature found, the treatment facilities are not considered as actual decision-makers. They are seen as players within IS water networks that always take part.

3.5. Conclusions from the literature study and knowledge gap

It can be concluded from the results of this literature study that the owners of the chemical factories and the owners of the treatment facilities are the most important stakeholders, namely the local symbiosis partners, within chemical parks. The MCDA method suits best to quantify the different decisions of these stakeholders for joining or not joining an IS water network. The decision criteria of technical feasibility, revenue growth, compliance to regulations, internal sustainability policy, trust and awareness are the impacting decision criteria for stakeholders within a chemical park. However, in some studies are the treatment facility owners not considered as decision-makers.

This concludes the literature review. The most important contributions of this study can be summarized into two main points. Firstly, this study will bridge the gap between the economic and environmental optimal networks and on the other hand the social optimal networks. Secondly, this study will research which specific decision criteria have a big influence on the optimal designs of IS water networks.

4

Overview of the Model Design

In order to answer the research question, a model of a water network within chemical parks is constructed, that incorporates all three pillars of industrial symbiotic performance. This chapter will discuss the narrative behind the model, the high-over design, and the components which form the basis of the model. The model consists of two main parts: the technical optimization part and the social behaviour part. Both designs are elaborately explained in the following two chapters, chapters 5 and 6. This chapter forms the basis for the entire model structure, incorporating both parts of the model.

4.1. Model Narrative

As the conclusion from the literature study of Chapter 2 stated, there are no optimal water network designs that incorporate the social aspect of industrial symbiosis, namely the behaviour of the stakeholders. In the model, the bridge between economical and environmentally optimal models, and on the other hand social optimal models need to be solved. Within this research, it has been chosen to incorporate the social behaviour of stakeholders as the choice between joining or not joining the IS water network. The effect on the IS performance is compared with the IS performance of a network after the stakeholders have decided on wanting to join the IS network or not. By comparing the different IS performances, the resilience of stakeholder behaviour in the IS water network can be defined. This process is visualized in Figure 4.1. Within the design of the model, the two different parts, the technical optimization part, and the social behaviour part have been incorporated in a different manner. The technical optimization part uses the method of network theory, part of graph theory. The social behaviour part of the model design uses the multi-criteria decision analysis method. In both parts, different methods are used but are eventually combined in the overall model. The technical optimization part of the model is used twice in an entire run, as can be seen in Figure 4.1. A run means the model is executed entirely for a single experiment.

4.1.1. Network theory for the technical optimization model

For this research, a water network within a chemical park needs to be imitated, to be able to analyze if different IS connections are possible between different chemical companies or treatment facilities in a chemical park. Therefore, the different stakeholders within the chemical park and the water and wastewater flows need to be represented. Within previous studies, analyzed in Chapter 2, network theory is often used for this. Network theory is part of graph theory. In the field of mathematics, graph theory is concerned with the study of graphs, which are mathematical structures used to represent relationships between objects. A graph consists of vertices (also known as nodes) that are connected by edges (also known as links). Network theory extends the concept of graphs by adding attributes to both the nodes and edges. This theory analyzes networks based on the symmetric or asymmetric relationships between their components, which are typically discrete (Barnes & Harary, 1983). In the common sense of the term, a directed graph is represented as an ordered pair G=(V,E), where:

- V, a set of vertices (also called nodes or points)
- E$\subseteq \{(x, y) \mid (x, y) \in V^2$ and $x \neq y\}$

Network problems often involve finding an optimal way of doing something (Barnes & Harary, 1983). With

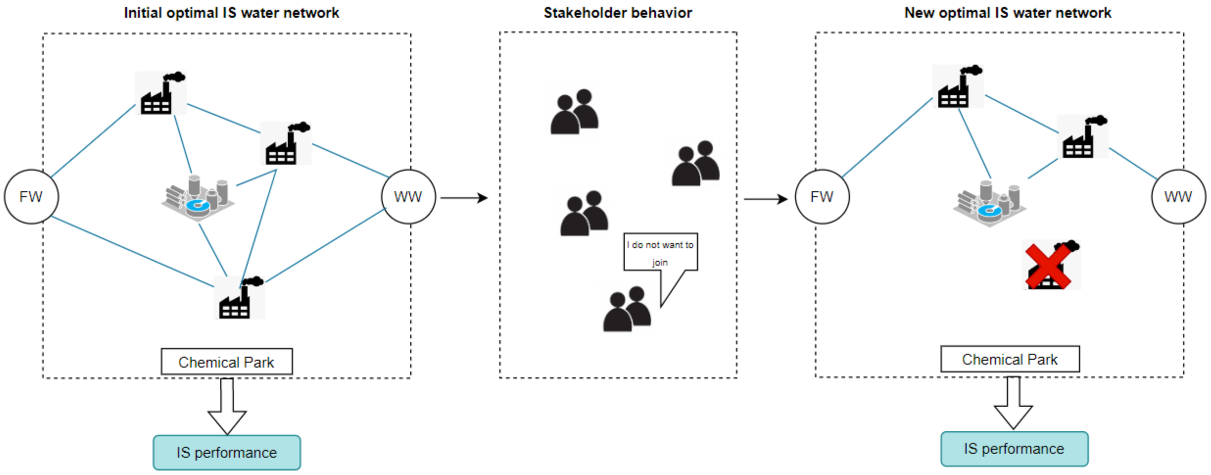


Figure 4.1: Visualization of the model design, FW=Freshwater, WW=Wastewater

the network analysis, an optimal combination of stakeholders (nodes) and water pipes (edges) will be searched according to the IS performance metrics. The information found in literature chapter 2.1 forms the basis for the network design of this research.

4.1.2. Multi-criteria Decision Analysis for the social behaviour model

The other aspect of the model is to research how stakeholders behave in deciding on whether to join an IS water network or not and process this decision in the IS water network. Many different methods exist to analyze and identify stakeholder behaviour, however, for this research, the choice has been made to use multi-criteria decision analysis (MCDA), defined by the literature study in paragraph 3.1.3. As in the decision-making process for joining an IS water network, many criteria could play a role, each stakeholder can represent different behaviour. The outcome of the decision can be combined with the designed network model. The most important criteria for stakeholders to make their decision in joining an IS water network in a chemical park have already been defined in Chapter 3.

4.2. Choice for generic design

The designed model has been formulated in a generic manner to allow for its applicability across various contexts. Specifically, the model aims to evaluate the impact of stakeholders' social behaviour on the technical IS water network systems within a chemical park. Nonetheless, given that each chemical park is different with respect to a number of factors, for example, the physical location, number of factories, and water contaminants produced, not a single model could function for an analysis of the IS potential of all chemical parks. Therefore, it is important the IS performance could be analyzed for any chemical park located in a bottom-up regulated country. To achieve this, the model has been designed in a highly generic way such that the number of stakeholders involved, the number of water sources and sinks, the type and number of treatment facilities, and the location of the stakeholders could differ. The chemical park visualized in Figure 4.1, could be any chemical park in a bottom-up regulated country.

4.3. High-over structure of the IS water network model

In the previous paragraph, the narrative behind the model is explained. Moreover, the two different parts the model consists of are elaborated a bit more. In this paragraph, the actual high-over structure of the model containing both parts, shown in Figure 4.2, is explained according to different steps. The initial IS water network of a chemical park is designed according to input variables. These input variables define the topology of the network. First, the complete network of a chemical park will be defined according to all possible links, defined by the water demands of all stakeholders. From this complete network, all different kinds of routes for the water flow are possible. All the different routes are analyzed and the optimal routes are searched. However, this complete IS water network design has not considered stakeholder behaviour yet. In step 4, different stakeholder behaviour options are defined according to social scenarios. These social scenarios define if stakeholders are wanting to join the IS water network, or not, and are more elaborately explained in Chapter 6. The setup of the network differs according to the involved stakeholders. After step 4, the impact of the social behaviour of stakeholders has been incorporated, and the new combination of stakeholders within the network needs to be analyzed again according to the IS performance metrics. This is why the optimization function, from step 3, is performed again in step 5 with the new setups of the network. All different outputs from all different setups of the network are taken together for further analysis (step 6).

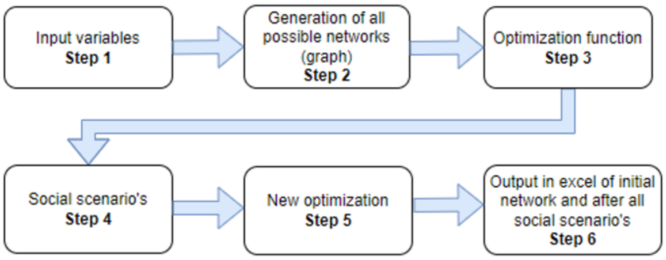


Figure 4.2: Visualization of the high-over structure of the model

4.4. Choice of modelling tool

Since a customized IS water network of a chemical park needs to be developed and network optimization and social stakeholder behaviour needed to be included, using an existing optimal water network tool was not an option. To construct a water network optimization model for this research, the choice of the programming environment is important. There are various programming languages available such as Python, C++, and Matlab. In this study, Python was selected as the preferred programming language for two primary reasons. Firstly, Python is a versatile language with numerous packages that can provide additional features to the model, including packages for network analysis. Secondly, Python is a widely used programming language, which allows other researchers to easily use and reproduce the model.

4.4.1. Choice of networking package in Python

To perform the water network analysis and optimization, a package called NetworkX (Hagberg, Schult Swart, 2004) in Python is used. This Python package functions for *“the creation, manipulation and study of the structure, dynamics, and functions of complex networks.”* There were many reasons for choosing this Python package. NetworkX is easy to implement, has much online documentation, nodes can be any Python object, edges can contain any arbitrary data, it allows for full customization of the network, and includes functions for searching specific flows within the network (Brandes, 2005). An important aspect of this research is to include all the different water qualities required and produced in chemical parks, which could be represented by the attributes of the edges within this package. Moreover, another important aspect of this research is that optimal routes are searched regarding different IS performance metrics, which is possible with different functions part of the Networkx package. As the network can be customized to a high extent, the specific customization of the network for this model design will be explained below, according to all the different network components.

4.5. Defining the network topology for the IS water network

The customization of the network analyzed in the model requires a good definition and demarcation of all components the network should consist of. The arrangement of these components defines the network topology. The components column in Table 2.2 in Chapter 2.3 gives a good overview of how different the network topology designs could be for wastewater networks. What has been found in the literature is that each study used a different set of components to model an optimal wastewater network. For this model, a set of components and attributes have been included according to the most used components in the literature. Moreover, this research specifically focuses on water network designs for chemical parks. Therefore, it is of utmost importance to create a network topology design that could represent a chemical park. To achieve this, a specific chemical park in the Netherlands has been analyzed and taken as an example case to define the minimal set of components and attributes the network should consist of. This chemical park is called Chemelot, located in Geleen, on which all different kinds of chemical factories exist (Brightside, 2021). A design of the water flow and wastewater production of the chemical park Chemelot is shown in Figure 4.3. The different components will be discussed in the following paragraph and how these form an eventual complete network is shown in Figure 4.4.

4.5.1. Scope of the model

First of all, the scope of the model needs to be explained. The designed model focuses on the possibilities for constructing IS water connections within a single chemical park. The only flow of water flowing into the chemical park is the water that is needed for the chemical processes of the site users. No other water usage flows, like for cooling, represented in Figure 4.3 as the other lines stemming from the source, are considered in the model. Moreover, the only possible flow of water flowing out of the chemical park is the wastewater flow. No other possible ways, like evaporation, shown in Figure 4.3 in green, are considered. Lastly, no time component has been incorporated into the model. The model will analyze whether IS water connections are possible at all, regarding pre-set amounts of water. This amount will not differ for each stakeholder, as there is no time lapse incorporated.

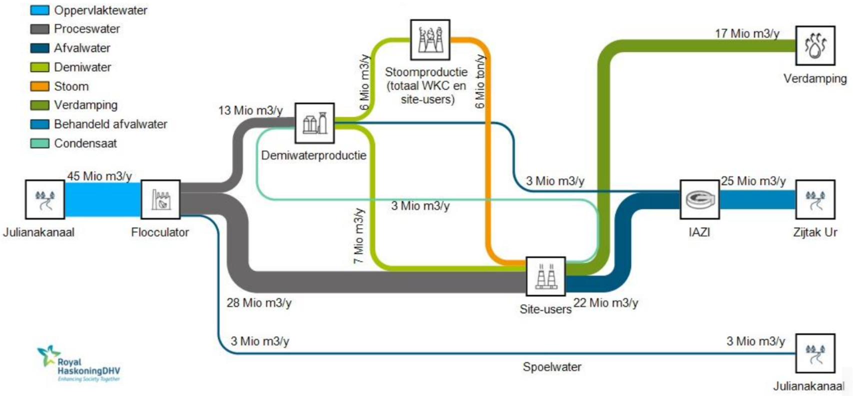


Figure 4.3: Example of the water flow at Chemelot

4.5.2. Stakeholders

The most important component within the network topology is defining the nodes. The nodes are represented as stakeholders within the chemical park in this model.

Chemical factories

The chemical factories form the basis of an IS water network of a chemical park, as depicted in Figure 4.3 where they are referred to as site users. These are the stakeholders that need water for their chemical processes and produce wastewater. Consequently, these players have to cooperate to create IS connections. In all studies analyzed in the literature review, the chemical factories are included as components and represented as nodes. In the network, the chemical factories are represented as nodes, with a specific attribute distinguishing them from other nodes. Within the model, the assumption is made that the chemical companies require a specific quality of water for their own process and that within the factory, the water quality is always downgraded (producing wastewater). As stated in paragraph 2.1 of the literature review, this is also reflective of reality. Each chemical company requires a specific water quality, concerning factors such as the level of pH and total suspended solids (J. Liu & Tang, 2018). Furthermore, chemical factories inevitably produce wastewater as a byproduct of their chemical processes (Long et al., 2018).

Treatment facilities

Another important type of node forming the basis of the network is the treatment facility within a chemical park is, represented as the 'IAZI' in Figure 4.3. In the literature research, it was found that in chemical parks, often the treatment facility is managed by a different stakeholder than the chemical factory itself (EPSC, 2005). Each chemical park has at least one treatment facility located in it, as this is required by most laws set by each government (Lyu et al., 2020). Moreover, recent scandals regarding the quality of wastewater flowing into rivers again have resulted in more strict regulations on the treatment of wastewater in chemical parks (Lyu et al., 2020). Therefore, the inclusion of the treatment facilities as a type of node in this network is very important. In all studies analyzed in the literature review, the treatment facilities are included as components and represented as nodes. The attribute of these nodes represents that the treatment facilities always upgrade the water quality from the wastewater. In reality, this is also the case, as the literature study of 2.1.4 explains the treatment facilities treat the water so it can be discharged into receiving water bodies such as rivers, lakes, or oceans (Agrawal & Verma, 2022).

Freshwater

Each network consists of a source. This is the node from which the flow in a network originates (Barnes & Harary, 1983). In a chemical park, this is just the place from which the freshwater comes, such as a nearby river, or a groundwater basin, in Figure'4.3 represented as 'Julianakanaal'. From this node, all the water flows into chemical factories. In all studies analyzed in the literature review, represented in Table 2.2, the source is a solid component always included in the network.

Wastewater

Each network also consists of a sink. This is the node in which the water flow always ends (Barnes & Harary, 1983). A chemical park is a place where the wastewater is disposed into nature, which could be a river, dwell, or basin, in Figure 4.3 represented as 'Zijtak Ur'. The wastewater produced by chemical factories is firstly treated by treatment facilities and afterwards, flows into the sink node. In all studies analyzed in the literature review, represented in Table 2.2, the sink is a solid component always included in the network.

4.5.3. Water pipes

The second basic component the network topology consists of, are the edges. In a chemical park, the edges represent the pipes through which the water flows. In Figure 4.3 the individual pipes between the different site-users and the water source and sink are not visualized, but the different lines in the image represent the water flow. As edges are a basic component of a network, logically water pipes are a basic component in all optimal water networks analyzed in the literature in chapter 2.3. Within the designed model, the edges are given certain attributes, to customize the network more as a water network of a chemical park. The edges are given a certain capacity for the amount of water that can flow through. Moreover, the edges are given the attribute of specific water quality, meaning the specific water pipe only transports water of a certain quality. Lastly, the edges are given certain costs. The water pipe becomes more expensive if its size becomes larger.

4.5.4. Water qualities

An important attribute coupled to the nodes of the network are the demanded and supplied water qualities. As explained in Chapter 2.1.1, do different types of chemical processes have different demands for the quality of the water. A certain chemical factory that manufactures paint, has regulations implemented that require water only for 90% cleaned. Within the model, four different water qualities are included. Quality A represent treated water up to a 100%, quality B represents treated water up to 95%, quality C represents treated water up to 92% and quality D represents treated water up to 86%. In Figure 4.4, the different water qualities are represented by colour.

4.5.5. Water demand

During the literature study, it became clear many optimal water network designs contained the component flow rate or demand. In Figure 4.3, the water demand is represented as million m3/year. The flow rate can be modelled in a way it differs per time step per factory. However, there are no different time steps in the designed model for this research. Another way to model the flow rate is to use averages of water demand per stakeholder. In the designed model, the nodes that represent a chemical factory are given a specific water demand.

4.5.6. Location

Within chemical parks, different factories are located quite near each other, this brings one of the main advantages of an industrial park (EPSC, 2005). Each factory is located on a specific location within the chemical park. To reconstruct this, it is important specific locations are given to the nodes within the network. These locations are defined by coordinates (Sousa et al., 2002). The location of a certain node is solid, and cannot change during different runs of the model.

4.5.7. Advancement treatment facilities

Another important component which let the customized network represent a chemical park, even more, is the advancement of the treatment facilities. Within chemical parks, the treatment facilities are an important component (J. Liu & Tang, 2018). They define how much the wastewater is treated and what quality of wastewater is disposed into nature again. Within the literature study of chapter 2.2 it has been found that some optimal water network designs contain the component named 'removal ratio' or 'treatment technology', which defines to what quality the wastewater is treated (Tudor et al., 2007). In this model, this component is called the advancement of the treatment facility. It defines how many water qualities the treatment facility can treat. The higher the advancement, the more water qualities the treatment facility can upgrade. A treatment facility with the highest advancement level can upgrade the lowest water quality to the highest quality, this is three levels.

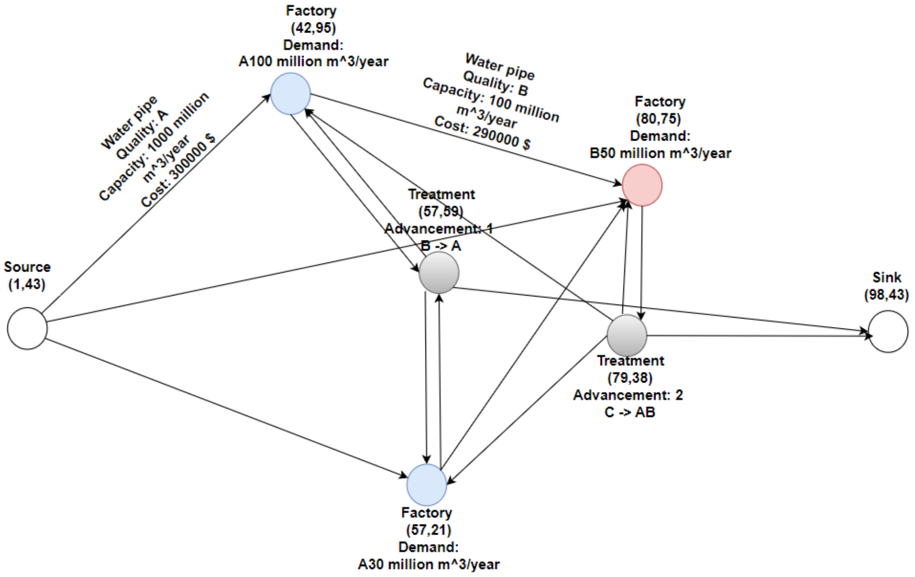


Figure 4.4: Visualization of the structure of networks with pretreatment facilities inhouse

4.6. Defining the two different model setups

Globally, two different structures of wastewater treatment models exist, as explained in Chapter 2.1. The wastewater treatment solutions in chemical parks range from solutions where each chemical plant treats its wastewater separately, to solutions where all the wastewater produced in the region is sent to a single treatment plant. No consensus exists on which model is most effective. Lyu et al. (2020) states that many wastewater operating models have substantial room for improvement. Industrial water pollution prevention is still a hot potato for eco-industrial transformation of the intensive industrial parks in China and there is considerable progress to be made. Combining the design of both models could be effective. This is why the two different structures of network designs have been constructed and analyzed in the model, shown in Figure 4.5 and Figure 4.6.

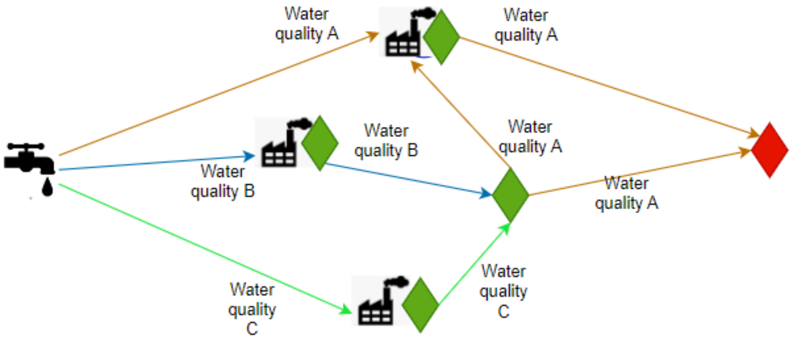


Figure 4.5: Visualization of the structure of networks with pretreatment facilities inhouse

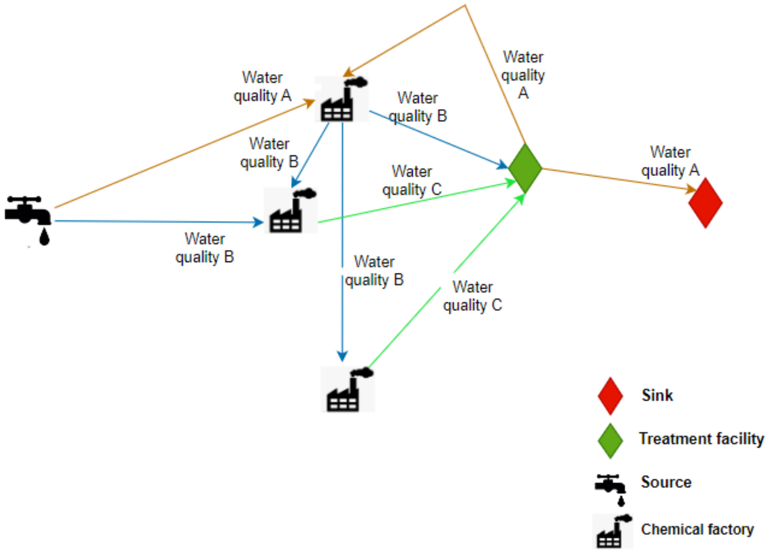


Figure 4.6: Visualization of the structure of networks with separate treatment facilities

As shown in the two figures, a clear distinction is being made between a network including separate treatment facilities and inhouse treatment facilities. The difference means that in the first network structure, the treatment facilities are seen as separate actors. It is assumed that the chemical factories do not have pre-treatment facilities attached to their own factories. The raw wastewater directly flows to the treatment facilities used in the specific network. On the other hand, as was researched in the literature study of chapter 2.1, there are chemical factories with treatment facilities in-house, and the water flowing out of these factories is already treated. This means the treatment facility is part of the same stakeholder that owns the chemical factory.

To include this difference in the network structure in the model, two different network topologies are used. In the network structure with inhouse treatment facilities, the quality of the water flowing out of the chemical factory stay the same as the quality flowing into the chemical factory, while in the network structure with separate treatment facilities, does the quality of the water flowing out of the chemical factory always downgrade by one level compared to the quality of the water flowing in. This is a simplified version of reality.

The inhouse treatment facilities only function for the chemical factories they are part of. This means these facilities only treat the water of a dedicated chemical factory and should not be seen as separate actors (nodes) within the IS water network. If these treatment facilities were considered as separate nodes, the designed model would consider these treatment facilities as nodes to which other wastewater streams from other factories could be sent to, to be treated.

Moreover, the reason for representing the outflow of the water as the same quality as the inflow is because it is the only option to represent the water is treated inhouse. As the most crucial difference between these network structures is that the water leaving the chemical factory is of higher quality in the network structure with inhouse treatment facilities than in the network structure with separate treatment facilities, as explained in the study of Lyu et al. (2020). In the original network topology, with separate treatment facilities, the water always downgrades by one level in a chemical factory. Therefore, the only option in the network structure with inhouse treatment facilities to keep the water quality higher, is not to downgrade the water quality by one level and therefore keep the water quality of the outflow the same as the inflow. This represents the water is treated inside a chemical factory.

The effect of this difference is that the number of water qualities present in some networks with inhouse treatment facilities is lower than in networks with separate treatment facilities. In reality, the same difference applies as Lyu et al. (2020) states the central treatment facility within the chemical park with inhouse treatment facilities treats less water qualities than in the other treatment structure.

4.7. Mathematical formulation of the model

The narrative of the model, the topology of the network of the chemical park and the two different network structures have now been defined in previous paragraphs. In this section, the mathematical formulation of the model is provided below as an entirely new model had to be designed, containing varying mathematical formulations. Table 4.1 shows all sets, parameters, and variables used in the formulas below.

4.7.1. Defining the sets for the model

Different sets are defined in Table 4.1. It is important to discuss the difference between the first two sets (R and N). The two sets look like each other, but an important distinction exists. The first set contains all stakeholders involved in the route within a chemical park (R), while the second set (N) contains all stakeholders involved in the complete network of the chemical park. The difference between a route and the complete network is visualized in Figure 4.7. According to specific input parameters, the complete network is designed containing all possible links between the involved stakeholders (nodes). From this complete network, all different kinds of subnetworks can be generated in which a single route performs best. This difference and process of finding the optimal route is explained more elaborately in Chapter 5. A single subnetwork contains an optimal route that involves different stakeholders. For all the different routes the outcome for the output parameters needs to be defined, this is why it is important to make this distinction. A more elaborate explanation of the generation of routes is given in Chapter 5.

In the previously discussed two sets, the elements are described as stakeholders. However, within this research, two stakeholders exist, namely chemical factories and treatment facilities, which function differently within the model. This is why two different sets have been defined, gathering all involved chemical factories (C) and treatment facilities (F) from the involved stakeholders.

	Sets
Notation	*Description and range*
R	Set of all stakeholders within the considered route
N	Set of all stakeholders within the complete network of the chemical park
C	Set of all chemical factories within the involved stakeholders
F	Set of all treatment facilities within the involved stakeholders
L	Set of all water pipes within the considered route
I	Set of all sources considered in the network
J	Set of all sinks considered in the network
Q	Set of all qualities of the water
T	Set of all considered treatment technologies (anaerobic-anoxic-oxic, aerobic biological, membrane bioreactor)

	Parameters	
Notation	*Description*	*Unit*
CTS_f	Fixed costs for separate wastewater treatment facility f (f∈R)	€/year
CTI_f	Fixed costs for the inplant wastewater treatment facility f (f∈R)	€/year
CTE_t	Variable costs for the wastewater treatment technology (t∈T)	€/year
C_{fresh}	Costs for freshwater	€/m^3
C_{constr}	Costs for the construction of a water pipe	€/m^3
FR_l	Capacity of the water pipes	$m^3/year$
f_l	Flow rate of a water pipe	$m^3/year$
LE	Location of the source, sink, chemical factories or treatment facility	coordinates(x,y) in km
$D_{c, q}$	Water demand of a chemical factory (c) of a certain water quality q	$m^3/year$

	Variables	
Notation	*Description*	*Unit*
$C_{tinhouse}$	Costs for the industrial symbiosis water route with inhouse treatment facilities	€/year
$C_{tseparate}$	Costs for the industrial symbiosis water route with separate treatment facilities	€/year
$C_{tinhousepark}$	Costs for the industrial symbiosis complete water network with inhouse treatment facilities	€/year
$C_{tseparatepark}$	Costs for the industrial symbiosis complete water network with separate treatment facilities	€/year
$C_{waterusage}$	Costs for the freshwater usage	€/year
d	Length of a water pipe	km
C_{con}	Costs for the construction of the additional water pipes	€
$PC_{inhouse}$	Additional costs for the specific route compared to the costs for the entire IS network	%
$PC_{separate}$	Additional costs for the specific route compared to the costs for the entire IS network	%
FW_{total}	Total freshwater demand of all chemical factories within the considered network (c∈R)	$m^3/year$
FW_{target}	Total freshwater target	$m^3/year$
$FW_{targettry,R}$	Minimum total freshwater target for one optimization try per route	$m^3/year$
$FW_{targetmin}$	Minimum total freshwater target	$m^3/year$
$WW_{produced}$	Total wastewater produced within the considered network	$m^3/year$
$FW_{i,c,q}$	Freshwater flow from source to chemical factory	$m^3/year$
$F_{f,c,q}$	Water flow from treatment facility to chemical factory	$m^3/year$
$F_{c1,c2,q}$	Water flow from chemical factory to chemical factory	$m^3/year$
$W_{f,j,q}$	Wastewater flow from the treatment facility to sink	$m^3/year$
$W_{c,j,q}$	Wastewater flow from chemical factory to sink	$m^3/year$
RW_{total}	Total recycled water	$m^3/year$
RW	Amount of recycled water compared to the total freshwater demand	%

Table 4.1: Overview of all sets, parameters, and variables used in the model

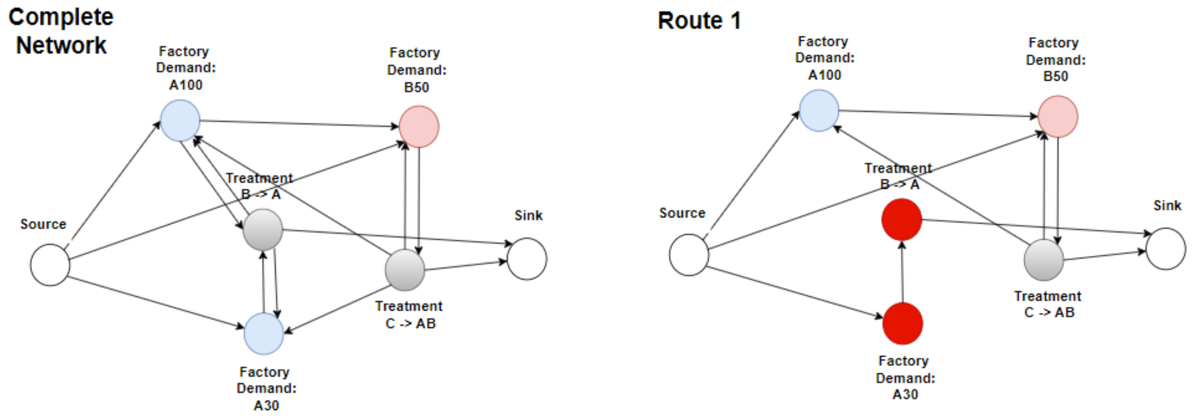


Figure 4.7: Visualization of the difference between the complete network and the route

4.8. Mathematical formulation of the model output parameters

To measure the IS performance, the model should include output parameters related to the three most important performance topics defined in Chapter 2.2: economic, environmental and social. To be able to compare the industrial symbiotic performance between the different scenarios, involving different stakeholders, treatment facilities, and pipes, most output parameters are defined in percentages. Below are the formulas used to calculate each of the relevant criteria enlisted.

4.8.1. Environmental performance

In paragraph 2.2.2 is stated that environmental performance is an important criteria for defining the industrial symbiotic performance of a water network in a chemical park. This criteria is in quantification terms related to water efficiency (Boix et al., 2015). In this model, water efficiency is measured in the amount of water that is recycled in the specific water network.

The amount of recycled water is calculated according to all the water demands of the chemical factories (c) involved in the initial network. According to Lyu et al. (2020), most enterprises use less than 2 million tons of wastewater annually. The different water demands (D) per stakeholder are defined according to the same scale for the network setup. The total water demand (FW_{total}) is the total value considering all different water qualities. So, the demands of all stakeholder that take part in a specific route for a specific water quality are summed into a total freshwater demand consisting of all water qualities. The formula for the total water demand of the initial network is:

$$FW_{\text{total}} = \sum_{c \in R \cap C} \sum_{q \in Q} D_{\text{c,q}} \tag{4.1}$$

The amount of wastewater that is received in the sink ($WW_{produced}$), and in reality disposed into nature again is calculated by the amount of wastewater flowing from the treatment facilities towards the sink ($W_{f,j,q}$) and from the chemical companies towards the sink ($W_{c,j,q}$), again considering all water qualities. The final amount of wastewater produced contains all different water qualities, therefore, amounts of water are always summed up for each water quality.

$$WW_{\text{produced}} = \sum_{f \in R \cap F} \sum_{j \in R \cap J} \sum_{q \in Q} W_{f,j,q} + \sum_{c \in R \cap C} \sum_{j \in R \cap J} \sum_{q \in Q} W_{c,j,q} \tag{4.2}$$

The most important aspect of the model is the optimization function to find the lowest amount of water that could flow through a network while all water demands of the chemical factories are satisfied. This amount of water is called the freshwater target, FW_{target}. The freshwater target for each try (explained in Chapter 5) $\text{FW}_{\text{targettry}}$ is calculated per route by the amount of freshwater that flows from the source into the network to the chemical companies, $FW_{i,c,q}$ minus the amount of water that flows from the treatment facilities (f) towards the chemical factories (c), $F_{f,c,q}$ or from the chemical factories (c) towards other chemical factories (c), $F_{c1,c2,q}$, meaning this amount of water will be recycled. Important to note is that this freshwater target is again incorporating all different water qualities (q).

$$FW_{\text{targettry}} = \sum_{c \in R \cap C} \sum_{i \in R \cap I} \sum_{q \in Q} FW_{i,c,q} - \sum_{f \in R \cap F} \sum_{c \in R \cap C} \sum_{q \in Q} F_{f,c,q} - \sum_{c_1 \in R \cap C} \sum_{c_2 \in R \cap C} \sum_{q \in Q} F_{c_1,c_2,q} \tag{4.3}$$

Within the model, two important objectives are identified when searching for the optimal water flow in the network. First of all, it is essential to note that the target amount of freshwater needs to be minimized to find an optimal IS water route. Secondly, the amount of target water flowing into the chemical park (network) must be the same as the amount of wastewater flowing out of the chemical park for the optimization function to work. The resource objectives are defined according to a study in which an optimal water flow is also calculated from Chin et al. (2021). The scope defined in section 4.5.1 explained no other wastewater routes, like evaporation, are considered within this model.

$$FW_{\text{targetmin}} = \text{min} FW_{\text{targettry,R}} \forall R \tag{4.4}$$

$$FW_{\text{target}} = \begin{cases} FW_{\text{targetmin}}, & FW_{\text{targetmin}} = WW_{\text{produced}} \\ 0, & \text{otherwise.} \end{cases} \tag{4.5}$$

Eventually, the amount of recycled water defines the environmental performance of a specific network. The amount is defined as the difference in the total demand of all stakeholders taking part in the initial network (FW_{total}) and the target amount of freshwater (FW_{target}), shown in this function:

$$RW_{\text{total}} = FW_{\text{total}} - FW_{\text{target}} \tag{4.6}$$

Lastly, a formula is set up that enables comparison between different structures of networks. Each network analyzed has a different topology, also dependent on the number of stakeholders that partake in the network. The amount of recycled water (RW) is defined in percentages to compare these different networks. To know what this percentage is compared to the water demand of the entire initial network, this value is divided by the sum. The formula for Recycled Water (RW) is:

$$RW = \left(\frac{RW_{\text{total}}}{FW_{\text{total}}} \right) \cdot 100\% \tag{4.7}$$

Any networks no longer connected after removing stakeholders are assigned a value of 0 for the optimal flow. These networks are included in the calculation of output parameters, as it is crucial to account for networks that no longer have any performance in the final analysis.

4.8.2. Economic performance

The second criterion for measuring the industrial symbiotic performance of a water network in a chemical park is the economic performance. The economic aspect is the easiest criteria to measure through a mathematical formulation (Boix et al., 2015). To implement an IS water network, it needs to be economically viable. The model calculates the costs for the entire new network as the net present value (NPV).

The costs of a specific water network are calculated according to several factors. The first factor is the costs that have to be invested for new water pipes to enable more IS connections within the chemical park (C_{con}). The length of a new pipe in the network (d) is defined according to the locations of the two involved stakeholders, i and j. The locations of the stakeholders are defined according to the coordinates (x,y), visualized in Figure 4.8.

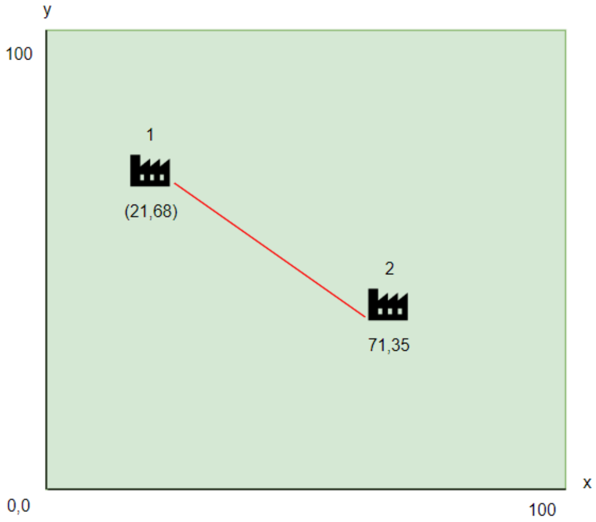


Figure 4.8: Visualization of locations according to the coordinates and the length of the edges

$$d(i,j) = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2} (\forall i, j \in N) \tag{4.8}$$

The lengths of all involved water pipes within the specific route are summed and multiplied by the average cost for the construction of a water pipe per kilometre (C_{constr}).

$$C_{\text{con}} = C_{\text{constr}} \cdot \sum_{(i,j) \in R} d(i,j) \tag{4.9}$$

The second factor impacting the total costs for the IS water network is the cost of the freshwater intake ($C_{waterusage}$). This cost is calculated by the amount of the exact freshwater intake per network multiplied by the costs for freshwater (C_{fresh}). The costs for freshwater differ per country. Therefore, an average will be used. The costs for the different water qualities are all the same. The different water qualities are not presented in this equation as the variables, (FW_{total}) and (RW_{total}), already contain the amount for all different water qualities. The costs for freshwater

$$C_{\text{waterusage}} = C_{\text{fresh}} \cdot (FW_{\text{total}} - RW_{\text{total}}) \tag{4.10}$$

The third factor impacting the total costs for the IS water network is the cost for the treatment of wastewater in the chemical park. As explained in paragraph 3.6, two different types of networks have been constructed within this research. A network with inhouse treatment facilities, and another network with all separate treatment facilities. According to Lyu et al. (2020), does the wastewater treatment calculation in chemical parks differ between these two models. The fixed costs for inhouse treatment facilities differ from those of separate treatment facilities. Therefore, a different cost parameter (CTS_f, CTI_f) is used (elaborated in Chapter 7) for each of the two model structures resulting in separate equations for the two treatment models.

The advancement of a treatment facility can greatly differ, as detailed in section 2.1.3. The model developed for this study incorporates three distinct advanced technologies for the treatment of water. Each of the technologies has different costs, explained elaborately in Chapter 7, notated as variable cost in this research (CTE_t).

The costs for the treatment facilities is directly incorporated into the equation for the calculation of the final costs for the IS water network. The final costs for the the IS water network with separate treatment facilities ($C_{tseparate}$) and with inhouse treatment facilities ($C_{tinhouse}$) are calculated by taking the trhee different factors, construction costs, water usage costs and the wastewater treatment costs together:

$$C_{\text{tseparate}} = (\sum_{f\in R\cap F} CTS_f + \sum_{t\in F} CTE_t) + C_{\text{con}} + C_{\text{waterusage}} \tag{4.11}$$

$$C_{\text{tinhouse}} = (\sum_{f\in R\cap F} CTI_f + \sum_{t\in F} CTE_t) + C_{\text{con}} + C_{\text{waterusage}} \tag{4.12}$$

With previous formulas, the costs for the IS water network can be calculated for a specific route. However, to be able to compare the costs of a certain route with the maximum the IS water network could cost, the costs for the complete network need to be calculated, which is performed in the equations for $\text{C}_{\text{tseparatepark}}$ and $\text{C}_{\text{tinhousepark}}$. By calculating what percentage of the costs of a specific route are compared to the maximum costs of the specific complete network, a comparison can be made between all existing routes. This percentage ($PC_{separate}$, $PC_{inhouse}$) is calculated for the two different network structures enlisted below:

$$C_{\text{tseparatepark}} = (\sum_{f\in N\cap F} CTS_f + \sum_{t\in F} CTE_t) + (C_{\text{constr}} \cdot \sum_{(i,j)\in N} d(i,j)) + (C_{\text{fresh}} \cdot \sum_{c\in N\cap C}\sum_{q\in Q} D_{\text{c,q}}) \tag{4.13}$$

$$C_{\text{tinhousepark}} = (\sum_{f\in N\cap F} CTI_f + \sum_{t\in F} CTE_t) + (C_{\text{constr}} \cdot \sum_{(i,j)\in N} d(i,j)) + (C_{\text{fresh}} \cdot \sum_{c\in N\cap C}\sum_{q\in Q} D_{\text{c,q}}) \tag{4.14}$$

$$PC_{\text{separate}} = \left(\frac{C_{\text{tseparate}}}{C_{\text{tseparatepark}}}\right) \cdot 100\% \tag{4.15}$$

$$PC_{\text{inhouse}} = \left(\frac{C_{\text{tinhouse}}}{C_{\text{tinhousepark}}}\right) \cdot 100\% \tag{4.16}$$

4.8.3. Social performance

The third performance metric for IS is the social aspect. As concluded in Chapter 2, this aspect is not represented enough and measured in optimal water network designs of existing studies. The social performance metric can be interpreted in different ways. In this research, the social performance is measured as the robustness towards stakeholders not partaking in the network on the water network with social network analysis. However, there is a limited possibility to measure the robustness within the network theory mathematically.

Many existing approaches for assessing sustainability, including those based on life cycle thinking, typically rely on biophysical methods to quantify resource flows and environmental impacts of products and processes. However, these approaches often assume a straightforward cause-and-effect relationship and may overlook indirect effects resulting from the complex interactions among components within the system (Ruth and Davidsdottir, 2009a, Ruth and Davidsdottir, 2009b). In contrast, network analysis employs techniques and metrics such as centrality or connectivity indices to comprehend the structure of a network and the intricate relationships among its nodes (Zhu and Ruth, 2013).

Nevertheless, network analysis has not been extensively employed to enhance the understanding of resilience in engineered networks. To address this gap, the principles of network theory are integrated with information about resource (specifically water) flows to comprehend the robustness of industrial symbiotic networks. The network metric 'network efficiency' is utilized to gain insights into the resilience of specific water networks within industrial symbiotic systems in response to stakeholder behaviour.

In a network, the efficiency between a pair of nodes refers to the inverse of the shortest path distance between them. This means that if two nodes have a short distance between them, their efficiency value will be higher. The average global efficiency of a graph is obtained by calculating the average efficiency value of all possible pairs of nodes in the graph.

Social relationships are based on water flow connections. If a specific stakeholder drops out, not only will the relationships of their immediate stakeholders be affected, but the overall throughput of the network (chemical park) will also change. The amount of water that can be recycled depends not only on direct connections but also on indirect connections. For instance, if one factory sends water to a treatment facility and another chemical factory uses the water from that treatment facility, it is important to measure the efficiency between these two stakeholders, as it directly affects water recycling. Since robustness to the failure of specific stakeholders needs to be measured, it is crucial to assess the impact on the entire network (all shortest paths) rather than solely focusing on direct relationships.

$$E = \frac{1}{|N|(|N|-1)} \sum_{(i,j)\in N, i\neq j} \frac{1}{d(i,j)} \tag{4.17}$$

The most natural distance for unweighted networks is the length of a shortest path between nodes i and j. A shortest path between i,j is a path with a minimum number of edges and its length. Observe that if i = j then dij = 0 and that is why the sum above is over i≠j while if there is no path connecting i and j, d_{ij}=∞ and their pairwise efficiency is zero. The network efficiency (E) is bounded between 0 and 1, meaning it is a normalised descriptor.

The network efficiency of an IS network is used to calculate the importance of each of the nodes by examining the change in the network efficiency on removal or change in the flows from the nodes. Removal of a node in the network leads to a reduction in the total throughput in the network, which decreases the efficiency of the network. Large reductions in efficiency mean the network structure is less robust to certain stakeholder behaviour. The total network efficiency of a network with less stakeholders joining is compared to the total network efficiency of the initial network, to gain insights on the importance of different stakeholders in the chemical park, and see the robustness of certain networks (chemical parks) towards stakeholder behaviour.

This concludes the formulation of the designed model. All calculations and outputs of the model have been defined. The outputs are reached by first using the optimization part of the model, and, afterwards, the social behaviour part of the model. The technical optimization part of the model, including the objectives, constraints, and several steps, will be introduced in the next chapter.

5

Technical Optimization System Description

In the previous chapter, an overview of the entire model design has been given. It is explained that the model contains two parts, the technical optimization part, and the social behaviour part. The first part of the model is explained elaborately in this chapter. First, an overview is given of all steps involved in the model, followed by a summary of the most important tasks that are performed to prepare for the optimization algorithm and the simplifications that are made in this process. Finishing with an elaborate explanation of the optimization algorithm used within this research.

The technical optimization model consists of different steps involved in the design, presented in Figure 5.1. The diagram displays all the input and output for each step, as well as the relationships between them. Although the following section will provide a more detailed explanation of the most important steps, it is essential to keep this diagram in mind to understand the overall structure and relationships.

5.1. Generation of all possible water routes and simplifications

The model aims to conduct a network analysis to determine if there is potential for improved industrial symbiosis performance within specific water networks. In order to carry out this analysis, it is first necessary to initiate a network. The design of a complete network is possible for each unique combination of network components and their corresponding attributes (defined input parameters). From this complete network, all possible water routes are identified. This complete network and possible water routes serve as the foundation for the subsequent model analysis. The design of the complete network and possible water routes exists out of a few steps of which the most important steps are explained in the next paragraphs, and the explanation of the other steps are attached in Appendix C.

In the process of developing the model, some simplifications were made to avoid lengthy computation times or excessive network complexity. These simplifications and their possible impact are discussed per step. Additionally, the possible alternatives that could have been adopted are also discussed.

5.1.1. Input parameters

The input parameters form the basis for the customization of the network. The inputs are required to define the initial setup of the network.

In the first step of the model, these input parameters are defined. It gives the setup for the number of nodes, the type of nodes, and all their accompanied attributes. The attributes that are given to each node are defined by their types, such as ’chemical factory’, ’treatment facility’, ’source’ or ’sink’, and are their location, defined in coordinates, their demand of water defined in m3 per year, and the type of water quality demanded and afterwards supplied.

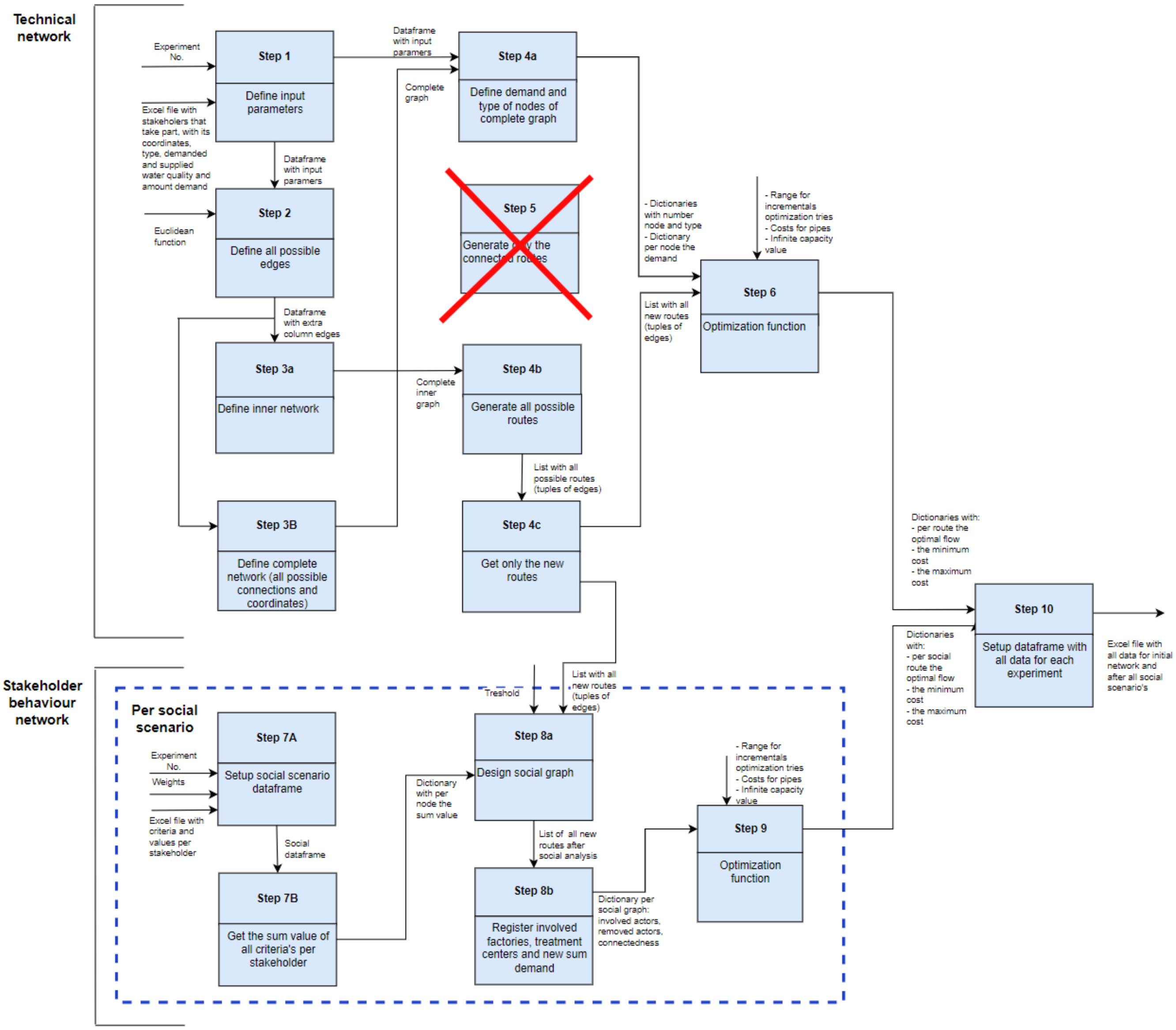


Figure 5.1: High-over scheme of the model design

A few simplifications are made in this step having different possible impacts, summarized in Table 5.1. First of all, regarding the water quality. The water quality is defined in letters, specifically A, B, C, D, of which A is the water quality of the highest level, having 100% cleaned water. Chemical factories always downgrade the water quality by one level. Chemical factories that require a certain water quality, can also use water of higher quality. Treatment facilities always upgrade the water quality, how many levels are defined by the advancement of the treatment facility. As the chemical factories only reduce the water quality by one level, while the treatment facilities upgrade the water quality in some cases by more levels, this simplification could imply that the water network potentially contains more water flows of higher quality than is actually realistic.

Secondly, the treatment facilities do not have an attribute of the amount of water demand or supply, as they just process the amount of water that is sent to them from the chemical companies. Notwithstanding, this presupposes that the treatment facilities possess the capability to treat all quantities of water, thereby implying the feasibility of a more efficient water distribution network than what is realistically achievable.

Lastly, each node representing a stakeholder contains for a set of attributes the same values for all experiments. Meaning, if a certain chemical factory is involved in the network, this factory always has the same location, water demand, and water quality demand and supply. This is an important aspect, as in this way the different networks can be compared with each other. If the values of the attributes would differ per experiment, the effect of the involvement of certain stakeholders (nodes) on the performance of the network cannot be analyzed.

Step 1	Task	Simplification	Possible impact	Alternative	Computation time
Define input parameters	Create overview per experiment with the number of nodes and their attributes: • Type; • Amount water demand; • Water quality demand; • Water quality supply; • Coordinates	1. Chemical factories are downgrading water quality only by one level 2. Treatment facilities have no water demand 3. All values of a set of attributes per node stay the same	1. Water network with potentially higher water qualities than realistic 2. More efficient water network than feasible 3. Enabling analysis of the impact of involvement of certain stakeholders	1. Defining per chemical factory different number of levels the water is downgraded 2. Set maximum of water flow per different treatment facility 3. Use time steps with varying demand per stakeholder	Very short

Table 5.1: Overview of the task, simplifications, alternative, and computation time of step 1 in the designed technical optimization model

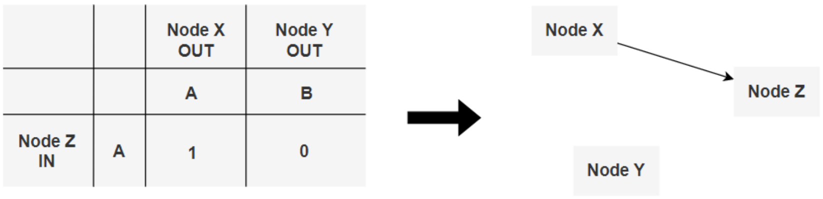
5.1.2. Finding all possible connections between stakeholders

In the previous paragraph, the setup for the input parameters identifying the nodes of the network and the simplifications made were explained. In this paragraph, will be explained how all possible water pipes between the stakeholders in the chemical park are defined, and the simplifications made in this process.

In step 2, all possible edges of the specific network are searched and defined. The method for defining all possible edges is shown in Figure 5.2. If the supplied (out) water quality of a certain node matches the demanded (in) quality of another node, a link is possible between these nodes.

In step 3a, the inner-directed graph is defined. This means the network is defined without the source, the sink, and its in-out flowing edges. This step is necessary as differences exist between the edges of the inner network and the edges connected to the source and the sink, explained in the next paragraph. According to all the possible edges per node defined in step 2, the directed edges are added to the network between the nodes. A directed network is a graph consisting of a set of objects (called vertices or nodes) that are connected together, where all the edges are directional (Barnes & Harary, 1983).

In step 3b, the source and the sink nodes and their according edges are added to the inner network again, shown in Table C.3. However, the edges are added according to some extra rules. Specifically, all chemical factories are connected to the source and a treatment facility, as it is assumed that in current chemical parks, every chemical factory already receives freshwater and has an outflow of wastewater



		Node X OUT	Node Y OUT
		A	B
Node Z IN	A	1	0

Figure 5.2: Defining network edges according to rules for matching water qualities

which needs to be treated according to regulations. All treatment facilities have no direct connection (edge) with the source as treatment facilities will not have to treat freshwater, in reality (AkzoNobel, 2021). Moreover, every treatment facility is connected to the sink, as all water needs to be treated before it is dismissed into surrounding water basins again (Abdel Wahaab & Alseroury, 2019).

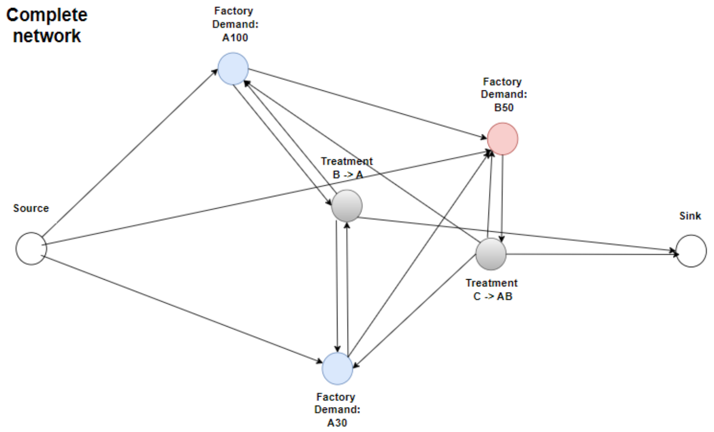


Figure 5.3: Visualization of the complete network according to a set of input parameters

5.1.3. Finding all possible water routes within the network

Now that the entire network in the chemical park has been defined, all possible water routes within this network, have to be defined, consisting of a few steps explained below.

In step 4b of the designed model, first, all different subnetworks are identified and second, all potential water routes are established within this subnetwork by combining edges between the source and the sink. Per subnetwork, a huge number of different combinations and orders of edges can be defined. A single route (specific order of edges) is searched per subnetwork, which performs optimally compared to all other routes stemming from a subnetwork. A single node can be present in this route more than once, as it should be able to use wastewater of multiple treatment facilities and chemical factories (other nodes).

In Figure 5.4, a few examples are given from subnetworks that are generated from the complete network in Figure 5.1. Figure 5.5 shows two different routes (order of edges) that are established from a single subnetwork (3) of Figure 5.4. These routes form the basis of the IS water network as the performance of these routes is analyzed to find the optimal route. To simplify this process, two important assumptions are made.

Firstly, a maximum length is set for the generated routes. This length defines the maximum amount of edges the different routes within the network consist of. The first reason for this simplification is that the computation time grows exponentially according to the length of the possible routes. The second reason is that, in reality, it would become too expensive if all possible pipes were built between all stakeholders within the park. However, this simplification could limit the amount of water that is being recycled in the network. A maximum has to be set before the optimization is performed. This means a limit is already given before the optimal route (and its length) is known. It could be possible the optimal route is not included in the outcomes as the length of this route is larger than the limit set beforehand.

Secondly, a graph does not have to be constructed for each route to check if the route is connected from the source to the sink (step 5). A graph is connected if at least one branch exists between any of the two nodes of a graph so that no node will present as isolated or separated (Barnes & Harary, 1983). This connectedness check is unnecessary as it is assumed that every water pipe already located in the chemical park can be used and included in all routes. In reality, these water pipes are already constructed and will no longer have to be paid for. This means that every node in the network is already connected. These simplifications save significant computation time and cost, with the alternative being to include all possible lengths for the routes and not make hypotheses about their economic performance.

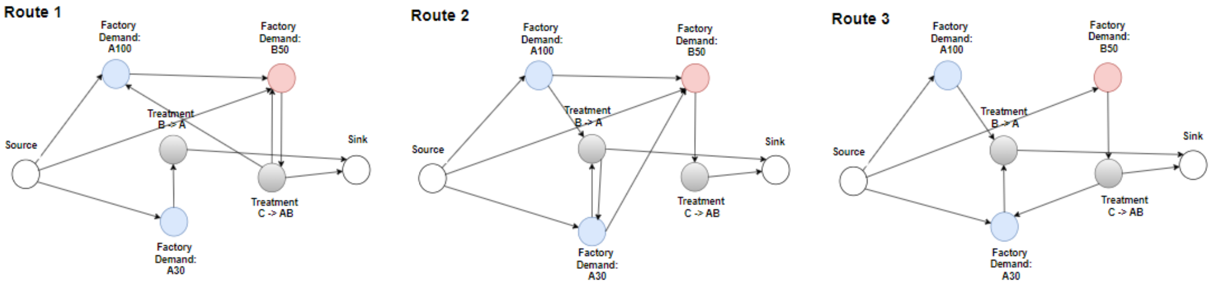


Figure 5.4: Visualization of a few different subnetworks that stem from the complete network

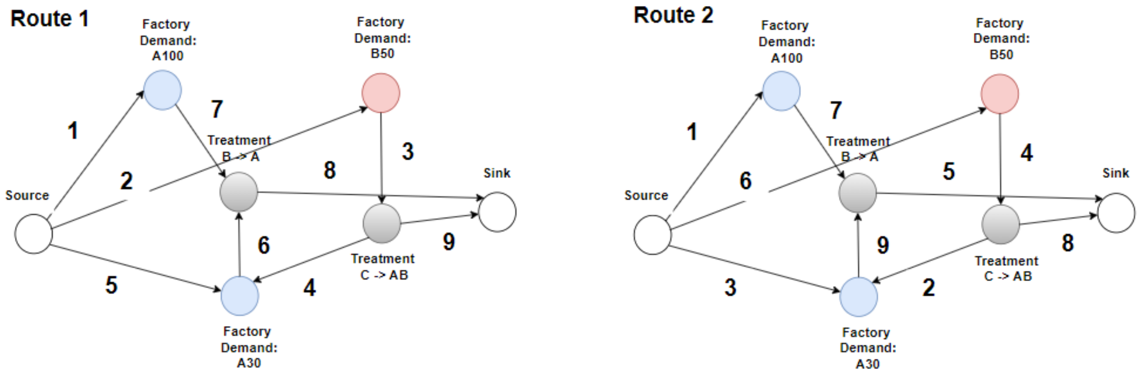


Figure 5.5: Visualization of a few different routes that can be identified by making different orders of the edges in a subnetwork

5.2. Description of the optimization algorithm

The technical optimization model comprises several steps, with Step 6 being of paramount importance. This step involves optimization, which seeks to identify the optimal water flow for each specific route based on the costs and the amount of recycled water. It encompasses several tasks and simplifications

Step	Task	Simplification	Possible impact	Alternative	Computation time
Step 4b Generate all possible water routes	Generate all possible combinations from the possible edges of the inner network	1. Length of possible routes set to 9 2. No connectedness check has to be performed	Limit the possibilities for water recycling	1. Generate routes from the complete network 2. Put no limit on the length of the routes	Medium

Table 5.2: Overview of the task, simplifications, alternative, and computation time of step 4b in the designed technical optimization model

Step 6	Task	Simplification	Possible impact	Alternative	Computation time
Optimization function	For each route perform different tries for the minimal amount of flow through the network until accepted.	1. Set capacity edges to infinity 2. Make the incrementations of each try for the minimum demand and supply for each network bigger	Higher or lower amount of recycled water than in reality	1. Conduct optimization only for the inner network routes 2. Find another optimization method	Very long

Table 5.3: Overview of the task, simplifications, alternative, and computation time of step 6 in the designed technical optimization model

that are explained in detail below and presented in Table 5.3.

5.2.1. Explanation of the Maximum Flow Minimum Cost Algorithm

The algorithm used for the optimization function in step 6, is called the maximum flow minimum cost algorithm (Hagberg, Schult Swart, 2004). The maximum flow minimum cost algorithm is an optimization and decision problem to find the cheapest possible way of sending a certain amount of flow through a flow network. A flow network is directed graph G=(V,E) with a source vertex i$\in$V and a sink vertex j$\in$V where each edge l $\in$E has capacity c_l>0, cost a_l and flow f_l. The cost of sending this flow along an edge (l) is $a_l \cdot f_l$ (Hagberg, Schult Swart, 2004).

5.2.2. Defining the constraints

This research uses a constrained optimization algorithm to solve the optimization problem. The solution space is restricted by multiple constraints that must be satisfied by the solution. These constraints will be elaborated on below.

The first constraint for finding the optimal route within a water network is that the water flow rate f_l within a water pipe should never exceed the capacity (FR_l). Not more water can flow through a water pipe than the capacity the water pipe consists of (Dinitz, 2006).

$$f_l \leq FR_l \tag{5.1}$$

The second constraint is set for the amount of water that can flow from stakeholder towards stakeholder in the network. The amount of water that is sent to a node (sum of f_l of all edges that go into the node) is always the same as the amount of water that the same node is sending to other nodes (sum of f_l of all edges that go out of the node), except for the source and sink nodes. In this research is assumed that no water is lost within chemical factories or treatment facilities, and therefore, the amount of water that flows out of these facilities will always be the same as flows in (Dinitz, 2006).

5.2.3. Defining the objectives

In Chapter 2 have the different criteria for the industrial symbiotic performance been defined. According to these criteria, the mathematical output parameters are set up in Chapter 4. The optimal routes must be defined according to certain objectives during the optimization. The objectives are enlisted below. The first objective, PC, needs to be minimized and the second objective, RW, needs to be maximized. An optimal IS water network requires the least amount of costs and the most amount of recycled water.

1. *Additional costs for the specific route compared to the costs of the entire IS water network (PC)*
2. *Total amount of recycled water (RW)*

An important note for these objectives is that the social aspect, network efficiency, is not included as an objective for the optimisation function. This can be explained by the fact that the social performance is measured within this research as the influence of certain stakeholders not taking part on the entire network. The IS water network cannot be optimized according to its network efficiency because the decisions of the stakeholders cannot be changed. The network efficiency represents the stakeholder behaviour's effect on the IS water network instead of an objective for defining the optimal route within a chemical park (Heeres et al., 2004, Mirata, 2004).

5.2.4. Defining the solution to the limitation of the maximum flow minimum cost algorithm

However, specific to this research, the algorithm contains an important limitation. The algorithm searches for the route within a network containing the minimum costs but the maximum flow. While for this research, the route needs to be searched within the network in which the most water is recycled, so the least amount of freshwater is required. Therefore, for the optimization to work, the costs of the edges from the source to the nodes and from the nodes to the sink are set to a very high amount to ensure with the maximum flow minimum cost algorithm, the route is searched in which most of the water is recycled.

5.2.5. Defining the optimization within the model

The actual optimization designed in step 6 uses the maximum flow minimum cost function. The optimization works as a trial and error. A minimum amount is set for the water supply in the source and inherently as demand in the sink. If the minimum cost maximum flow function works with this amount, this amount is used as optimal water flow for the specific route. If the function does not work, a new try is performed with each time a higher amount of water set as supply and demand, meaning less water is able to be recycled. The process is shown in Figure 5.6 and in Figure 5.7. In Figure 5.6 is illustrated the first try is performed with a water demand of 120 million per year. In Figure 5.7 is illustrated what happens within the specific route if the amount of water is set to 120, what can be seen is that the water demand of two factories is not satisfied, so this try does not work. The third try is performed with a water demand of 150 million liter per year, and what can be seen in the network on the right in Figure 5.7, that all water demands of factories are satisfied, and 30 million liter of the water is being recycled (in green).

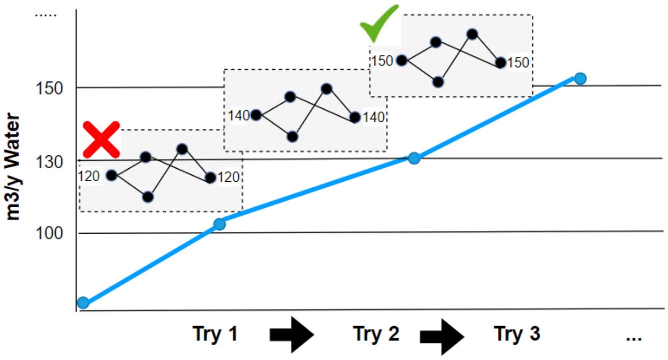


Figure 5.6: Visualization of the operation of the optimization function within the model

A few simplifications are made in order for the optimization to work and to reduce the computation time. First of all, the capacity of every edge of the inner network is set to infinity to ensure all edges could always be used. This does initiate that all water pipes located in the chemical parks, or that will have to

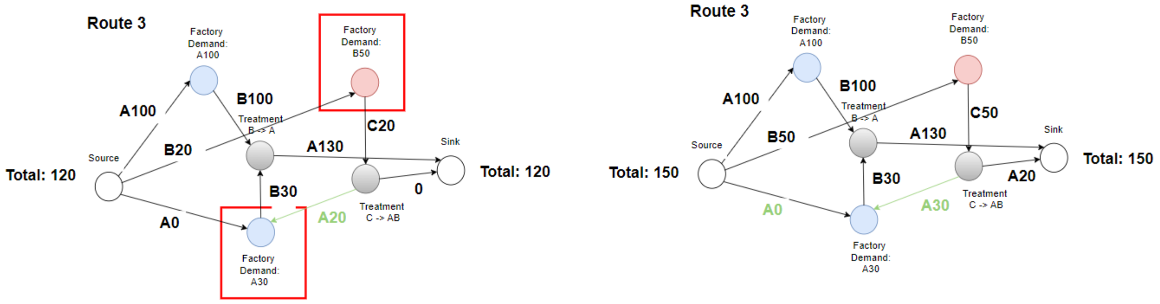


Figure 5.7: Visualization of the tries with water flow of the optimization function within the network

be built are always large enough to transport all water. So, all water can always flow from stakeholder to stakeholder, while in reality water pipes have a maximum volume, limiting the maximum amount of water that can flow through. This means the optimal water flow could in reality be higher than the outcome of the model shows.

Furthermore, a simplification is made in order to reduce the computation time. The differences in incrementations between amounts of water with which the tries are performed have been enlarged, to reduce the number of tries. Instead of trying per 10 million liters of water per year, the model performs tries per every 20 million litres of water per year. This saves a lot of computation time. However, this does have an effect on the possible optimal water flow within a network. The optimal water flow could in reality, be slightly lower than the outcome of the model shows.

5.2.6. Analysis of the water networks after social behaviour has been incorporated

After the social behaviour part of the model has run, new compositions of networks compared to the initial network have to be analyzed. During the social behaviour part of the model, the social behaviour of each individual stakeholder (node) in the network defines if it wants to take part in the network or not. From the initial network, some stakeholders will need to be removed. The newly defined networks have to be analyzed on their performance again. To see what their optimal performance is regarding costs and recycled water, the networks will run through the optimization step again, defined as step 9 in Figure 5.1.

This concludes the formulation of the technical optimization part of the designed model. The different steps to generate all possible water routes within a chemical park have been explained and the coupled simplifications have been elaborated. Afterwards, the optimization function designed for the model has been explained and illustrated. The next chapter will discuss the stakeholder behaviour part of the model.

6

Stakeholder Behaviour Model Description

All the steps of the technical optimization model have been defined in the previous chapter. In this chapter, the steps of the social behaviour part of the model will be explained. Moreover, the specific method for performing the MCDA is motivated and defined.

6.1. Multi Criteria Decision Analysis method: Weighted Sum Method

To research the robustness of a certain IS water network in a chemical park towards stakeholder behaviour, all kinds of different types of stakeholder behaviour should be represented. A method to reach this in a quantifiable manner is working with weights. By adding different weights to certain decision criteria for the stakeholders, the stakeholder behaviour differs in different contexts (J. Wang & Zionts, 2006). This is why the choice for the Weighted Sum Method (WSM) has been made for the implementation of de MCDA in this model. It is probably the simplest and still the widest-used MCDA method. A systematic and logical approach is typically used in the planning and decision-making process to arrive at a solution. In dealing with uncertainty, the theory of multi-criteria decision analysis is often the most common method used. This model is utilized as a multi-attribute decision analysis tool with multiple alternatives and criteria in various fields (Kahraman, 2008). In the weighted sum model, each decision criteria (x_{ij}) is multiplied by a user-supplied weight (w_j) $\forall j \in C$, $\forall i \in A$. Where C is the number of criteria and A is the number of stakeholders. The formula to derive the weighted sum per stakeholder is shown in equation 6.1 and the matrix for deriving these weighted sums with multiple criteria, weights and stakeholders is shown in Figure 6.1. In the maximization case, the best alternative is the one that corresponds to the largest preference value.

$$X_i^{\text{WSM-score}} = \sum_{j=1}^{n} w_j x_{ij}, \text{ for } i = 1, 2, 3, \ldots, m. \qquad (6.1)$$

$$\begin{array}{lc} & \begin{array}{lcccc} \text{criteria} & C_1 & C_2 & \cdots & C_n \\ \text{(weights} & w_1 & w_2 & \cdots & w_n\text{)} \end{array} \\ \text{alternatives} & \text{— — — — — — — — —} \\ X = \begin{array}{c} A_1 \\ A_2 \\ \vdots \\ A_m \end{array} & \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{pmatrix}_{m \times n} \end{array}$$

Figure 6.1: Multi Criteria Decision Making Matrix (Kahraman, 2008)

6.1.1. Defining values for the decision criteria

The choice for using WSM in the social behaviour model part of the model design has been explained in the previous paragraph. Moreover, in the paragraph is explained what the decision matrix consists of, weights and decision criteria, and how it is constructed, to get to the weighted sum. The social behaviour model aims to represent stakeholders' different social behaviour according to their decisions for joining or not joining IS water networks, which they make according to several criteria. The most relevant criteria for the decision to join or not join an IS water network in a chemical park have been defined in the literature study of Chapter 3. This paragraph will explain how values for these decision criteria, are defined. An aspect of the WSM is that it is a subjective method. Generating the values for the criteria and weights will always contain a part of subjectivity (Kahraman, 2008). The values are defined according to interviews and company analysis.

Interviews

Interviews have been conducted during this research to get a more deliberate and accurate overview of the current trends and problems within the chemical parks related to industrial symbiosis. To be able to decide which decision criteria should be included in the social behaviour part of the model, the literature study must be supported by knowledge specific to the chemical industry. Most literature studies are not analyzing decisions specifically for the chemical industry. Moreover, not all literature studies are from recent years, meaning industry trends could already have changed. Therefore, the identified criteria which could be relevant for stakeholders in chemical parks deciding on whether to join an IS wastewater network or not, are tested during the interviews. An overview of the performed interviews is given in Table 6.1 and the summaries of the interviews are given in Appendix A.

Company	Company type	Employee's position
1	Chemical company producing paints	Global director environment
2	Chemical company for health, nutrition and materials	Plant Improvement Engineer facility
3	Coalition for defining sustainability goals for the industry in the Netherlands	Manager Water Sustainability
4	IT consultant	Utilities Manager specialized in Water
1	Chemical company producing paints	Technology Lead
5	Research institution for sustainability in chemical industry	Technology Manager
6	Producer of membrane distillation	Technology officer

Table 6.1: Overview of the different social scenarios

To generate the actual values for the decision criteria, during the interviews the number of mentioned important decision criteria was noted and counted afterwards. This resulted in the following list, shown in Table 6.2. The values are normalized for all decision criteria, by substituting each count by the maximum number of performed interviews.

Company Analysis: Stakeholder properties

During the explanation of the applied WSM within this research, the importance was stressed for using different values for the decision criteria per stakeholder. According to the interviews, values for the decision criteria of each stakeholder type have been defined. Multiple chemical factories take part in a chemical park, but are all the same stakeholder type within this model, meaning they would have the same results for each criteria from the interview. This is why a slight difference of a range from 0 to 10%

Criteria	Count
Feasibility	2
Increase revenue	7
Compliance	8
Internal sustainability policy	5
Trust	5
Awareness	3

Table 6.2: Overview of the output of the interviews for the different decision criteria

in values for the decision criteria has been given between the different partaking chemical factories. The same goes for treatment facilities.

The treatment facilities have been included as stakeholders in the MCDA, although in Chapter 3 was explained that some studies do not consider them as stakeholders. However, in Chapter 3 is also explained that treatment facilities can be publicly or privately owned. Privately owned treatment facilities do have their own consideration for joining or not joining a water network, making their own decision. This is why the treatment facilities have been included in the company analysis.

6.1.2. Defining the weights according to social scenarios

The goal of this research is to find the influence of different criteria influencing the decisions of stakeholders on joining IS water networks and the possibilities for creating an IS water network. Therefore, the different criteria influencing the social behaviour of stakeholders should be tested with different proportions as then the severity and difference in impact can be tested best. This is why social scenarios have been defined, which all represent a different combination and set of weights. According to different social scenarios, the combinations of the criteria and attached weights will differ accordingly.

Huge research according to the European Social Survey, conducting interviews with 46000 Europeans, found six different social attitudes towards sustainability within businesses (Otto & Gugushvili, 2020). Eco-social enthusiasts are defined in this research as the part of Europeans that have a positive stance towards climate change policies and public welfare. ’Welfare enthusiasts’ are the businesses that reject the idea of carbon taxes, make high investments in renewable energy and ban the sale of the least energy-efficient appliances. The group known as ”environment devotees” is characterized as those who are skeptical of the welfare state but supportive of policies aimed at addressing climate change. On the other hand, ”eco-social skeptics” are individuals who hold negative views towards both public welfare and environmental policies. Surprisingly, this group is the largest in Europe. The other two scenarios are combinations of these scenarios, making the set complete, and combining sets of the three pillars. The different social scenarios are shown in Table 6.3. All social scenarios are relevant to one or more of the three performance metrics for industrial symbiosis: social, economic and environmental. Which of the pillars it describes defines which criteria are given specific weights. All the other criteria which are not impacted, are given the medium weight, explained in the paragraph below.

Scenario number	Scenario name	Impacted criteria	Weight
Scenario 1	Environmental-social enthusiast	Trust, Internal policy, Awareness	High, High, High
Scenario 2	Welfare enthusiast	Compliance, Revenue growth	High, High
Scenario 3	Environmental devotee	Internal Policy, Revenue growth, Compliance	High, Low, Low
Scenario 4	Social scepsis	Trust, Awareness	Low, Low
Scenario 5	Environmental-social scepsis	Trust, Awareness, Internal Policy	Low, Low, Low
Scenario 6	Economic-social scepsis	Compliance, Revenue growth, Trust, Awareness	Low, Low, Low

Table 6.3: Overview of the different social scenarios and the impacted criteria

Initial scenario within the model
Within this research, all performances of each network considering stakeholder behaviour are compared to the 'initial scenario'. This is the scenario in which all stakeholders would participate within the IS water network.

Ranges within the weights for the scenarios
The importance of ensuring the objectivity of decision criteria weights cannot be overstated as they can significantly impact the outcome of the decision-making process (Odu, 2019). According to J. Wang and Zionts (2006), a gap exists between the theoretical work and the practical needs of a decision-maker often exists. This is mainly caused because the preferences of the decision maker are not exactly known, which results in wrong implemented or translated preferences in the theoretical model. To prevent the highest subjectivity and wrong translated preferences, this model uses ranges for the weights. This means that it is not possible to further define or determine the weights of the decision criteria due to a lack of specific information about the preferences of the actors involved.The weights are represented as high, medium and low, shown in Table 6.3 and have the actual value scheme enlisted below:

Low = random value between 0.01 - 0.33
Medium = random value between 0.33 - 0.66
High = random value between 0.67 - 1.0

The selection parameters for alternative suppliers are often uncertain, and decision-makers usually express evaluation data and criteria weights in linguistic terms due to a lack of specific information about preferences. Additionally, human judgment on qualitative criteria is subjective and imprecise. Traditional multi-criteria decision analysis (MCDA) methods assume that criteria and weights are expressed in precise values, allowing for straightforward rating and ranking of alternatives (Jamwal et al., 2021).

6.1.3. Implementation of the Weighted Sum Method in the model

Previous paragraphs explained all aspects of the WSM and how values for this research are generated for each aspect, decision criteria and weights according to scenarios. This paragraph will explain how the WSM has been specifically implemented in this model. A small dynamic in stakeholder behaviour is created by varying the values for the criteria per stakeholder and by changing the weights per scenario. Moreover, the robustness to stakeholder behaviour will be measured in this research. Therefore, it is essential the differences in performance are compared every time with the initial network (the network in which all stakeholders would join the IS water network). To create these two aspects, dynamics and resilience comparisons, different steps have been incorporated in the model design. The different steps within the entire model design that are part of the social behaviour part of the model, are represented in Figure 5.1 between the brackets of 'Social Behaviour Network'. A summary of the most critical steps is shown in Table 6.4, and will be explained below.

In step 7a, shown in Table 6.4, the social decision matrix is created, by a specific combination of values and weights multiplied by each other. The choice has been made to focus on specific decision criteria and to research their influence. Therefore only a few criteria will be multiplied by weights per experiment. The weights are determined based on Table 6.3. Moreover, according to Deb (2008), the WSM model only works when the decision criteria can be expressed in the identical unit of measure, and the decision criteria have the same magnitude. This requires the data to be normalized. The normalization step will not have to be performed anymore as the values for the criteria are already normalized, explained in 6.1.1. The decision matrix consists of the values for each of the six criteria per stakeholder: xij, i $\in$A, $\forall$j $\in$C. Where C is the number of criteria, and A is the number of stakeholders.

In step 7b, the weighted sum value for each stakeholder's weighted normalized decision matrix is defined (A), shown in equation 6.1.

After the sum of all criteria per stakeholder has been calculated in step 7b, the new social graph of all partaking stakeholders in the IS water network per scenario can be designed. If certain stakeholders do not want to join the IS water network anymore, no contracts will have to be and can be signed. The stakeholders will be disconnected from the designed IS water network and the remaining network will be analyzed according to the industrial symbiotic performance measures. The source and sink are not

Step	Task	Simplification	Alternative	Computation time
Step 7a Setup social scenario dataframe	Multiply certain decision criteria with the weights specified for the specific scenario	1. Only focus on certain criteria per scenario 2. Use three different sets of values for the criteria	1. Give all criteria different weights 2. Adjust more differences in values per stakeholder to analyze the effect	Short
Step 7b Get the weighted sum value of all criteria per stakeholder	Generate an overview with the sum value per stakeholder			Very short
Step 8a Design the social graph for each scenario	Create an undirected social graph per route and delete the nodes of which their weighted sum value does not reach the threshold	1. Only assume social relations exist between stakeholders that exchange water 2. Use a single threshold	1. Include other relations between stakeholders 2. Use multiple thresholds to analyze the effect	Medium

Table 6.4: Overview of the task, simplifications, alternative, and computation time of step 7a, 7b and 8a in the designed stakeholder behaviour model

considered as stakeholders in the model. This process is shown in Figure 6.2 and the equation below in which TR represents the threshold. The stakeholders will not want to join the IS water network if the sum of all the criteria does not reach the pre-set threshold. A threshold declares the height of the willingness of the stakeholders. If the threshold is lower, the stakeholders will join the IS water network faster, with the same values for the criteria. The values defined for each criteria per stakeholder should differ to analyze the decision of the same stakeholders in the model when they value certain decision criteria differently (Purvis et al., 2019). However, the values for the criteria can be changed in numerous ways, as a simplification for this research has been chosen to change the values for the criteria for each stakeholder three times.

The threshold for this research has been defined according to the lowest weighted sum value of a stakeholder within the initial scenario. All stakeholders join the network in the initial scenario, so the lowest weighted sum value should be above the threshold.

$$X_i^{\text{WSM-score}} \geq TR \forall i \in A \tag{6.2}$$

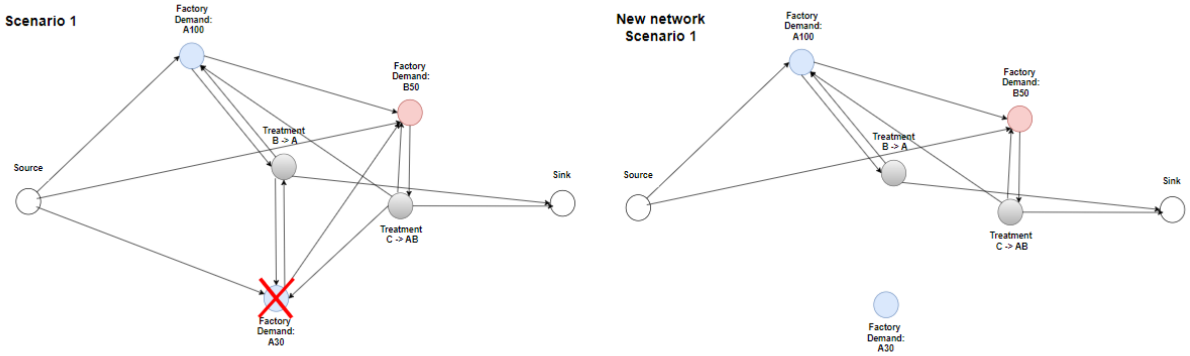


Figure 6.2: Visualization of the effect on the network if a stakeholder does not participate in a certain social scenario

A few important simplifications are made in this step. Firstly, social relations only exist between stakeholders that should or would have exchanged water of a certain quality, as these stakeholders will have to sign a contract. In a social network graph, the social relations between stakeholders are analyzed. It could be possible the stakeholders have a social relationship within the chemical park that do not exchange wastewater. However, this has not been incorporated in the model and in the social graph, as this does not impact the possibilities for IS connections of water within the chemical park. Secondly, only a single threshold is tested in the social behaviour model part, otherwise, the number of experiments becomes too high. The definition for the value of the threshold within this research has been explained above. If another higher or lower threshold were included in the model, all steps of the stakeholder behaviour part of the model would have to be performed again for every scenario, drastically increasing the computation time per experiment.

According to the new social graph for each scenario, the new possible routes within the technical model can be constructed and run through the optimization part again.

This concluded the formulation of the stakeholder behaviour part of the model. The reason for using the WSM, the generation of the values for the decision criteria per stakeholder, the social scenarios and their weights and the different steps part of the implementation in the model have all been defined. The definition of the model analysis and the experimental setup will be defined in the next chapter.

7

Definition of the model analysis, data input and model parameters

In the previous chapters, the narrative, goals of the model, the mathematical formulation, and most important simplifications of the two different parts of the model have been defined. This chapter will introduce the simplified case on which the generic mode is based. The model input parameters will be defined and explained, the experimental setup is explained in 7.3, the different incentives that will be tested are introduced in 7.4, and finally, the behaviour of the model is verified in 7.5.

7.1. Simplified Case Conceptualisation

In Chapter 4, the narrative behind the designed model is explained, moreover, the example of the chemical park on which the network topology is based is explained.

The proposed model has a generic design that enables the use of data from any chemical park. However, the model's computation time increases exponentially as more stakeholders are included in the setup. Therefore, to simplify and optimize the model, it was run on ”dummy data.” Nonetheless, the input data, network structures, experimental setup, and incentives are based on a real-life case study of the chemical park Chemelot.

In an interview with the program manager of Brightside, it was revealed that Chemelot had just initiated a project aimed at identifying options for reducing water intake, one of which was the recycling of wastewater represented by ’recycling effluent 1 and 2’ in Figure 7.1. While the research for this project has not yet begun, it is considered to be of high potential. Chemelot is also considering the construction of another treatment facility, IAZI 2.0. They are interested in finding out if this would be a beneficial project regarding the amount of water that is being recycled and the costs and if site users would use this treatment facility. Or if it would be more beneficial to let the chemical factories implement more pretreatment facilities themselves. Moreover, the decision on what technologies to include in the treatment facility is still under consideration. The experimental setup has been based on this data from Chemelot.

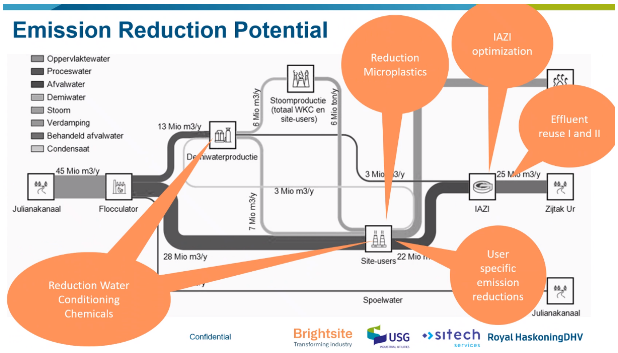


Figure 7.1: Different options for water reductions in Chemelot, Source: Brightside

Notation	*Description*	*Unit*	*Value (in millions)*	*Source*
CTS_f	Fixed costs per separate wastewater treatment facility	€/year	65	Majumdar and Sinha (2021)
C_{constr}	Costs for the construction of a water pipe	€/m^3	0.0125	Geng et al. (2007)
C_{fresh}	Costs for freshwater	€/m^3	0.000003	Hallman (2020)
CTE_t	Variable costs for the wastewater treatment technology anaerobic-anoxic-oxic	€/year	30	Rodiguez-Miranda (2015)
CTE_t	Variable costs for the wastewater treatment technology membrane bioreactor	€/year	20	Rodiguez-Miranda (2015)
CTE_t	Variable costs for the wastewater treatment technology aerobic biological	€/year	10	Rodiguez-Miranda (2015)
CTI_f	Fixed costs for the inhouse treatment of wastewater	€/year	27	Geng et al. (2007)

Table 7.1: Overview of the values for the input parameters

7.2. Data input for the model

To be able to analyze the possibilities for IS in chemical parks, the model requires some data input. The different data inputs are enlisted in Table 7.1. For each input parameter, the source of the data will be discussed, including any concerns about the reliability of the data.

Costs for the construction of water pipes
The average costs for the construction of water pipes has been set to 12500 euro per cubic metre. This average is derived from the study of (Geng et al., 2007). In this study, the average piping costs are derived from research from the Tianjin University in which the entire North China plain was analyzed. The construction costs formula is based on non-corrodable PVC pipes and flat land.

Costs for freshwater
The costs for freshwater differ per country. Impacting factors on the price for water is water scarcity in that location and the availability of treatment facilities. WaterNews (2021) made an analysis of the water prices per m3 per European city. As this research focuses on chemical parks located in bottom-up regulated regions, of which Europe is an important region, this source is used. The costs vary from 0.40 euro per m3 up to 5.6 euro per m3. The average water price for this research has been chosen, which is 3.0 euros per m3.

Costs for separate treatment facilities
The fixed costs for separate treatment facilities, CTS_f, could differ heavily. According to Rodiguez-Miranda (2015), the costs for a treatment plant can be categorised under two heads, namely, capital cost (such as land, cost of consulting and knowledge, civil works for road and other facilities, diesel generator sets, piping, plants and instrument cost, laboratory costs) and operating cost (such as power, transportation, plant maintenance, disposal, consumables, laboratory, third-party charges for analysis, all kinds of spares). The selection of wastewater treatment plants is predominantly influenced by investment costs, according to Majumdar and Sinha (2021). These costs are interrelated with various factors such as the treatment level, quality of raw wastewater, design flow, and purpose of treated wastewater. In a study conducted by Majumdar and Sinha (2021), data from 51 new treatment plant projects were analyzed using multivariable exponential regression analysis. This study revealed the cost scale elasticity of each treatment technology, in slow growth relative to the design flow. In this study, the total annualized equivalent cost (TAEC) is used, which can be calculated by adding the annualized capital investment cost to the annual OM cost. To express the total cost in present values, the expected life of each WWTP is assumed to be 20 years, and the discount rate is 5.5% (Bhoye et al. 2016). From this analysis it can be concluded that the average annual investment costs for a treatment facility are 63 million and a year of

operational costs is 2 million, concluding to 65 million. This amount excluded the initial investment for the pipes connected to the treatment facility as the costs for the pipes are already included in the calculation of the total cost. So, according to the literature, the average costs for a treatment facility will be set to 65 million euro's on average per year.

Costs for inhouse treatment facilities

Costs for the model setup with pretreatment facilities differ as the companies will also have to pay for their internal treatment processes. The pretreatment costs is very volatile and difficult to accs. ount for all companies featured in heavy-organic loads. As this cost could vary in so many ways, and the model that is being designed is for generic usage, an average amount of costs has been taken for this variable (Lyu et al., 2020). The average cost set for every inhouse treatment facility linked to every chemical factory within the model is 27 million euros, derived from Singh and Kazmi (2018). The main difference with separate treatment facilities exist that land does not have to be bought anymore and the operational costs are lower. Moreover, ss mostly the in-house treatment facilities include secondary treatment, instead of more expensive tertiary treatment, the annual investment costs are lower. This study explained the pretreatment costs could vary widely, according to the regulations set for wastewater in the specific country, the substance of the wastewater from the chemical process and the treatment technology implemented.An average has been used, as 26 million euros per year, derived from all different annual prices of the analyzed secondary treatment facilities in this study. An extra 1 million euros is added to this cost for the annual operation costs.

Costs for the treatment technology per level

Rodiguez-Miranda (2015) and Singh and Kazmi (2018) conducted analyses on the difference in investment costs for different treatment technologies. It included different treatment technologies in the analyses, of which anaerobic-anoxic-oxic, anaerobic biological and membrane reactor were part of which all information is provided in appendix A. However, different types exist within these treatment technologies. For example, four different types of membrane reactor technologies exist. Furthermore, the capacity of the treatment technology is not specifically captured within this research. Therefore, an average of annual investment costs has been taken per treatment technology type. On average, there was a difference between investment costs of 30 million euros between the less advanced and most advanced treatment technology. As the model included three different advancement levels, it was derived that each level of advancement is estimated to require a cost of 10 million. However, in reality, this amount can vary widely.

7.3. Experimental setup

The experimentation setup is a combination of social scenarios and networks. The networks are formed according to the input variables and are separated according to the two different types of network structures. This results in the experimentation matrix shown in Tables 7.2.

To gain better insight into how the model operates under different conditions and explore its behaviour on a larger scale, this section explains how data has been generated through experiments. Subsequently, this data will be utilized in the upcoming sections to examine how input parameters affect the model's results.

7.3.1. Centralized vs. decentralized treatment facilities

This is an important difference in the construction of the network model, as explained in Chapter 4. Therefore, separate experiments are constructed. In the present experimental setup, all the input variables are the same for the separate sets of experiments, except for the number of treatment facilities. Specifically, in the second set of experiments, it is assumed that all chemical factories have treatment facilities attached to their chemical factories, obviating the need for separate treatment facilities within the network. Nevertheless, it is evident that one treatment facility still remains in the network, which can be explained by the fact that in real-world cases, every chemical park typically contains one central treatment facility. The primary purpose of this treatment facility is to treat and monitor all diverse treated wastewater streams from the chemical factories before they are released into the environment. This practice is globally required by law (Hu et al., 2019).

Input variables	**Variety values separate treatment facilities**	**Variety values incorporated treatment facilities**
Number of chemical factories	3,4,5	3,4,5
Number of treatment facilities	1,2,3	1
Number of water qualities	2,3,4	2,3,4
Technological advancement treatment facilities	1,2,3	1,2,3

Table 7.2: Content of the experimental setup

7.3.2. Explanation for input variables experimental setup

Further choices for the actual numerical filling of the parameters will be discussed in this paragraph. The goal of this research is to analyze the resilience of the different technical components to a certain behaviour of stakeholders. To research this, the sizes of the technical components should differ, to be able to compare the effect of specific components.

A minimum amount of three factories has been chosen because different routes can be created upward of three nodes. A maximum of five chemical factories has been chosen with regard to the computational effort needed for networks with more nodes. The more nodes the network contains, the number of routes that need to be analyzed grows exponentially. Therefore, the computational power required grows exponentially as well. This is why a maximum of five chemical factories have been chosen.

The number of treatment facilities must be a minimum of one, as explained in paragraph 2.1, required by law. The maximum number of treatment facilities is set to three. This choice has been made because of the exponential growth computation time, and as the number should be lower than the number of involved chemical factories.

The number of different water qualities tested in the experiments is made according to logical reasoning. As explained in paragraph 4.5, each chemical factory downgrades the water quality by one level, so the minimum number of water qualities for the network to work is two. Moreover, as the narrative of the model is to test how resilient certain technical components are toward stakeholder behaviour stimulated by social factors, a network needs to be designed that is technically working. If a high number of water qualities are incorporated into the design of the network, the network becomes technically very challenging, according to Rodiguez-Miranda (2015). This explains that it will not add value to the initial goal of this thesis to include a high number of water qualities. Therefore, the number of water qualities stops at four.

Lastly, The technological advancement of treatment facilities is intrinsically linked to the number of water qualities. If the experiments involve a maximum of four water qualities, the technology in the treatment facilities can only upgrade the water quality by three levels. This is because the maximum difference between the lowest quality and the highest quality is three steps.

7.3.3. The demand of stakeholders

An important note to make regarding the experimental setup is that each experiment consists of a set of chemical factories and treatment facilities. As explained in the technical system description chapter, each chemical factory requires a specific water quality and each treatment facility treats a specific water quality into one, two, or three different higher water qualities. As a complete set of experiments is performed, meaning all different possible variations of the four input variables are tested in experiments, the characteristics of certain chemical factories and treatment facilities differ per experiment. In some experiments, only two water qualities are incorporated, this means the included chemical factories and treatment facilities can only require or treat two different water qualities. However, in other experiments, the same chemical factories and treatment facilities can require or treat four different types of water qualities. However, their initial water quality demand stays the same for all different experimental setups. There is no other possible way to test all the different varieties of input parameters and the chemical factories and treatment facilities always have the same characteristics in this thesis research. In the discussion chapter, the effect of this note will be reflected upon.

Parameter *Notation*	*Description*	*Unit*	*Adjustment*
	Incentive 1: Subsidy for water pipe construction		
C_{constr}	Costs for the construction of a water pipe	€/m^3	10% lower
C_{constr}	Costs for the construction of a water pipe	€/m^3	20% lower
	Incentive 2: Subsidy for advanced treatment technologies		
CTE_t	Costs for the wastewater treatment technology	€/year	10% Lower
CTE_t	Costs for the wastewater treatment technology	€/year	20% Lower
	Incentive 3: Freshwater tax		
C_{fresh}	Costs for freshwater	€/m^3	10% higher
C_{fresh}	Costs for freshwater	€/m^3	20% higher
C_{fresh}	Costs for freshwater	€/m^3	1000% higher

Table 7.3: Overview of the adjustment of the parameters per incentive

7.4. Testing different incentives

According to (Navarro Martínez et al., 2020), the main drivers for taking environmental actions are regulations for wastewater treatment facilities. Their focus is on legislation compliance and on sound execution of technical procedures. However, new thinking, going beyond the end-of-pipe traditional service, needs to be spread off to be able to close the loop and walk towards circularity. To research what could possibly stimulate more circularity, specifically more IS connections within chemical parks, different incentives are introduced. The different incentives are explained below and shown in Table 7.3.

7.4.1. Subsidies

Chin et al. (2021) studied what kind of initiatives could stimulate more water symbiosis within eco-industrial parks. The study concluded that: ”*implementing the symbiosis requires an expensive capital cost on the site and may need cost compensation by the authority to facilitate the operation*”. Cost compensations by authorities are effectuated by subsidies. Despite the identification of the minimal total annual costs through optimization, individual plants in the industrial site may be hesitant to participate in the symbiosis program. This reluctance could be attributed to the potential additional costs they may have to incur to construct the overall system, which may surpass any cost savings they could attain, thereby resulting in no profit. This poses a challenge to the practical implementation of the proposed scheme. To overcome this challenge, it is necessary for the authority to play a central role in providing subsidies to incentivize the plants to participate in the industrial symbiosis program. By offering these subsidies, the authority can persuade the plants to participate in the program, resulting in greater environmental benefits (Chin et al., 2021). To ensure the stakeholders’ willingness to participate in the symbiosis and achieve complete integration, it is crucial to ensure that the subsidies offered for the grand cooperation exceed the subsidies they would receive if they choose not to participate (Chin et al., 2021).

Subsidy for the construction of water pipes

Authorities could subsidize the construction of IS water integrations on the one hand. By subsidizing the construction of the water pipes, it is possible the stakeholders are more quickly stimulated to construct the easy, ’low hanging’ IS water integrations. Stakeholders are only concerned about their own benefits. Government subsidies often lead to stakeholder dissatisfaction as the height of subsidies are differently provided to each stakeholder. With this incentive, a subsidy is given to each kilometre of newly constructed water pipe. To whom this subsidy is given, is not incorporated in the model as the overall costs for the water pipes will be reduced by 5 and 10%. Higher values than this will not be realistic (Chin et al., 2021).

Subsidy for the implementation of advanced treatment facilities
On the other hand, could authorities subsidize the advancement of treatment technologies to stimulate an increase in IS water connection possibilities. With more advanced treatment technologies, water can be treated towards higher quality. However, these technologies are very expensive and therefore less attractive (Majumdar & Sinha, 2021). In this model, this incentive will be researched by introducing a subsidy of 5 or 10% for the advancement of the treatment facility.

7.4.2. Freshwater tax

According to Chin et al. (2021) is, introducing a tax on freshwater or the production of wastewater a possibility as well. A potential method of encouraging stakeholders to participate in the symbiosis program is to offer incentives, such as a reward scheme for their recycling efforts. This allows stakeholders to determine the recycling quantity that maximizes their economic interests. Additionally, an authority could impose a freshwater tax on stakeholders to incentivize their participation in the symbiosis program, while also generating funds for subsidization (Chin et al., 2021). In this research, the effect of the incentive of a freshwater tax is analyzed by increasing the costs for freshwater by 10% and 20%. This is a high increase because currently water is considered very cheap. This is why according to a study from EuropeanCommission, 2000, the price elasticity of water is very high.

7.5. Model verification

After defining the model, the mathematical formulation, and inputting all data, it is essential to ensure that the model and its outcomes are adequate. Two critical steps need to be taken before drawing meaningful conclusions from the model: verification and validation. Verification is aimed at determining if the final model accurately represents the mathematical conceptualization. It does not aim to check whether the results from the model represent the real world, which is done during the validation of the model results in Chapter 9. In this section, the model is verified to represent the conceptual model correctly and to provide a proper translation of theory into a model.

Several methods can be employed to confirm the accuracy of a model. These methods encompass a variety of techniques, such as having an expert review the model, creating logical flow charts that consider every possible action, evaluating the model output to ensure it is reasonable across different input parameter values, and utilizing an interactive debugger. This research verifies the model by examining the expected outcomes if specific input parameters change.

7.5.1. Verifying the network topology per performance metric: does the model behave as expected?

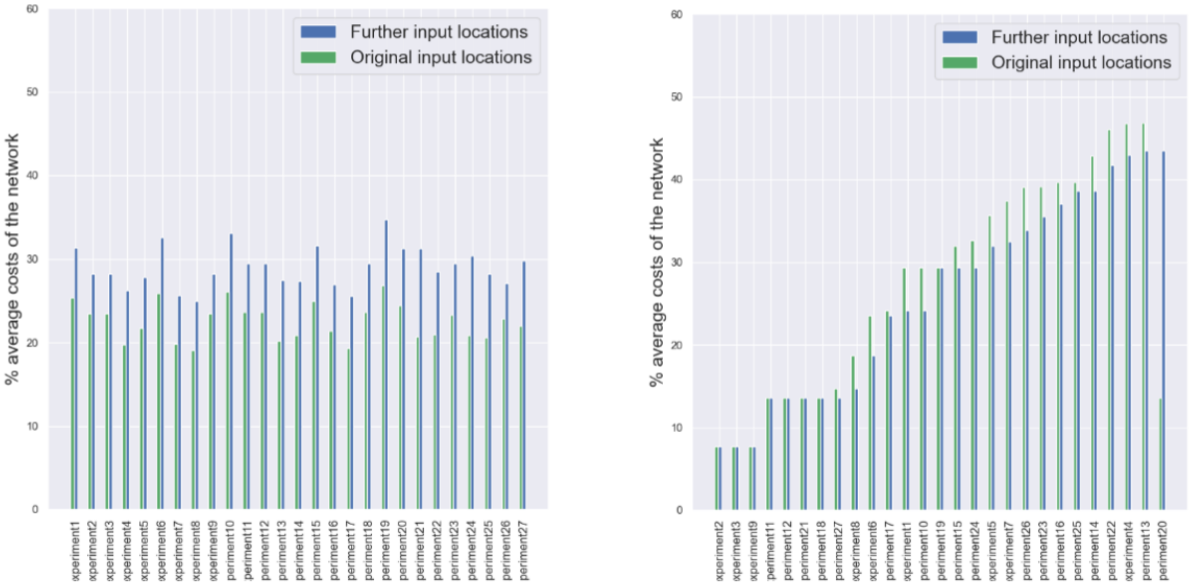
To verify the expected outcomes of the model, a specific input parameter is changed on which the entire model is based: the locations of the stakeholders. The network topology is defined according to this input parameter. The coordinates are changed so that the stakeholders are located much further away from each other. An illustration of how the coordinates are changed for a part of the stakeholders is shown in Table 7.4. The model that has been designed searches for the optimal routes within a network according to the lowest costs and the most possible water that could be recycled. It is expected that the outcomes for the performance metrics: average amount of costs and recycled water, will change with different locations for the nodes, meaning other links could become more efficient. The model is verified according to the change in performance for the initial scenario, in which all stakeholders involved join the network.

First of all, if the locations are further from each other, it is expected that the costs of building an IS water network will be higher because the construction of the pipes will be more costly. This is expected according to the two formulas, 4.8 and 4.9 explained in Chapter 4. In Figure 7.2, this expectation is verified.

Secondly, the average amount of water that could be recycled per experiment is dependent on the different routes identified within the chemical park. In the experiments in which, on average, much water is recycled in the original network topology, it can be seen that less water is being recycled in the new network topology. This is a logical consequence as many water pipes are probably used in these experiments, which is much more expensive in the new network. The model has identified routes with

Old coordinates	New coordinates
source (1,43)	source (1,43)
(83,24)	(183,24)
(11,1)	(111,1)
(46,66)	(146,66)
(72,3)	(172,3)
(17,81)	(117,81)
(22,51)	(121,51)
(41,89)	(141,89)
(53,28)	(153,28)
sink (88,45,89)	(188,45)

Table 7.4: Illustration of adjustment coordinates of the stakeholders



(a) Change in costs

(b) Change in recycled water

Figure 7.2: Verification of the change in costs and recycled water of the network for the initial scenario

fewer connections; otherwise, the economic performance would be far from optimal.

7.5.2. Verifying the model outcomes for the economic performance: does the model behave as expected when changing the input costs?

In the second part of the model verification, all the input parameters defining different costs within the network are changed to see if the outcome for the economic performance changes as well. The different input parameters are costs for the treatment facility, costs for the construction of water pipes, costs for freshwater and costs for the wastewater treatment technology. The costs will be varied by -20% and +20%. The results are visualized by comparing the average optimal costs and percentage of recycled water for the initial scenario per input parameter with the reference situation (REF). It is expected that when certain costs increase, it would become more expensive to construct additional infrastructure for IS connections. On the other hand, when certain costs become cheaper, for example of a treatment facility, it is expected that constructing additional infrastructure for IS water connections would become less expensive. The results are shown in Figure 7.3.

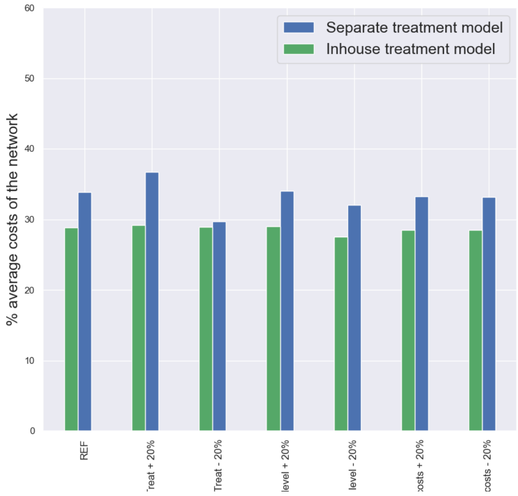


Figure 7.3: Sensitivity of the final average result for the two different networks to different inputparameters

It can be seen in Figure 7.3 that the costs for the network become higher if the input costs increase with 20% and the costs for the entire IS water network decrease if the input costs decrease with 20%. So, the model behaves as expected.

By looking at the outcomes for the different network topologies and different cost input parameters, it can be verified that the model behaves as expected. Changes in other input parameters used within the model are tested in Chapter 9.1.

8

Analysis of the results

The previous chapters have defined the designed model, the data inputs and the experimental setup. The model is completely described and experimentation can begin. This chapter will present the main results of the optimized routes per network structure for each scenario defined in section 6.1. Analyzing the results of all different optimal routes is not straightforward, however. The methods used to analyze the results will be discussed first.

8.1. Explanation scenario 0

Prior to discussing the results, it is imperative to define the current status of the chemical parks with regard to the IS water network, referred to as scenario 0 in this research. This research analyzes to what extent a higher industrial symbiotic performance is possible. This research assumes that in the present situation at a chemical park, there are no IS water relations between stakeholders. It differs per chemical park which chemical factories have water pipes connected to certain treatment facilities. However, it is assumed that in scenario 0, no additional water pipes exist that enable water reuse at the park. Chapter 4 defines that each chemical factory initially has a water pipe connection to a source and a sink, and each treatment facility has a water pipe connection to a sink. The water network of a chemical park in scenario 0 is illustrated in Figure 8.1. This also means the outcomes for the metrics defining the industrial symbiotic performance of a water network in a chemical park are 0 in scenario 0, shown below. It could be possible that the efficiency of the water network in scenario 0 is actually higher than 0 because some connections exist between nodes, however, this differs per network and for ease of comparison, it is assumed the network efficiency is 0 in scenario 0.

- Extra costs of the water network: 0
- Amount of water that is being recycled: 0
- Efficiency of the water network: 0

All different scenarios that will be shown in the results have been defined in Chapter 6. However, scenario 0 will not be displayed in the results. As mentioned in the previous paragraph, the goal of this research is to find out if industrial symbiosis is still possible if stakeholder behaviour is taken into account. Therefore, it is important to make comparisons between the results of the initial network in which all stakeholders partake, compared to the networks in which certain stakeholders do not partake. In scenario 0, no stakeholders partake at all, meaning the results will always be 0, which will not have to be displayed in the graphs.

8.2. Methods used to analyze the results of the optimizations

The run for each experiment resulted in a dataset of on average 10000000 possible outcomes, for each scenario. As the number of nodes through which all possible routes are constructed, span from 4 to 8 nodes, and the length of the route is set to a maximum of 9, on average 6^9 routes can be identified. The output datasets contain 50 columns enlisting for each route the optimal water flow, the optimal costs, the maximum costs, the involved stakeholders, the removed stakeholders, the network efficiency, and the

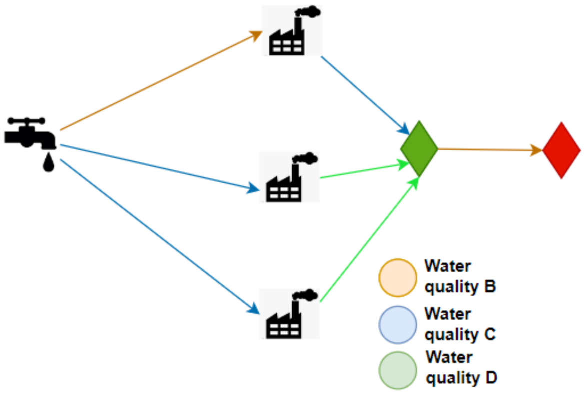


Figure 8.1: Visualization of the possible water network in scenario 0

sum of the demand, per scenario. Respectively to a large amount of data in the output files, processing the results is challenging. A structured approach is necessary to analyze the results. The results are analyzed in different steps. The general structure of the analysis and the goal per step is represented in Figure 8.2. The different steps will be elaborated in the following paragraphs.

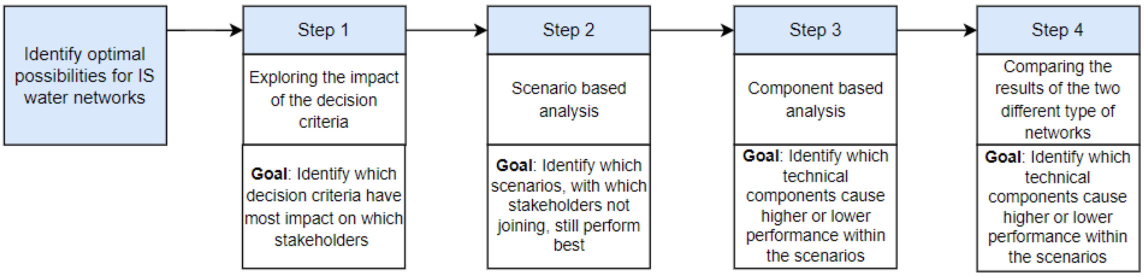


Figure 8.2: Structure in steps of the analysis and the goal

8.2.1. Step 1: Exploring the impact of the decision criteria

In this step, the individual impact of the decision criteria will be analyzed on the establishment of the different scenarios. The proposed model evaluates the robustness towards various stakeholder behaviours in deciding to join or not to join an IS water network. Several decision criteria influence the decision-making process of stakeholders, each assigned different weights in different scenarios as outlined in Chapter 6. The average number of stakeholders not joining the IS water network has been taken as a guideline from the three different tries with different values per criteria per stakeholders, as explained in Chapter 6. The impact of these different scenarios on stakeholder behaviour is presented in Table 8.1. In scenario 1, high weights are assigned to several decision criteria, yet a chemical company is still not willing to join the network. This may be explained by the fact that the other criteria not mentioned in scenario 1 are given a medium weight, meaning that the influence of compliance and revenue growth, which are given low weights in other scenarios, are still significant enough to discourage a chemical factory from joining the network.

In scenario 2, high weights are assigned to several other decision criteria, yet a treatment facility is still not willing to join the network. This may be explained by the fact that other criteria not mentioned in scenario 2 are given a medium weight, meaning that the influence of trust, awareness and internal policy, are still significant enough to discourage a treatment facility from joining the network.

Notably, when the weights assigned to compliance and revenue increase are low, the number of chemical companies unwilling to join the network is observed to increase in scenarios 3 and 6. Simi-

Scenario number	**Scenario name**	**Adjusted criteria**	**Exp 1: Removed stakeholders**	**Exp 2: Removed stakeholders**	**Exp 3: Removed stakeholders**	**Average Removed stakeholders**	**Average percentage decrease**
Scenario 1	Environmental-social enthusiast	Trust, Internal Policy, Awareness	1 Chemical company	1 Chemical company	0 Stakeholders	1 Chemical company	20%
Scenario 2	Welfare enthusiast	Compliance, Increase Revenue	2 Chemical companies	3 Chemical companies	2 Chemical companies	2 Chemical companies	40%
Scenario 3	Environmental devotee	Internal Policy, Revenue growth, Compliance	0 Stakeholders	1 Treatment facility	1 Treatment facility	1 Treatment facility y	33.3%
Scenario 4	Social scepsis	Trust, Awareness	2 Treatment facilities	2 Treatment facilities	2 Treatment facilities	2 Treatment facilities	66.6%
Scenario 5	Eco-social scepsis	Trust, Awareness, Internal Policy	0 Treatment facilities, 3 Chemical companies	2 Treatment facilities, 1 chemical company	2 Treatment facilities, 2 chemical companies	2 Treatment facilities, 2 chemical companies	66.6%, 40%
Scenario 6	Economic-social scepsis	Compliance, Increase revenue, Trust, Awareness	4 chemical companies	5 chemical companies	4 chemical companies	4 chemical companies	80%

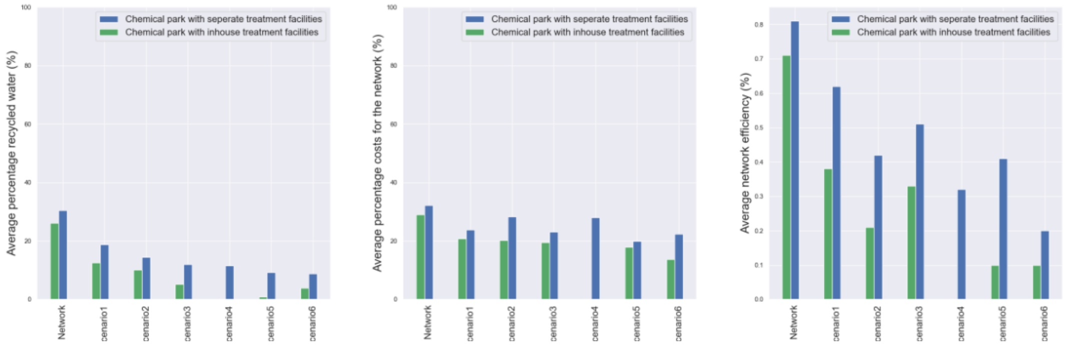
Table 8.1: Overview of the different social scenarios

larly, when the weight assigned to trust and awareness is low, it leads to an increase in the number of stakeholders unwilling to join the network as seen in the comparison between scenarios 4 and 5.

In scenario 6, most decision criteria are given a low value. This resulted in almost all stakeholders not joining the IS water network.

8.2.2. Step 2: Scenario-based analysis

After the establishment of the different scenarios has been analyzed, the average results for the performance of the different scenarios will be identified. Moreover, pareto fronts will be analyzed per scenario regarding different performance metrics and possible positive outliers will be identified. This analysis is done by examining pairwise plots for the performance metrics and the scenarios. Please note that the pairwise plots do not have matching x- and y-axes. The choice is made to use different axes because the most important conclusions from this section are the relationships between the different scenarios, not the absolute values for the performance metrics. Figure 8.3 shows the averages of each performance metric per scenario. A summary of the results per graph is enlisted in Table 8.2.



(a) Amount of recycled water

(b) Costs for the additional network compared to the maximum costs

(c) Robustness towards stakeholder behaviour

Figure 8.3: Average performance per scenario of each performance metric

Besides the graphs in which the total average performance per scenario is analyzed, have several boxplots been generated to perform a more detailed analysis of the performance of each different network structure per scenario. An example of the boxplot is shown in Figure 8.4. All other boxplots are attached in Appendix E1. When looking at figure 8.4, it shows in some specific networks consisting of a specific set of technical components, the percentage of recycled water is 10 to 20% higher than the average. The graphs of all the other scenarios are shown in a large extent in Appendix E. Moreover, the boxplots of the economic performance reveals that many networks have higher costs than the average represented in Figure 8.3. It stands out in this figure that the costs do not become less than 20% and have a higher upper range than a lower range. This can be explained by the fact that at the initiation of the model, it is assumed that costs for the treatment facilities are included, and these treatment facilities will always remain in the chemical park. However, they do not participate in the IS water network. Another notable aspect shown in the boxplot for costs attached in appendix E1 is that scenario 1 shows a clear division in the distribution for the percentage of costs. A set of 18 experiments have a lower percentage of cost distribution than the average percentage of costs of scenario 1.

Aspect	Network with separate treatment facilities	Network with inhouse treatment facilities
Environmental	1. Average maximum of 30% water recycled 2. Some specific networks perform 10 to 20% higher 3. A decrease towards 10 to 19% when stakeholders not partake	1. Average maximum of 25% water recycled 2. Some specific networks perform 5 to 20% higher 3. A decrease towards 0 to 15% when stakeholders not partake
Economic	1. Cheaper when chemical factories not partake compared to treatment facilities 2. Change in costs between 5% and 10% 3. Maximum change of 12% in costs compared to initial scenario	1. Cheaper when chemical factories not partake compared to treatment facilities 2. Change in costs between 1% and 5% 3. Maximum change of 12% in costs compared to initial scenario
Social	1. Average decrease in robustness when chemical factories not partake by 0.4 2. Average decrease in robustness when treatment facilities not partake by 0.6	1. Average decrease in robustness when chemical factories not partake by 0.4 2. Average decrease in robustness when treatment facilities not partake by 0.8

Table 8.2: Summary of conclusion Step 2

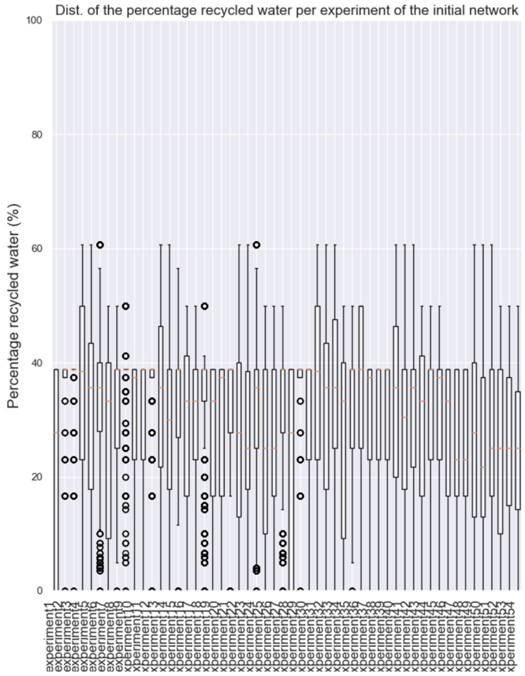
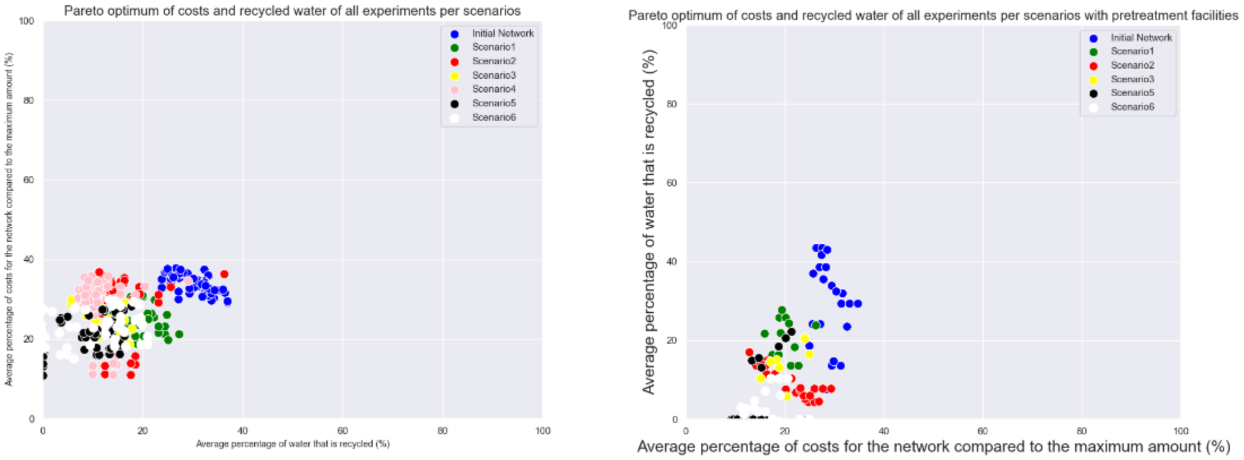


Figure 8.4: Distribution of the % recycled water per different network structure for the initial scenario

Average Pareto optimum analysis

The different performance metrics are combined into a Pareto optimum analysis. Pareto efficiency refers to a solution that is best for all measured criteria. This means that improving a solution based on one criteria would lead to a worsened result for the other criteria, and vice versa, leaving a balanced pareto best solution for both criteria. Often, Pareto-optimal solutions can be connected by a line or surface, forming what is called the Pareto-optimal front. In multi-objective optimization, the aim is to identify a set of solutions as close as possible to the Pareto front. The pareto front in this research consists of economic and environmental performance metrics. This can be substantiated by the fact that the IS water networks are also optimized according to these two objectives, explained in Chapter 5. In further analysis, different technical components are combined as well to analyze their performance for multiple performance metrics.

Figure 8.5 shows the pareto optimal distribution of the different network structures per scenario. It becomes clear that both the amount of recycled water and the costs for the network do not exceed 40% on average. It shows that most of the initial network structures have the highest percentage of recycled water, but are also expensive. However, some network structures containing less stakeholders have a high percentage of recycled water, which is worth identifying further in next paragraph.



(a) Pareto optimum visualization of the average outcome per experiment per scenario for chemical parks with separate treatment facilities

(b) Pareto optimum visualization of the average outcome per experiment per scenario for chemical parks with inhouse treatment facilities

Figure 8.5: Difference in all Pareto solutions of the average outcome per experiment per scenario between the different network types

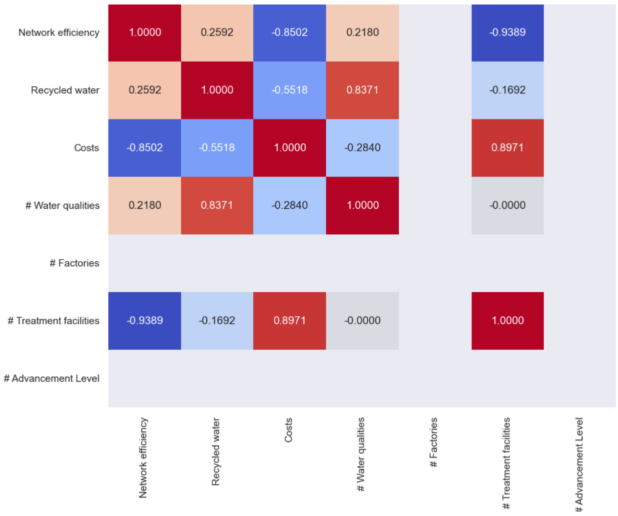
Conclusions from analyzing the performances according to the different scenarios

From this section, it is clear that the economic, environmental, and social performance of both types of network structures of each scenario in which different decision criteria are valued high is lower than the initial scenario's performance, on average. When comparing the two different network types, it becomes evident that, on average the network with in-house treatment facilities is cheaper, but less water is being recycled, even until no water is recycled, compared to the network with separate treatment facilities. Moreover, it is less robust to stakeholder behaviour overall. However, when analyzing the distributions of all individual network structures per scenario, it can be concluded that for some specific network structures of both types, the environmental and economic performance is higher than the average of a particular scenario. This requires a more detailed look at the combination of the components the networks consist of. An important note is that this only subjects to scenarios 1 and 2, as for the other scenarios, the individual distributions are much lower.

8.2.3. Step 3: Component-based analysis

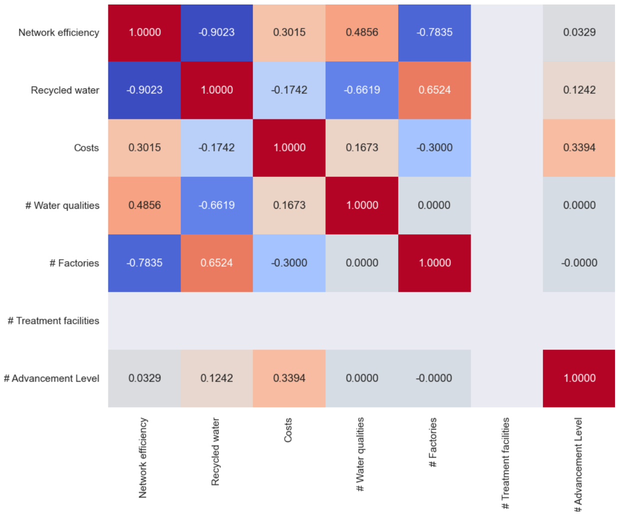
As concluded in the previous paragraph, do certain experiments, which determine the combination of components the network consists of, perform high for a certain performance metric. In this step, an analysis is performed on the performance of the individual network components related to the individual performance metrics, to identify possible components that determine or influence higher or lower performance on the performance metrics. This analysis is performed in a structured manner in order to prevent having to analyze each experiment individually. In the first exploratory analysis, correlation matrices are constructed. Correlation matrices measure the correlation between different variables, which in this research is used to measure the correlation between the IS performance metrics and the technical network components.

The correlation matrices for the initial scenario are shown in Figure 8.7. The correlation matrices of the other scenarios are attached in Appendix E. Notably, the figures representing the network structures with in-house treatment facilities miss a specific row for the number of treatment facilities. This can be explained by the fact that these networks always contain a single separate treatment facility, defined in Chapter 7.3.1.



	Network efficiency	Recycled water	Costs	# Water qualities	# Factories	# Treatment facilities	# Advancement Level
Network efficiency	1.0000	0.2592	-0.8502	0.2180		-0.9389	
Recycled water	0.2592	1.0000	-0.5518	0.8371		-0.1692	
Costs	-0.8502	-0.5518	1.0000	-0.2840		0.8971	
# Water qualities	0.2180	0.8371	-0.2840	1.0000		-0.0000	
# Factories							
# Treatment facilities	-0.9389	-0.1692	0.8971	-0.0000		1.0000	
# Advancement Level							

Figure 8.6: Correlation matrix of the initial scenario for the network with separate treatment facilities



	Network efficiency	Recycled water	Costs	# Water qualities	# Factories	# Treatment facilities	# Advancement Level
Network efficiency	1.0000	-0.9023	0.3015	0.4856	-0.7835		0.0329
Recycled water	-0.9023	1.0000	-0.1742	-0.6619	0.6524		0.1242
Costs	0.3015	-0.1742	1.0000	0.1673	-0.3000		0.3394
# Water qualities	0.4856	-0.6619	0.1673	1.0000	0.0000		0.0000
# Factories	-0.7835	0.6524	-0.3000	0.0000	1.0000		-0.0000
# Treatment facilities							
# Advancement Level	0.0329	0.1242	0.3394	0.0000	-0.0000		1.0000

Figure 8.7: Correlation matrix of the initial scenario for the network with inhouse treatment facilities

Technical component	Network with separate treatment facilities	Network with in-house treatment facilities
Water quality	1. With more water qualities, 3% more water recycled on average 2. When fewer chemical companies join, chemical parks with three water qualities 1% to 5% more water can still be recycled 3. Networks with most (4) water qualities have lowest costs	1. With fewer water qualities, 8% more water recycled on average 2. When fewer chemical companies join, chemical parks with three water qualities 1% to 5% more water can still be recycled 3. Networks with most (4) water qualities have lowest costs
Advancement level treatment technology	1. Per level 2% higher costs 2. When fewer chemical factories do not join, the higher the advancement level, 1% up to 8% more water can be recycled 3. Advancement does not make any impact when treatment facilities itself do not join the IS water network	1. Per level 1% higher costs 2. When fewer chemical factories do not join, the higher the advancement level, 1% up to 3% more water can be recycled 3. Advancement does not make any impact when treatment facilities itself do not join the IS water network

Table 8.3: Summary of results single components step 3

It can be seen in these figures that a big difference exists in the correlations between the same variables of the two types of network structures. The only similar result in correlation for all different scenarios is between the number of factories and the percentage of recycled water. Moreover, a slight similarity exists in the advancement of the treatment facility and the costs. Both are positive correlations, meaning the more advancement levels the network contains, the more the network will cost.

In the networks with in-house treatment facilities does the network become more efficient, meaning more stakeholders have a social relationship with each other if more water qualities are considered. The number of factories involved positively impacts the amount of water recycled and does the advancement of the treatment facility positively influence the costs (become more expensive).

Within the network with separate treatment facilities do the number of water qualities positively influence the amount of water recycled and do the number of treatment facilities and the advancement levels positively influence the costs (become more expensive). Moreover, it can be seen that the number of treatment facilities greatly impacts the amount of water recycled.

Analysis of single technical components

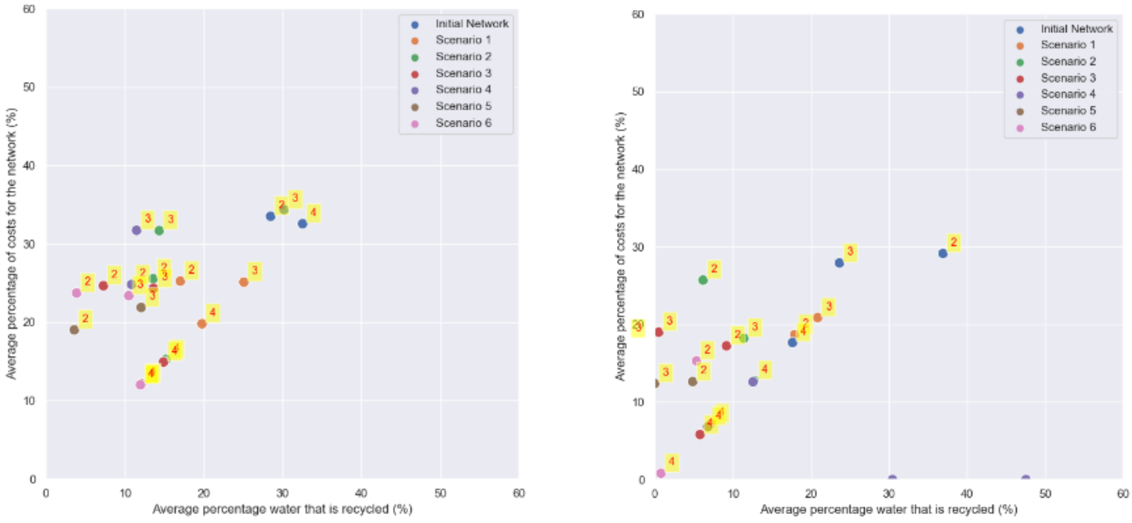
According to the correlation matrices, relations are found between single technical components and single performance metrics. This already gave some results and implications. However, it is also interesting to research how the single technical components, water quality and advancement level of the treatmetn technologies, perform regarding multiple performance criteria, analysed in the pareto plot in figure 8.8 and attached in appendix E. The most important results are summarized in Table 8.4.

Table 8.4 shows that for the specific component type, the water quality, positively or negatively influences the performance of the IS water networks. While the other component type, advancement level, has a lower impact, especially in chemical parks with in-house treatment facilities. However, when less chemical factories join, a higher level of advancement could increase the amount of water recycled highly.

Analysis of couples of technical components

A more extended analysis is performed of couples of components, identifying if even higher performances are possible, with regards to the single technical component analysis of the previous paragraph. All graphs resulting from this analysis are attached in appendix E, see E.16 and E.17. The sets of components are combined according to the high-performing components in the correlation matrices. The plots show only the initial scenario and scenarios 1, 2, and 3. This choice is made as otherwise, the graphs would become unreadable, and, scenarios 1, 2, and 3, all are formed according to different sets of decision criteria valued higher or lower, resulting in a different set of stakeholders not joining. All results stemming from these graphs are summarized in Table 8.4.

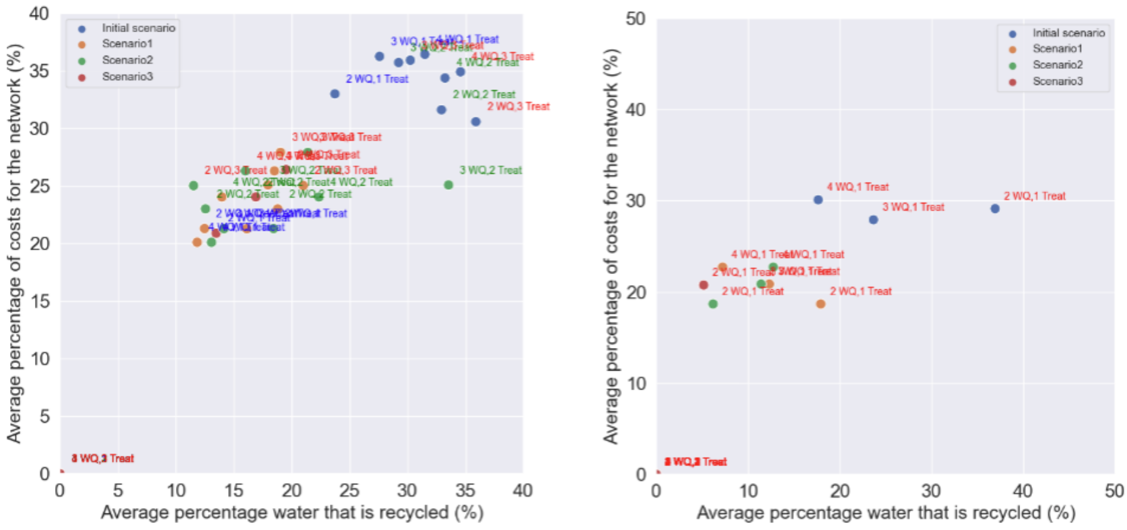
In figure 8.9 the graph is shown for one of the analyses performed for a couple of technical components, namely the number of water qualities and treatment facilities. The plot for the in-house treatment



(a) Pareto optimum for the chemical park with separate treatment facilities (b) Pareto optimum for the chemical park with inhouse treatment facilities

Figure 8.8: Difference in the pareto optimum for the different network structures according to the number of water qualities, between the different types of networks

facility contains less data as in this chemical park only a maximum of one treatment facility exists. The figure shows that in every scenario, the networks containing more treatment facilities perform higher on the amount of water recycled. However, these networks are also more expensive.



(a) Pareto optimum for the chemical park with separate treatment facilities (b) Pareto optimum for the chemical park with inhouse treatment facilities

Figure 8.9: Difference in the pareto optimum for the different network structures according to networks with specific components of treatment facilities and water qualities, between the different scenarios (*Red text applies to 5 factories, green text to 4 factories, blue text to 3 factories)*

Technical component	Network with separate treatment facilities	Network with in-house treatment facilities
Water quality and number of factories	1. Range of recycled water between 7% and 34% 2. Cost range between 23% and 35% 3. Highest performance, 34% recycled water, with most wq and most factories 4. When fewer treatment facilities join, costs increase with 5% with more factories	1. Range of recycled water between 0% and 43% 2. Cost range between 18% and 33% 3. Highest performance, 43% recycled water, with least wq and most factories 4. When fewer treatment facilities join, costs increase with 3% with more factories
Water quality and treatment facility	1. With fewer wq 4% lower costs 2. The more treatment facilities, 5& higher costs 3. Combination 2 treatment and 3 wq perform best with recycling 18% more than average 4. When fewer stakeholders join, performance is still highest with most treatment facilities and average number of wq	Only a single treatment facility involved
Treatment facility and advancement level	1.Per advancement level, 2% higher costs 2. When fewer stakeholders join, 5% more water is being recycled with the highest advancement level	1.Per advancement level, 3% higher costs 2. When fewer stakeholders join, 10% more water is being recycled with highest advancement level

Table 8.4: Summary of results couples of components step 3

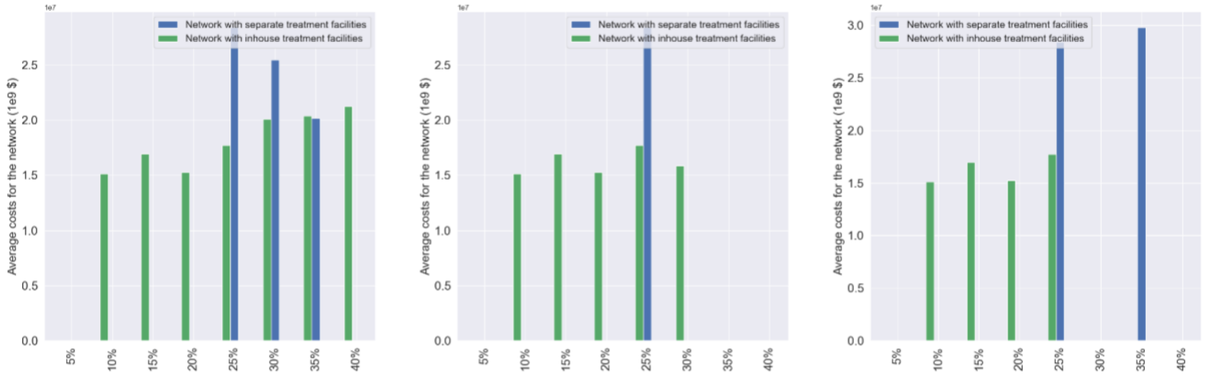
Conclusions from analyzing certain combinations of network components

From this paragraph, a few important conclusions can be drawn. First of all, the amount of recycled water differs to a greater extent in chemical parks with in-house treatment facilities, between 0% and 45%, compared to the chemical park with separate treatment facilities, 12 % and 35%. Secondly, the impact of the different technical components on the costs for the network is not very high. The range between the costs range is small for both network types. This can be explained by the fact that several treatment facilities already exist within the chemical park, which are included in the annual costs of the chemical park.

Lastly, the two different network types perform very differently according to the technical components. Respectively to the network with separate treatment facilities is a higher number of water qualities beneficial for the economic and environmental performance. More treatment facilities enable more water to be recycled, but also more costs. For the advancement level and for the number of factories the same. In scenarios when fewer chemical factories want to join, the networks still perform best that contain fewer water qualities, and a higher advancement level. In scenarios with less treatment facilities, the only option for still recycling water is to include the minimum number of water qualities. In network types with inhouse treatment facilities, do the networks perform best with the most possible number of factories and the least amount of water qualities. In scenarios with fewer chemical factories, the networks with the least amount of water qualities perform best. In scenarios with the treatment facility not joining, the only option for recycling water is if the minimum number of water qualities are included. The level of advancement does not have an impact.

8.2.4. Step 4: Comparison of the performance of the two different types of networks

In previous analyses, the performances of the different network types, scenarios and specific single or couples of components are analyzed according to percentages. This paragraph shows the performance of all optimal routes within the specific network structures compared to the highest possible performance regarding recycled water or the highest costs for the network. However, to make a sophisticated comparison between the network types, actual numbers should be given to the costs or the amount of water recycled. It could be possible a certain network type is much cheaper, which cannot be seen in the percentages. Figure 8.10 shows the actual average costs per percentage of recycled water for the different network types in the initial scenario. It can be seen that the more water is being recycled, the cheaper the networks with separate treatment facilities become. Moreover, when 25% of the water is being recycled, the network type with separate treatment facilities is a billion euros more expensive than within the network with in-house treatment facilities. In contrast, when 35% of the water is being recycled, both networks are as expensive. In scenarios 1 and 2, the networks with separate treatment facilities are more expensive and have less variety in the percentage of water that is being recycled. In scenario 1, the networks with separate treatment facilities are 1 billion euros more expensive; in scenario 2 this is 1.5 billion euros.



(a) Initial scenario (b) Scenario1 (c) Scenario2

Figure 8.10: Difference in the costs for the two types of networks per percentage of recycled water for the initial scenario, scenario 1 and 2

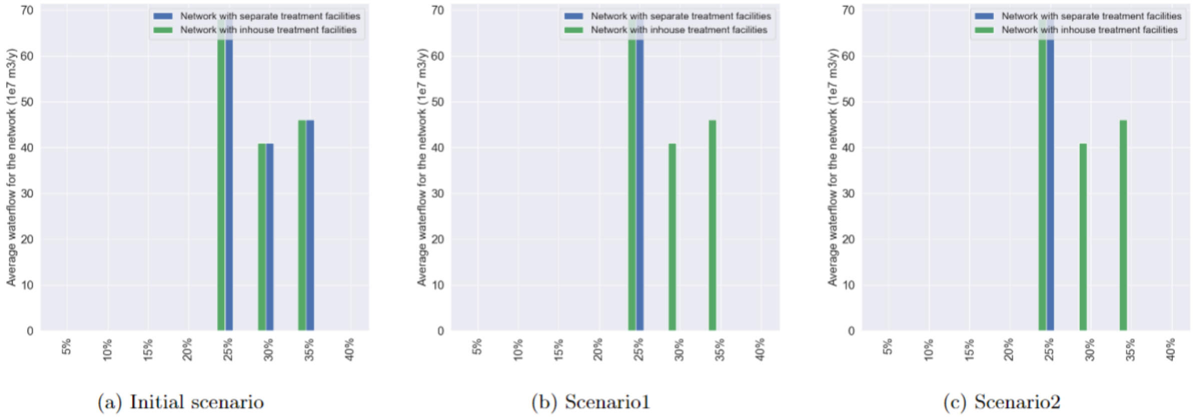
Figure 8.11 shows the average amount of water that is recycled per percentage of costs that are paid compared to the maximum costs that would be paid for the different network types in the initial scenario. Notably, a low number of bars consist in the plots. This can be explained by the fact that the percentages of costs for each network do not differ that much. It can be seen that not a big difference exists in the average amount of water that is being recycled between the two network types.

Conclusion from the analysis between the two network types

It can be concluded from the previous two analyses that the more water is recycled, the lower the relative costs within the initial scenario are. But, overall, the networks with separate treatment facilities are more expensive when looking at the actual costs in euros. When the costs are measured in percentages of the maximum costs that could be paid, it becomes clear that the same amount of water is being recycled in millions of liters per year for both network types.

8.3. Testing of the impact of the different incentives

Chapter 7 introduces a few possible incentives that could stimulate more circularity within industrial parks. The results for these incentives are explained in the following paragraph.



(a) Initial scenario (b) Scenario1 (c) Scenario2

Figure 8.11: Difference in the amount of recycled water for the two types of networks per percentage of costs for the initial scenario, scenario 1 and 2

Freshwater tax

The aim of the freshwater tax was to make the costs for using a litre of freshwater more expensive. This incentive is focused on the economic benefit for stakeholders to recycle more water. When looking at Figure 8.12, the focus is not on the difference per tax addition in the scenario but instead on examining whether the cost difference between the various scenarios and the initial scenario becomes smaller. If the costs are approximately the same in the initial network as in the network of a particular scenario, it would become more advantageous for stakeholders to participate in IS water networks. However, the difference is not significant for the water taxes of 10% and 20%.

However, the beneficial impact can be seen when looking at the yellow bar, representing a water tax increase of 1000%, which is an enormous increase. The networks in which fewer stakeholders take part, are more expensive. This means it would be economically stimulating for stakeholders to recycle water, and reduce costs for freshwater usage. However, it only becomes considerably more attractive to recycle water for an unreal increase of costs for freshwater.

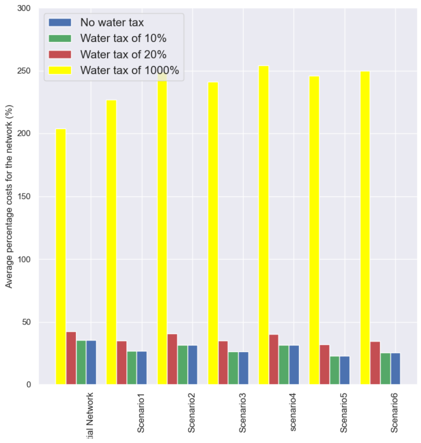


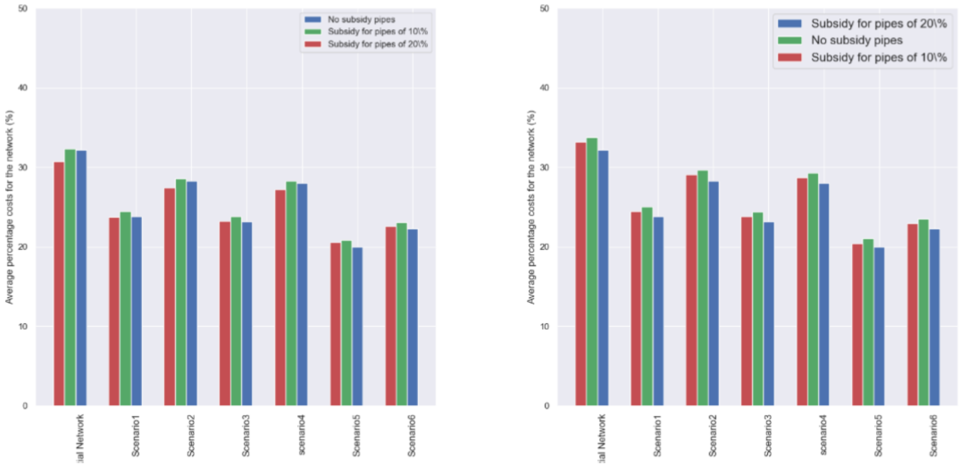
Figure 8.12: Difference in the costs for the networks regarding different heights in tax for freshwater

Subsidy for the construction of the water pipes

The subsidy for the construction of the water pipes does have an impact on the costs for the IS water network. The higher the subsidy becomes, the lower the costs for the network become. What can be seen is that the reduction in costs is higher in the initial scenario, comparing the bar with no subsidy to the bar with 20% subsidy. This difference in costs becomes less, with fewer stakeholders taking part. This is supported by the fact that more water pipes have to be constructed when more stakeholders join the IS water network. This subsidy will probably not change the behaviour of the stakeholders, as the difference in cost reduction is not very high.

Subsidy for treatment technologies

In Figure 8.13, is the effect of the subsidy for the advancement technologies of the treatment facilities shown. It can be seen that the difference in costs between the three bars stays the same in every scenario. So, the costs for the IS water network do not become less if more stakeholders join. This can be substantiated by the fact that the costs for the treatment technology need to be paid for, although certain stakeholders do not partake in the IS water network. They do need to treat their wastewater, meaning they will always have to pay for the treatment technology. It does not change the economic incentive for stakeholders for joining the IS water network.



(a) Subsidy for the construction op the water pipes

(b) Subsidy for the treatment technolgies

Figure 8.13: Difference in the costs for the networks regarding two different heights of subsidies

9

Validation and testing

In the preceding chapter, the model's results were presented. This chapter will validate the model's outcomes with real-world experiences and compare them to previous research. Additionally, section 9.4 will analyze the sensitivity of the results to a change in input values.

9.1. Validation of the results for chemical parks

In section 7.5, the model was verified if it represents the real-life conceptual model correctly. In this paragraph, several results of the model will be validated by comparing the results to other research and according to a validation interview performed with the program manager for water at Chemelot. A verbal validation has been performed as no real-life data is available from a certain chemical park, as explained in Chapter 7. Several statements resulting as conclusions from the research, displayed in Table 9.1, have been validated according to the interviewee's answers and according to the literature. A ✓means it is confirmed in literature or by the verbal interview, a X sign means it is not validated and the '-' sign means nothing is stated about this in literature or the interviewee did not know the answer.

Result	**Validated in interview**	**Validated by source**
The costs for recycling the same amount of water are higher in chemical parks with separate treatment facilities	✓	(Lyu et al., 2020), (Navarro Martínez et al., 2020)
In chemical parks with inhouse treatment facilities, the possibility to recycle water is lower compared to chemical parks with external treatment facilities	✓	(Hu et al., 2019)
Chemical parks with inhouse treatment facilities is more sensitive to the decisions of the chemical factories regarding the possibilities for recycling water, compared to the chemical park with separate treatment facilities	-	-
In water networks with inhouse treatment facilities and large number of different water qualities, the possibilities to recycle water are limited	-	-
In water networks with separate treatment facilities, the possibility to recycle more water increases by including more water qualities	✓	(UNIDO, 2019),(Lyu et al., 2020)
In water networks with separate treatment facilities, the additional costs for the IS water network are mainly influenced by the treatment facilities	×	(Rodiguez-Miranda, 2015)
In water networks with separate treatment facilities, when fewer chemical factories want to join, the possibilities to recycle water increase with higher levels of advancement within the treatment facilities	✓	(Kaviya, 2022)

Table 9.1: Summary of validation of the model results by an interview and literature

The results that have been identified in this research have been validated during the interview and according to the sources. A short illustration per result will be given on how the literature validates this, the summary of the validation interview has been attached in Appendix A2.

First of all, Lyu et al. (2020) validates that the costs for recycling water in chemical parks with separate treatment facilities is higher. It states the separate treatment facilities impose a very high economic burden on the chemical park. In particular, it states that within chemical parks, for each chemical factory at least 30% of the costs are for the treatment of the water. Moreover, Navarro Martínez et al. (2020) explained in his research that parks with separate treatment facilities have more possibilities to recycle water. The interviewee confirmed Chemelot bore all the investment costs of the central treatment facility 'IAZI 1.0' and is hesitating about building IAZI 2.0 because of the extremely high costs.

Secondly, Hu et al. (2019) states the optimal solution for the treatment of wastewater within chemical parks is probably situated between the two extremes. Partly consisting of inhouse treatment facilities and partly of separate treatment facilities. However, the study concludes that chemical parks with only inhouse treatment facilities have less possibilities to recycle water; approximately a maximum of 25% of the water can be recycled. This is also almost the same outcome as the average outcome for the environmental performance of this research for the chemical park with inhouse treatment facilities. The interviewee highlighted that the likelihood of recycling discharged water is higher with the treatment facility at Chemelot, as it is separate from the chemical factories and capable of processing various water qualities after extensive research had been conducted to the network structure. However, trust in the Chemelot governance and the other connected chemical factories is deemed crucial.

Thirdly, (UNIDO, 2019) has written a report on international guidelines for industrial parks, mainly related to improving sustainability. Several feasibility studies have been performed to be able to give these guidelines. One of these studies researched the possibility of recycling water in chemical parks, stating the chances increase when more qualities of water are involved that could be treated by a treatment facility. The interviewee believed that the total amount of recycled water in Chemelot could be higher than the outcome predicted by the model. This is because many chemical companies can handle multiple water qualities, and there is already a high level of trust within the chemical park due to the presence of a single large central treatment facility.

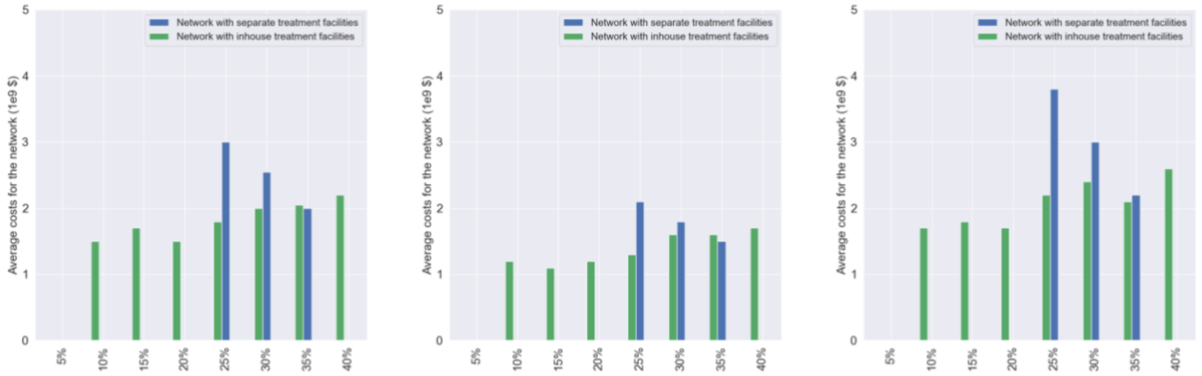
Lastly, Kaviya (2022) states that higher advancements of treatment facilities cause higher costs for the entire network, but, could also increase 13% more water to be recycled. The interviewee confirmed that currently complex chemicals cannot be completely removed from the water, which is vital for building trust among the chemical factories and enabling water recycling from IAZI. This has been identified as one of the most important aspects of their circularity plan for 2050.

9.2. Sensitivity Analysis

The outcomes of any model are dependent on the input parameters, including economic parameters. However, there is no widely accepted single value for these parameters, and different reports offer varying values for the costs of treatment and construction. Additionally, the MCDA method is subjective and prone to sensitivity. This section aims to perform a sensitivity analysis to assess the impact of changes in parameters on the average results. First, the sensitivity of the outcomes to input parameters is investigated. Section 9.3.2 examines the effect of stakeholders not joining the water network, and section 9.3.3 assesses the effect of changes in the threshold used for the MCDA. The sensitivity analysis in this section will focus on the initial scenario, where all stakeholders participate in the network. The results for this scenario represent the effect on the overall IS network.

9.2.1. Analyzing the sensitivity to the input parameters

Within the model, the water routes are optimized according to the costs of the network and the amount of water the network could recycle. However, the costs are based according to pre-set input parameters for the costs of different components within the model, explained in Chapter 7. The values have been substantiated by literature, however, no single value is widely accepted to be true, different reports give different values for costs of treatment and construction and for some costs, the average has been taken according to the literature. Moreover, the prices for freshwater differ per country. This is why a sensitivity analysis is performed to see if the model is sensitive to changes in the costs. The different input parameters are costs for the treatment facility, costs for the construction of water pipes, costs for freshwater and costs for the wastewater treatment technology. The costs will be varied by -20% and +20%. The results are visualized in Figure 9.1 by comparing changes in actual costs for the same percentage of recycled water between the two network structures. In the results was found that the network structure with in-house treatment facilities, it is cheaper to recycle water, but maybe this will differ with other values for input parameters.



(a) REF scenario (b) Sensitivity to 20% lower costs (c) Sensitivity to 20% higher costs

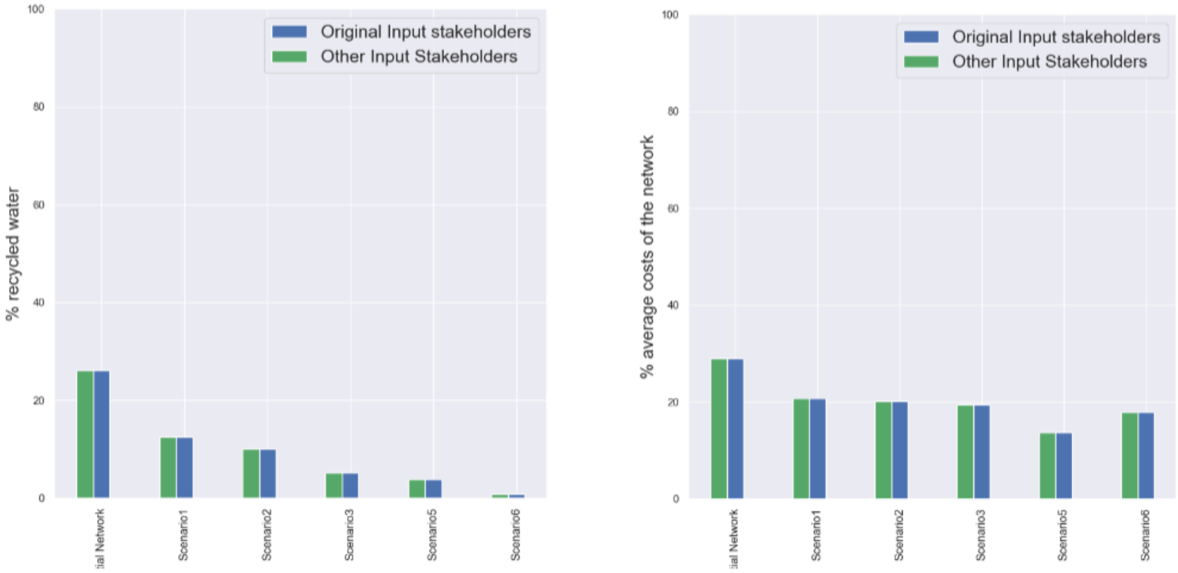
Figure 9.1: Sensitivity of an increase or decrease of all cost input parameters between the two different network structures

Figure 9.1 shows the model is sensitive to a 20% change in the costs. The network with separate treatment facilities becomes more expensive with an increase in the costs compared to the chemical park with in-house treatment facilities. However, an interesting change is that when the costs are 20% lower, the chemical park with separate treatment facilities becomes cheaper compared to the chemical park with in-house treatment facilities. With recycling 30% of the water, the costs only differ between 1.6 and 1.7 billion euros, changing the conclusion that in chemical parks with in-house treatment facilities, it is cheaper to recycle the same amount of water.

9.2.2. Analyzing the sensitivity to the involved input stakeholders

Another critical input the model is based on is the involved stakeholders with all their attributes. According to the involved stakeholders, the initial network topology is based. The involved stakeholders contain the attributes for the location of the nodes, the water quality, the demand and supply, and the amount of water they supply. The attributes per stakeholder never change, as explained in Chapter 4. In step 1 of the results in Chapter 8, which stakeholders will not join the network if different decision criteria are given a weight, has been analysed. However, as already explained in Chapter 8, the average of the stakeholders not joining has been taken, meaning and for the three different tries that have been performed sometimes other stakeholders would not have joined. This is why a sensitivity analysis has to be performed, to see if it would impact the result, if other stakeholders would have been selected per scenario not to join the network. The averages for the three different performance metrics for every scenario will be compared to the averages if other stakeholders, but of the same amount, would not have joined. However, this analysis is only performed for the networks with inhouse treatment facilities, because of a lack of time.

As can be seen in both the plots of Figure 9.2, is the model not sensitive for different stakeholders partaking in the initial network. Both the economic and environmental average results stay the same. This is an important finding because it shows that the model works the same on average per scenario when the same number of stakeholders do not join the network.



(a) Sensitivity for the environmental performance

(b) Sensitivity for the economic performance

Figure 9.2: Sensitivity of the final average result for the two different performances to different input stakeholders

9.2.3. Analyzing the sensitivity to the threshold applied in the MCDM

Data in multi-criteria decision-making (MCDM) problems are often imprecise and changeable. Therefore, an essential step in many applications of MCDM is to perform a sensitivity analysis on the input data. Many studies perform this by performing a sensitivity analysis on the weights (Triantaphyllou & Sánchez, 1997). However, as discussed in Chapter 6, subjectivity has already been tried to address by incorporating ranges for the weights. This is why no sensitivity analysis needs to be performed for the weights. Another influential aspect of the MCDA method within this research is the threshold. The threshold, which is a depicted number, is defined if stakeholders join or not join the IS water network. The threshold has been defined according to the sumvalue of the initial scenario. However, the threshold could be influenced by a culture of a country for example. If a country's culture is very individualistic, the threshold would become higher for companies to join the IS water network. This is why the impact of a 20% lower and a 20% higher threshold will be analysed towards the results for the number of stakeholders not joining the network.

Table 9.2 shows the sensitivity of the MCDA towards a 20% lower threshold. It shows the MCDA method is very sensitive to a different threshold. More stakeholders will decide to join the network, as the threshold is lower.

Scenario number	**Initial Removed stakeholders**	**New Removed stakeholders**
Scenario 1	1 Chemical company	0 stakeholders
Scenario 2	1 Treatment facility	0 stakeholders
Scenario 3	2 Chemical companies	0 stakeholders
Scenario 4	2 Treatment facilities	0 stakeholders
Scenario 5	2 Treatment facilities, 2 chemical companies	1 Treatment facility, 2 chemical companies
Scenario 6	4 chemical companies	2 chemical companies

Table 9.2: Sensitivity to a 20% lower threshold

Table 9.3 shows the sensitivity of the MCDA towards a 20% higher threshold. It shows the MCDA method is inevitably sensitive to a different threshold as well. Less stakeholders will decide to join the network, as the threshold is higher, which will result in almost no stakeholders joining the network. This will result in a very low performance for the industrial symbiotic performance metrics, as can be compared to scenario 5 and 6 in the results section.

Scenario number	**initial Removed stakeholders**	**New Removed stakeholders**
Scenario 1	1 Chemical company	3 Chemical companies
Scenario 2	1 Treatment facility	1 Treatment facility and 1 Chemical company
Scenario 3	2 Chemical companies	4 Chemical companies
Scenario 4	2 Treatment facilities	2 Treatment facilities and 2 Chemical companies
Scenario 5	2 Treatment facilities, 2 chemical companies	2 Treatment facilities, 4 chemical companies
Scenario 6	4 chemical companies	5 chemical companies

Table 9.3: Sensitivity to a 20% higher treshold

10

Discussion

Chapter 8 presented the results of this research, and the results were validated in Chapter 9. This chapter will discuss the implications of the results relevant to chemical park owners and policymakers. Section 10.3 will elaborate more on the limitations of this research.

First of all, the purpose of this research will be reiterated. This study aims to investigate whether it is possible to create more IS water connections in chemical parks in bottom-up regulated countries while considering certain stakeholders who may be unwilling to participate. Currently, there are few IS water networks in chemical parks that have not been established by government intervention. This research studies if such IS water networks can be created by stakeholders' initiatives within the chemical park themselves and will examine whether these networks are beneficial regarding the different performance metrics for industrial symbiosis. Therefore, this research is exploratory in nature.

This study extends the field of optimal water network designs in two main ways: firstly, by incorporating the influence of different stakeholder behaviour within the optimal design networks. This enabled a deeper understanding of which decision criteria, mainly compliance, revenue growth and trust, cause networks to perform better and are more likely to succeed in creating IS water connections. This design may be better suited for real-world implementation. Secondly, by performing optimization of two different structures of chemical parks, containing separate or in-house treatment facilities, the optimal results for the different structures can be compared. This leads to more insights into the possible designs for the chemical parks' water infrastructure and its potential for creating IS connections. The model created is generic for any chemical park. However, what should be noted is that a model has been developed specifically for this study, partly based on the literature and partly on original ideas. This means this exploratory study could have been conducted differently according to other ideas.

The results show that creating IS connections is possible, with significant performance, but it is very sensitive to stakeholder behaviour. The options become limited for recycling water already relatively fast if some stakeholders do not want to join the IS water network. This study has several interesting implications for chemical park owners and policymakers, which will be elaborated on in the following paragraph. A distinction has been made between chemical park owners and policymakers as part of the results give insight for chemical park owners. The other part of the results, specifically regarding the incentives, give insight to policymakers.

10.1. Discussions of the results and implications to chemical park owners

The ownership structure of chemical parks varies across Europe. Some parks are publicly owned, while other parks are privately owned (UNIDO, 2019). In this research, Chemelot has been taken as an example for the creation of the model. Therefore, the ownership structure of the Chemelot chemical park will also be used as an example in this research. It is managed by a separate company that aims to reduce water intake and achieve sustainability goals, including becoming fully circular by 2050 (Brightside, 2021). Therefore, implications for creating more IS water connections leading to more water recycling, are relevant for chemical park owners.

Overall, the model suggests that the more stakeholders that participate, the more opportunities and higher performance there will be for IS in chemical parks, which is also confirmed by the literature. Therefore, it is important for park owners to develop strategies to engage more stakeholders and to adjust to the stakeholders.

The strategies will be suggested to the chemical park owners. However, an important distinction has been made during the entire research, between chemical parks with in-house treatment facilities and chemical parks with separate treatment facilities. This was based on the big question globally of whether to centralize wastewater treatment facilities or build localized treatment facilities catering to smaller plants (UNIDO, 2019). This question will not be answered yet. However, it becomes evident in this research that a significant difference exists between these two treatment model structures regarding the IS water possibilities. This is why different strategies will be suggested to the chemical park owners for both types of network structures.

10.1.1. Strategies for Addressing Stakeholder Behaviour in Chemical Parks

Addressing stakeholder behaviour in the way they would join the IS water network is an important task for chemical park owners (Hewes & Lyons, 2008). In both types of chemical parks, the performance of IS water networks is much higher if more stakeholders join. In chemical parks with separate treatment facilities, the amount of water that is recycled could increase from 10% up to 30%, the total costs for the additional IS connections decrease relatively by 10%, and the robustness to stakeholder behaviour could increase from 40% up to 80%. In chemical parks with in-house treatment facilities, the amount of recycled water could increase from 0% up to 25% and the robustness to stakeholder behaviour could increase from 20% up to 80%. Especially in chemical parks with in-house treatment facilities, the environmental performance is sensitive to chemical factories' behaviour.

Chemical companies take compliance to regulations extremely seriously. If regulations become stricter, they will immediately adjust to these regulations because they want to prevent high fines for non-compliance at all costs. Moreover, it is bad for their own publicity if they do not comply to regulations. The most important asset for the chemical companies located on the chemical park, is their license to operate. If they lose their license to operate, they need to close their chemical factory, having crucial consequences for the chemical factory owners. The chemical park owners own this license to operate. Currently, no policies exist regarding the amount of water that needs to be recycled or the amount of wastewater discharge attached to this license to operate (Bahadorestani et al., 2020). If strict policies are set by the chemical park owners regarding these water usage parameters, it could increase the number of chemical factories joining the IS water network from 20% up to 80% as they do not want to lose their license to operate.

Creating trust between the different stakeholders in a chemical park is also an important strategy. It could increase the involvement of stakeholders by 33%. Especially in chemical parks with in-house treatment facilities, the trust is low. By creating trust, the amount of recycled water in this type of chemical park could be increased from 0% up to 15%. To include as many stakeholders as possible, creating trust between these stakeholders is necessary. According to Hewes and Lyons (2008), trust can be created in industrial parks by open and honest communication, clear coordination of tasks and maintaining surveillance of all included counterparts. An effective method in which these three tasks can be performed is to organize a monthly park stakeholder meeting.

However awareness of IS possibilities does not have the greatest influence on stakeholder behaviour, this criteria can be most easily addressed by chemical park owners. During this research, it became clear that the awareness of IS possibilities is not high, especially in the chemical industry, because of all the different water qualities present. Even the company responsible for the circularity of water at Chemelot had no insight into the possibilities yet. While in both types of chemical parks, when all stakeholders would join, it became clear that, on average 35% and 25% of the water can be recycled. Knowing this fact, chemical park owners should focus on creating more awareness that recycling water of different qualities is possible within chemical parks. Awareness can be created in multiple ways, however, within chemical parks the chemical park owners should address each chemical factory personally, explaining the possibilities and the factual advantages (Boix et al., 2015). Moreover, according to Cui et al. (2018), awareness could be raised gradually when single IS connections are created in chemical parks.

10.1.2. Strategies for Adjusting to Stakeholder Behaviour in Chemical Parks

Many IS water network initiatives eventually fail to be implemented in different bottom-up regulated countries because of multiple stakeholders not wanting to join this initiative (Ashton & Bain, 2012). In the previous paragraph, different strategies have been discussed to involve more stakeholders. However, when this is not possible anymore or is not worth the effort, other strategies can be implemented to adjust the IS water network initiative to certain stakeholders not partaking. Chemical park owners can make certain choices to create more possibilities for IS water connections or to generate as many connections as possible regarding the technical components the water network consists of or should consist of.

The costs of the treatment facilities are very influential for the costs of the possible overall IS water network. If it is assumed that the treatment facilities are already in the parks, then the additional costs are not as significant, namely only for the construction of the water pipelines. However, suppose these treatment facilities are not yet present, and the advancement level is low in a park where the chemical factories require high-quality water. In that case, the costs are incredibly high, spanning from 1.5 up to 3 billion euros. Generally, the additional costs for an IS water connection in chemical parks with in-house treatment facilities are lower.

In situations where only a few stakeholders would want to participate in the IS water network due to a lack of trust and awareness, the level of advancement of the treatment facilities is important. If this treatment facility or facilities contain high advanced treatment technology, advanced oxidation processes like anaerobic-oxic anoxic technology, in order to further remove pollutants including non-biodegradable organics, nutrients, and heavy metal, a significant number of IS connections can still be created with 1% up to 8% higher environmental performance. However, the economic performance of the IS connections depends on how advanced the current treatment technologies are. The same applies to the number of treatment facilities participating; the more, the better the percentage of water that can be recycled in chemical parks. Nonetheless, the economic performance will decline with a maximum of 12% if multiple treatment facilities need to be constructed.

Chemical park owners should prioritize creating IS water connections for a limited number of water qualities in parks with more in-house treatment facilities. In cases where stakeholders prioritize revenue growth and there are no penalties for recycling less water, park owners should target chemical factories that can utilize water of a quality that can already be upgraded by the treatment facility. Often these are the chemical factories with lower quality standards, like a pH level between 6.0 and 9.0, a total suspended solids level of 50 mg/L and a COD level of 250 mg/L. This approach may enable more IS water connections and respectively a 1% up to 5% increase in the amount of recycled water in these chemical parks. However, this solution is dependent on the chemical factories, treatment facilities and water qualities present in the chemical park. If only water of high quality is demanded, the opportunity of this solution becomes less attractive, because of higher costs and fewer IS connection possibilities.

Lastly, it is likely that the most effective solution both in terms of public expenditure, equipment reliability, and environmental impact will be found somewhere between the two extremes of separate treatment facilities and in-house treatment facilities (Sousa et al., 2002). Results showed that the technical components of an IS water network have a different impact on the industrial symbiotic performance of the two different types of network structures. Moreover, in chemical parks with separate treatment facilities, the costs for recycling water are higher than in chemical parks with in-house treatment facilities, while the possibilities of recycling water are also higher in the first chemical park structure. Therefore, it would be interesting to research if the advantages of both structures can be combined into a shared structure.

10.2. Discussions of the results and implications to policy makers

The research is focused on stakeholder participation in bottom-up regulated countries. Implementing actual laws for creating more IS water connections, as happened in China, is not a viable solution. However, creating certain incentives could be a more viable solution for policymakers. All considered incentives are economically focused. Based on the literature, accounts from experienced professionals in the chemical industry, and research findings, it is evident that participating in IS water networks will always be a cost-benefit consideration for companies. According to Song et al. (2018), without effective and efficient economic incentives, most firms would not like to engage in industrial symbiosis. However, after considering all three economic incentives, it becomes evident, that all have no significant impact in adjusting stakeholder behaviour. As Doménech and Davies (2009) researched, it is a contestable issue for policy mechanisms to enable more cooperation between actors anchoring in IS projects.

One of the most interesting incentives for policymakers is the implementation of a water tax, adding a 1000% of tax to the initial price for water per m^3. This is within their jurisdiction and has already had a significant impact on the world with respect to nitrogen taxes. Currently, water is very cheap. Song et al. (2018) states that if the prices of virgin materials are too low and cannot reflect their true values, firms will not care for resource efficiency. While the water tax incentive will not directly reduce the cost of creating IS water connections, it will affect stakeholder behaviour. An important criterion for stakeholders is revenue growth, which is precisely what the water tax targets. They will have to make a more significant consideration for choosing not to recycle water, as it will incur significant costs. Unfortunately, freshwater is so inexpensive that the tax would have to become extremely expensive before stakeholders alter their decision-making. Therefore, Singh and Kazmi (2018) introduced another incentive focused on limiting the freshwater intake, namely an actual freshwater limit. Within several municipalities in Europe, a limit has been given to enterprises according to their current use, for the amount of freshwater they can use. This policy could also be introduced within the chemical industrial sector.

An additional incentive that policymakers could consider is the provision of subsidies for the construction of water pipes that facilitate the IS of water. Although the effects of these subsidies might be relatively small, their impact is largely dependent on the height of the subsidies. However, there are two important considerations for the implementation of such subsidies. Firstly, the government must allocate these budgets carefully to support financially innovative industrial symbiosis activities, rather than simply redistributing them to support end-of-pipe treatment activities (Song et al., 2018). Secondly, policymakers should establish rules for the distribution of subsidies in advance, as stakeholders are primarily concerned with their own benefits. Discrepancies in the amounts of subsidies provided to different stakeholders often lead to dissatisfaction. Determining the contribution of each plant to the total cost, resource-saving, or waste discharge is a non-trivial task. For instance, a smaller plant may contribute less to resource-saving, as they require fewer fresh resources. The scale of the plant is also an important factor in cost allocation. Therefore, an analytical approach is required to determine a fair cost distribution among the plants, which will maximize the satisfaction of all stakeholders (Chin et al., 2021).

Finally, policymakers need not consider implementing subsidies for the advancement of treatment technologies. While this could be a useful subsidy for improving the quality of wastewater discharged into the environment, it has little effect on incentivizing stakeholders to participate in an IS water network. Subsidizing treatment technologies would benefit everyone in the chemical park, as costs would be lower for all. However, it would not persuade stakeholders to recycle more water as the costs of the treatment facility are already present. Thus, it is not a significant incentive for stakeholders to participate in IS water networks.

10.3. Limitations of this research

The outcomes demonstrated in Chapter 8 underwent testing and validation in Chapter 9. While the outcomes were determined to be a near approximation of a practical result, they were obtained using a model that possesses significant limitations. As Box and Draper (1975) noted, ”Essentially, all models are wrong, but some are useful.” Therefore, to draw significant inferences from the model developed in this research, this section will discuss the key limitations of the model.

10.3.1. Generic design, no real case study

This research exclusively focuses on simulated data, and no data from a real chemical park has been utilized to investigate the potential for IS water connections. As discussed in Section 10.1.2, the strategies heavily rely on the actual characteristics of the chemical park, including the existing treatment facilities, the level of advancement of treatment technologies, and the demanded and supplied water qualities. The absence of data from Chemelot, due to compliance agreements with all stakeholders, makes it unable to test the model on a real case, which is unfortunate in terms of the insights that could be identified. Furthermore, the network of Chemelot could not be tested as it would become computationally too intense. Nevertheless, the model has been designed to be run with data from any chemical park, meaning that if data is received, it could directly be implemented in the model.

10.3.2. Simplifications made in the model

Within the model, several simplifications have been made. Chapters 5 and 6 elaborately discussed all simplifications that are made in the model design, the impact and the alternatives. In this paragraph, the most important simplifications will be discussed.

Scope of the model

To begin with, the model assumes that all water remains within the system and only exits through the source, neglecting the effects of water loss through evaporation, which is a common occurrence in chemical processes. In section 4.5.1, the water flow within Chemelot's chemical park is depicted, demonstrating that 33% of the freshwater that enters the park is lost due to evaporation. This has a direct impact on the amount of water that can be recycled. The model assumes that 100% of the water entering the park can be recycled, whereas in reality, the maximum recyclable amount would be 67%. As a result, the environmental performance metrics obtained by the model are likely overestimated, as they do not consider the effects of water loss due to evaporation.

Secondly, yearly averages are used to define the water demand of the chemical factories. No time component has been incorporated in the model. While in reality the water demands of the chemical companies differ in time which means the flow rate from the freshwater source towards the chemical companies could actually greatly differ. At certain times, the water demand could be much higher than is averagely taken into account in the model. This means the capacity of the pipes could not transport these high values of water, resulting in the actual environmental performance could be lower.

Optimization of the routes within specific networks

In this research, optimal routes are searched within each specific network and designed according to input parameters using a self-designed optimization function. However, the design of this optimization function within the chosen Python package brings some limitations. The minimum-cost-maximum-flow function has been used to find the optimal route, while the aim of this model is to find an optimal route based on minimal costs and minimum flow (maximum recycled water). As a result, this function had to be redesigned into an optimization function specifically for this model, which made the function computationally heavy and increased the runtime of the model significantly.

Furthermore, to find optimal routes within the networks, a pre-set maximum route length had to be determined, which is used in every network type. However, the number of nodes within the network varies significantly, resulting in a maximum route length that is either too long and computationally heavy or too short, resulting in insufficient connections to recycle water effectively. To prevent the model from becoming computationally heavy, the maximum route length was set to a moderate value, which had a greater impact on the function's performance than expected, as explained in Section 8.2.3. As a result, it appeared that the participation of more treatment facilities had a negative effect on the recycling percentage of water in networks with separate treatment facilities. However, this was not logically sound, and experiments with longer maximum route lengths confirmed that more treatment facilities have a positive effect on the percentage of water that can be recycled.

Another limitation within the optimization function is that the social aspect has not been incorporated. The water routes within the network are optimized according to the economic and environmental aspect. Because the social aspect has been quantified as the network efficiency within this research, it was not needed to include the social aspect within the optimization function. However, this does limit the insight of the optimal defined routes regarding the social aspect.

Designed topology of the network

Within the model, network analysis is performed to research the performance of possible structures of chemical parks. For this analysis, the topology of the network is defined, however, some choices have been made in this design that could possibly have had an effect on the eventual performance of the chemical parks.

Firstly, in the model, the edges representing the water pipes are assigned an infinite capacity, meaning that all water supplied by a chemical factory or treatment facility can always flow to another stakeholder. However, in reality, water pipes have a specific size, which limits the amount of water that can flow through them at a certain flow rate. It is possible that not all water can flow through the pipes at all times, which would require the construction of additional pipelines. This, in turn, would have an impact on the economic performance of the network, as it would increase the cost of implementation. Furthermore, it would also limit the amount of water that could be recycled, which would negatively affect the entire network's environmental performance.

Similarly, the same issue arises for the treatment facilities. In the network, it is assumed that the nodes representing a treatment facility have no water demand, implying that they can process any amount of water. However, in reality, it is possible that the treatment facilities have a maximum capacity to purify water, which could affect the eventual environmental performance of the chemical parks.

Designed topology of the social network

In the part of the model where the influence of stakeholders is determined, it is assumed that stakeholders only make a social connection with each other if they must have a contract regarding water use and compliance. Therefore, it is not assumed that stakeholders have a social connection with each other for other reasons. This means that the social relationships between stakeholders are not included in the model and may lead to the network efficiency of the chemical park being actually higher than what is currently reflected in the results.

10.3.3. Influence of the MCDA

Chapter 6 of the thesis outlines the MCDA design and implementation of the model. The method used in this study is binary, where a stakeholder either participates or does not. Three different setups were employed to vary the impact of decision criteria among stakeholders and observe their effects on the identified scenarios. A sensitivity analysis can be performed on how different values for decision criteria influence the identification of participating stakeholders and the creation of scenarios used throughout the analysis.

Furthermore, subjectivity and uncertainties are inherent in determining the values of the criteria and weights. As J. Wang and Zionts (2006) noted, a gap often exists between theoretical work and practical decision-making needs because decision-makers' preferences are not precisely known, resulting in wrong translations or implementations in theoretical models. To mitigate the highest subjectivity and wrong translations of preferences, this model uses weight ranges. Due to the lack of specific information about the actors' preferences, further weight specification was not feasible. Nonetheless, another sensitivity analysis could be performed to determine the sensitivity to other precise weights, instead of ranges, for the number of stakeholders not participating in certain scenarios.

Although the model knows several limitations, the results are relevant and can be used as a basis for discussion between decision-makers. It paints a picture for possible strategies to address stakeholders within chemical parks and to improve the number of IS water connections in chemical parks. Also, the inclusion of stakeholder behaviour in the optimal water network design has led to a design that is more reflective of the decisions of different stakeholders. Performing a network optimization and analyzing the industrial symbiotic performances has shown that many possibilities exist for recycling more water within chemical parks, however, stakeholders' decisions eventually influence the most possibilities for IS water networks. Moreover, strategies can be created for the different structures of chemical parks, both having different requirements to increase the IS possibilities.

11

Conclusion and Recommendations

This chapter presents the conclusions and recommendations derived from the findings of the research conducted. Initially, the research questions formulated in the first chapter are addressed, followed by proposals for future research in section 11.3.

11.1. Answer to the main research question

The research question posed in Chapter 1 is repeated below for convenience.

Research Question 1

To what extent is industrial symbiosis of water within chemical parks possible, taking into account stakeholder behaviour?

The answer to this question is dependent on the characteristics of chemical parks and the type and number of stakeholders involved. The qualifications of the answer to this question are explained below.

The possibility of industrial symbiosis within chemical parks is analyzed in this research according to the industrial symbiotic performance of the IS water network. The industrial symbiotic performance is greatly influenced by the amount of water that could be recycled and the costs for the additional components within the IS water network. The cost of an IS water network is highly dependent on the existing treatment facilities and technologies within the park, as these are the biggest expenses. The environmental performance varies greatly between chemical parks with in-house treatment facilities and those with separate treatment facilities. In the latter type of chemical park, the maximum amount of water that can be recycled is limited to 30% if all stakeholders participate. As discussed in the limitations, this percentage will decrease further when evaporation is considered. In chemical parks with in-house treatment facilities, this percentage is slightly lower at 25% and will decrease faster if fewer stakeholders participate.

Therefore, it can be concluded that the possibilities for industrial symbiosis within chemical parks are highly dependent on the already existing treatment facilities within the park and the number of stakeholders participating in the network and their preferences. These differing optimal solutions are typical for a complex socio-technical system: the complexity of the challenge is increased by the different views of different involved stakeholders. However, this research has identified the decision criteria most influential for stakeholders to join the IS water network and the technical and policy-related optimal solutions to enable more IS water possibilities within the chemical park and stimulate more stakeholders to join the IS water network. These solutions are defined for the two different structures the chemical park could consist of, with separate or inhouse treatment facilities situated in bottom-up regulated countries.

Two key takeaways regarding chemical parks' different structures can already be given. The costs for recycling the same amount of water are higher in chemical parks with separate treatment facilities, spanning from 1 billion to 500 million euros for recycling respectively 25 or 30% of the water. And in chemical parks with inhouse treatment facilities, the possibility of recycling water is lower compared to chemical parks with separate treatment facilities. With fewer stakeholders or more water qualities, the chance of recycling water already does not surpass the 12%.

The most important decision criteria for stakeholders are the economic drive, compliance to regulations and trust. Efforts to increase the amount of participating stakeholders can improve the overall performance of IS water networks in chemical parks, however, only to a small extent.

Efforts could be taken by adjusting or constructing certain technical components within the chemical park to improve the possibilities for industrial symbiosis when certain stakeholders decide not to join. However, this will decrease the costs for the IS water network only by 3% and increase the amount of recycled water by 12%. In situations where the economic drive for joining the industrial symbiotic water network will not be high, and there will not be strict regulations set by the government/park owners, not many factories will want to join the network. To be able to still recycle as much wastewater as possible, an industrial symbiotic water network needs to be created for fewer water sorts of lower qualities, 86 up to 90% treated, if present in the chemical park. In this way, costs stay low and as much water as possible will be recycled. In situations where trust for joining the industrial symbiotic wastewater network, and the awareness of IS possibilities, will not be high, stakeholders will take less initiative to create IS water connections. To still be able to create industrial symbiosis possibilities within chemical parks with separate treatment facilities, the advancements of the treatment technologies need to be upgraded up to aerobic biological treatment. While in chemical parks with inhouse treatment facilities, the possibilities to recycle water become nihil.

Efforts could also be taken by convincing certain stakeholders to participate within an IS water network, which several policies could accomplish. This could decrease the costs for the IS water network with 10% and increase the amount of recycled water with 20%. First of all, the decision criteria of stakeholders to comply to regulations could be addressed by intensifying specific policies. The license to operate within a chemical park is the most crucial license for stakeholders to sustain. Stakeholders have to comply to specific policies to get such a license to operate. Setting more strict limits for the water intake, wastewater disposal or concentration, it would increase the chance that chemical factories will join the IS water network as they do not want to lose their license to operate. Moreover, the government or local municipality could also introduce a limit for the freshwater intake, which is a policy already introduced in the agricultural sector.

Secondly, the decision criteria of revenue growth can be addressed by introducing different economic-related policies: a carefully distributed subsidy for the construction of water pipes and a water tax. By increasing the subsidy for the construction of water pipes above 20% it could have a significant effect on the decision of stakeholders. By setting a water tax of unrealistically 1000% of the actual water price per litre, it will convince all stakeholders to join the IS water network, as it would incur extremely high costs if no water is being recycled.

Lastly, a policy relevant to creating trust among the stakeholders on a chemical park could be introduced. It could increase the participation of stakeholders by 33% and especially wihtin chemical parks with inhouse treatment facilities, the amount of recycled water could increase from 0% up to 15%. A policy could be introduced by chemical park owners to organize a monthly meeting for all stakeholders.

Scientific contribution

This research extends the existing optimal designs for IS water networks by incorporating the social aspect and different treatment model structures into the design. Current optimal wastewater network designs only include the environmental and economic aspects of industrial symbiosis. However, the possibility of stakeholders deciding not to join an IS water network is not incorporated. By including the social aspect within the IS water network design, and afterwards optimizing the new network, enables an analysis of the realistic possibilities of optimal IS water designs within chemical parks, as the decisions of stakeholders are the most critical aspect of creating industrial symbiosis of water. Moreover, the possibility for comparing two different treatment models within chemical parks has been added to the current optimal wastewater network design. It provides a more tailored insight into the differences and opportunities between the two different types of chemical parks.

Societal contribution
This research has given more insight into strategies to address or adjust to stakeholders to create more industrial symbiosis of water within chemical parks located in bottom-up regulated countries. Currently, almost no wastewater is being recycled. Several decision criteria have been identified that have the highest impact on stakeholder behaviour and, therefore, on the possibilities for industrial symbiosis. With this knowledge, chemical park owners and policymakers know which decision criteria should be addressed first to enable more industrial symbiosis in specific chemical parks. Different strategies for incentives and policies are identified that stimulate more stakeholders to join an IS water network. Moreover, several strategies for selecting or constructing technical components within the chemical park are identified to increase the performance of IS water connections. Lastly, this research also provides guidelines to see in which situation and chemical park structure it will be easier or more challenging to create industrial symbiosis possibilities of water.

11.2. Answers to the sub-questions

This chapter provides a brief overview of the primary recommendations for the future continuation of this research project.

How is water currently used within chemical parks and which aspects are relevant for industrial symbiosis?
Water is a crucial resource within chemical parks. Chemical factories require high volumes of water of a certain quality, regarding the levels of pH, total suspended solids, chemical oxygen demand, heavy metals, nutrients and organic solvents. The quality of the water always downgrades in chemical factories as different chemicals (all having different effects on the environment and humans) are added to the water, resulting in a diverse set of wastewater streams produced. The effluent water flow of chemical factories and treatment facilities is applicable for reuse and industrial symbiosis in chemical parks. As the laws and regulations for the consistency of waste within the water in chemical parks are very strict, water can only be reused if treated by a treatment facility first. Different treatment technologies exist, all treating different parts of the water. Technically, it is feasible to restore the quality of wastewater to a level that permits reuse as an inflow for chemical factories. The chemical park can be structured differently according to the treatment facilities. No consensus exists on which model, with inhouse treatment facilities or separate treatment facilities, works most efficiently in chemical parks.

It is imperative to design an industrial symbiosis water network to investigate the possibility of reusing more wastewater in chemical parks. An essential aspect of the designing process is understanding the water requirements of each factory part of the chemical park. Furthermore, the measurement of the performance of an IS water network is critical, as otherwise, no conclusions can be drawn if the design of an EIP for water in the chemical industry is effective and has specific opportunities.

What are important criteria to assess industrial symbiotic performance within a chemical park and how can these be measured?
The performance of industrial symbiosis of water will always be related to economic, environmental, and social aspects. The environmental performance criterion measures the environmental impacts of water-related IS exchanges within the park, in this research depicted as the water efficiency. The economic performance criterion measures the cost-effectiveness of the water reuse system and the financial benefits of resource recovery. The social performance criterion could be defined differently regarding the job creation, governance structure or collaboration effectiveness of stakeholders within the network.

A quantitative comparison of the input and output of different factories is the most effective way to measure the industrial symbiotic performance. Network analysis is the only method that could incorporate the social aspect within the design. Using this method, an optimal design can be created for a chemical park where opportunities for wastewater recycling can be determined and the most effective locations for treatment and reuse. However, the current optimal water network design mainly incorporates the environmental and economic aspects, excluding the social aspect. This can be substantiated because it is difficult to quantify the social aspect. In this research, social performance is measured as the change in the collaboration effectiveness of the stakeholders within the chemical park as they have decided to join an IS water network. These two designs must be combined to measure all three performance metrics of industrial symbiosis and define an optimal outcome.

Which stakeholders should be involved in industrial symbiotic wastewater networks and what are their decision criteria for joining such a network?
It becomes clear that the local industrial symbiosis partners within a chemical park need to collaborate to create the initial IS water network. These stakeholders are directly involved or plan to be involved in a water exchange. The relevant local industrial symbiosis stakeholders are the owners of chemical factories and the owners of treatment facilities. Because of different beliefs and internal policies, stakeholder behaviour is influenced, meaning it could differ per stakeholder if they take part in IS water networks.

This research has set out to define the most important decision criteria regarding whether to join an IS water network. The six most important decision criteria are identified: revenue growth, compliance to regulations, internal sustainability policy, trust, awareness of IS possibilities and technological feasibility of IS connections. Each of these is shortly discussed.

- Revenue growth: Considering joining an IS network will always be related to chances for generating extra revenue. The financial incentives associated with reduced water consumption, lower waste disposal costs, and the possibility of generating revenue from the sale of by-products can motivate stakeholders to join the network. Creating IS water connections, forces companies to make high investments. Hence, companies want to recover these costs and get a return on investment as quickly as possible.
- Compliance to regulations: Government regulations are one of the important external stimuli for IS. Stricter regulations on wastewater discharge can increase the need for wastewater treatment, making participating in IS networks of water more attractive. This need is essentially stimulated by the punishment combined with these stricter regulations. High fines or cancellations of licenses to operate are consequences of not complying to the regulations.
- The internal sustainability policies entail the goals regarding different sustainability topics, of which water is a part, set by the stakeholder. The goals set within this policy could be moderate or more challenging, requiring the stakeholder to make bolder initiatives regarding sustainability.
- The level of trust and collaboration among participants can also influence the willingness of stakeholders to participate in IS networks of water.
- By increasing stakeholders' understanding of the benefits of IS networks of water, as well as the technical and operational requirements of the network, stakeholders can make informed decisions and participate more effectively. Knowledge influences the acceptance to make IS-related investments.
- Especially within the chemical industry, could stakeholders' decisions to participate in IS networks of water also be influenced by the technical feasibility of the network. Factors such as water quality, availability, and compatibility of industrial processes can impact the ability to reuse wastewater, affecting stakeholders' willingness to participate.

How could the impact of stakeholder behaviour on the industrial symbiotic performance of a water network within a chemical park be tested?
A model needs to be created in which the bridge between economic and environmentally optimal models, and on the other hand, social optimal models can be solved. Within this research, it has been chosen to incorporate the social behaviour of stakeholders as the choice between joining or not joining the IS water network. The Multi-Criteria Decision Analysis method is used to quantify stakeholder behaviour. The IS performance is compared with the IS performance of a network after the stakeholders have decided on wanting to join the IS network or not. The robustness to stakeholder behaviour in the IS water network can be defined by comparing the different IS performances.

What is the effect of the different decision criteria on the industrial symbiotic performance of wastewater within chemical parks?

The decision criteria greatly impact the industrial symbiotic performance of the water networks within chemical parks. The decision criteria define if stakeholders join the IS water network or not. If the stakeholders do not join the network, the different economic, environmental and social performances inevitably decrease.

The revenue growth and compliance to regulations have the greatest impact on the industrial symbiotic performance of water networks within chemical parks. According to these decision criteria, most chemical factory owners depend their decision on. The revenue growth will currently be nihil as high investments need to be made by the chemical factory owners to create IS water connections while the economic benefit created, by reducing costs for the freshwater intake and wastewater production, is currently meagre. The prices for freshwater and wastewater disposal are very low in most parts of the world.

Moreover, compliance to regulations set by chemical park owners, regional municipalities or governments focused on freshwater intake or chemical wastewater disposal are currently not strict enough for chemical factory owners to change their decision to join IS water networks. All chemical factory owners are compliant to the regulations while most of them are not joining an IS water network.

As a result, in chemical parks in which the economic drive for joining the industrial symbiotic water network will not be high, and the government/park owners will not set strict regulations, few factories will want to join the network resulting in a low industrial symbiotic performance of the chemical park.

In chemical parks where the trust for joining the industrial symbiotic wastewater network, and the awareness of IS possibilities, will not be high, less initiative will be taken to create IS water connections. In chemical parks where the treatment facilities are privately owned, they may decide not to work with certain chemical factory owners. Substantiated that they do not trust these chemical park owners to discharge wastewater complying with all standards. This greatly decreases the environmental performance measure between up to 0 and 10% as it impacts the possibility of recycling water.

Which trade-offs between different technical components and decision criteria can be identified from analyzing the industrial symbiotic performance metrics?

In situations where few chemical factories would want to participate in the IS water network due to a lack of economic and legal drive and a lack of stimulation from internal sustainability policies, the treatment facilities' advancement level is very important. If this treatment facility or facilities contain high advanced treatment technology, a significant number of IS connections can still be created with a 12% higher environmental performance. However, the economic performance depends on how advanced the current treatment technologies are for the economic performance of the IS connections. The same applies to the number of treatment facilities participating; the more, the better the percentage of water that can be recycled in chemical parks. However, the economic performance will decline by 5% if multiple treatment facilities need to be constructed.

In situations where trust is low within the chemical park, which may occur because there are chemical factories in the park that produce wastewater with very high values of pollutants, the treatment facility may not want to take responsibility. This reduces the opportunities for chemical park owners to create IS connections, but in a park with multiple treatment facilities, there are still possibilities. It is then up to the chemical park owner to seek out chemical factories that require and process approximately the same quality. In this way, IS connections can still be created for lower qualities and for fewer water qualities.

When is the industrial symbiotic performance within chemical parks the highest?

It becomes evident that the industrial symbiotic performance of chemical parks is highest when all stakeholders participate in any type and situation of a water network. This is supported by existing literature. The greatest potential for water recycling occurs when both treatment facilities and stakeholders who can utilize the water produced from these facilities as inflow participate. In the initial scenario of this study, all stakeholders are considered who have the potential to establish connections with each other or with the treatment facility regarding water quality. The industrial symbiotic performance of the initial scenario is always the highest for every different type of network structure.

It does differ per chemical park structure when the highest performance of industrial symbiosis is reached. In chemical parks with separate treatment, the highest performance can be reached with multiple water qualities and a high advancement of treatment technologies. While in chemical parks with inhouse treatment facilities, even a higher performance can be reached with the least amount of water qualities.

What are the most important implications for policy-makers from this research?
The most important implications for policymakers, are related to the implementation of economic incentives to promote stakeholder participation in industrial symbiosis water networks and to policies intensifying the achievement of the license to operate.

On the one hand, should policymakers focus on implementing economic incentives that target stakeholder behaviour directly, such as freshwater taxes and carefully allocated subsidies, to promote IS water networks in bottom-up regulated countries. Given the decreasing availability of freshwater resources worldwide, the freshwater tax could be implemented. While this incentive may not directly reduce the cost of creating IS water connections, it will affect stakeholder behaviour by increasing the cost of not recycling water. However, the freshwater tax must be extremely high, around 1000 euros, to alter stakeholders' decision-making. Therefore, a more realistic policy would be to set a limit on the amount of freshwater intake per stakeholder on a chemical park. In several countries, limits are given within the agricultural sector on the freshwater intake. This policy could also be implemented within the chemical sector, which will force chemical factories to reduce their freshwater intake and use more recycled water. Another incentive that policymakers could consider is the provision of subsidies for the construction of water pipes that facilitate IS water. Policymakers should establish rules for the distribution of subsidies in advance and determine a fair cost distribution among the plants to maximize the satisfaction of all stakeholders.

Chemical companies take compliance to regulations extremely seriously. If regulations become stricter, they will immediately adjust to these regulations because they want to prevent high fines for non-compliance at all costs. The most important asset for the chemical companies located on the chemical park, is their license to operate. If they lose their license to operate, they need to close their chemical factory, having crucial consequences for the chemical factory owners. Policymakers should reset discharge standards customized to the industrial wastewater and local future-proof environmental capacity. Moreover, policymakers should include standards for freshwater intake regarding matching quality requirements between the water input and the required water within chemical processes, to prevent usage of over purified water. Intensifying the policies linked to the license to operate could have a positive impact on the decisions of stakeholders joining the IS water network.

11.3. Recommendations for further research

There are still numerous opportunities available for future research. Certain aspects were excluded from the scope of this study, and certain constraints were identified in section 10.3. Further investigation may address some of these limitations and extend upon the findings of this research. This section outlines some possibilities for future research.

Firstly, it would be beneficial to use real-life data from a chemical park for this research to determine whether the designed model is applicable to this data. Additionally, it would be worthwhile to investigate whether higher industrial symbiotic performance is possible with a different setup for the involved water qualities, treatment facilities, and water demands of an actual chemical park or whether the industrial symbiotic performance is lower due to the higher complexity of water qualities.

This model provides a good overview of all water quality demands and supplies within the entire chemical park. However, it could also be interesting to research certain parts within the chemical park. By scaling down the scope within the chemical park, it could be possible possibilities for industrial symbiosis are discovered requiring less investments.

Another interesting opportunity for future research would be to focus on chemical parks with 'cheaper' treatment technologies in the treatment facilities for finding IS possibilities. As it was found in this research that the treatment technologies with high advancements have a big impact on the costs, and therefore the economic performance of the IS water networks.

It would also be interesting to make certain adjustments to the model so that optimal routes do not have to be determined for the entire chemical park. This could first be achieved by establishing clusters consisting of certain chemical factories and treatment facilities within the entire chemical park. Alternatively, a specific key actor, such as a treatment facility, could be fixed so that the optimal route always includes this actor.

In this study, a clear distinction was made between networks with separate treatment facilities and in-house treatment facilities. This has resulted in conclusions being drawn only in relation to one of the two types of networks, while it would also be interesting to examine combinations of these two network types. In reality, there are also chemical parks in which certain chemical factories have their own pre-treatment facility, and there are also a few separate treatment facilities.

Additionally, water scarcity is a globally known issue with a high priority. This model includes the fact that the amount of water needed by the factories can always be delivered. However, it would be interesting, as well as future-proof, to include in this model that sometimes there is not enough water to be delivered and what this does to the environmental performance. This may also affect the behaviour of the stakeholders, which could cause the importance of the decision criteria to vary. It would then be interesting to develop a new prioritization of decision criteria for stakeholders in a water-scarce scenario.

Furthermore, MCDA was used in this study to differentiate stakeholder behaviour. The social behaviour part of the model is separate from the technical optimization network design in this study. Therefore, a different method could be used to investigate and represent stakeholder behaviour without having much influence on the further design of the model. For example, it would be interesting to apply agent-based modelling methods to introduce dynamics in the behaviour of stakeholders and examine whether this has a significant impact on the creation of scenarios in this model. Another opportunity for future research of this approach derives from the challenge of capturing the constantly evolving structural conditions of IS networks, as well as changes in the actors' composition, leadership, position, and power, providing another avenue for future research using this approach. To address this challenge, dynamic analysis and scenario building should be considered as complementary strategies in refining the method, as suggested by (Doménech & Davies, 2009).

Literature shows that it is difficult to create a water network design that highlights all three aspects of industrial symbiotic performance. The social aspect is still underrepresented in the results of this study. Network efficiency was chosen to be investigated, but it could be examined in much more detail and incorporated into performance metrics other than just network efficiency. More focus should be given to incorporating different aspects of the social performance, like job creation and the impact on governance structures, in a model design in future research.

Finally, the study examined the influences of different incentives on the performance of the IS water networks in various scenarios. However, it is also necessary to investigate whether these incentives actually affect the priorities of the decision criteria of the stakeholders. This would include incorporating stakeholder behaviour as a part of the model. Additionally, three different incentives have been tested, and the research demonstrates that these incentives can be effectively tested with this model. Thus, future research could further test the effects of additional incentives on the industrial symbiotic performance. For example, quotas could be established on water consumption (Song et al., 2018).

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A

Additional information for the treatment technologies considered in this research

This appendix identifies some extra information to the different treatment facilities that are considered in this research. The three treatment technologies are: anaerobic-anoxic-oxic, aerobic biological and membrane bioreactor. The information is summarized in the Table below and the data is gathered from Singh and Kazmi (2018).

WWTP	Preliminary treatment	Secondary treatment	Tertiary treatment	COD reduce	TSS reduce	TEAC (million euros)
Anaerobic-oxic-anoxic	Bar screening + gint chamber + fine screening	Anoxic aeration tank	Pressure sand filter + activated carbon filter + Chlorination	99%	98%	32
Aerobic biological	Screening	Aeration tank + settling tank + rapid mixing tank + Clariflocculator	Chlorination	90%	92%	10
Membrane bioreactor	Bar screening + equalization tank	Aeration tank + sedimentation tank	Chlorination + multigrade filter + activated carbon filter + softener	95%	96%	19

Table A.1: Overview of some information per treatment technology

B

Criteria that have not been included in this research

This appendix chapter complements Chapter 3 of the research by discussing criteria that were assessed but not utilized, as they may be valuable for other researchers. The criteria are categorized as economic, environmental, social, and technological, following the same classification as described in Chapter 3.

B.1. Economic criteria

In this research, two economic criteria, revenue growth and compliance to regulations, have been considered as most important for stakeholders in this research. However, two other economic criteria, gaining tax and reducing costs, have also been identified as possible decision criteria that could influence decisions of stakeholders for joining IS systems in industrial parks and will be discussed below.

B.1.1. Gain tax

The first economic criteria that has not been included as a criteria in this research is the criteria of gaining tax by joining an IS water network. With this wording is meant the encouragement provided by tax cuts and refund policies on resource utilization enterprises, that consumed water waste. For example, in the industrial park Hai Hua in China, a tax cut has been introduced by the local government of 10% by using other factories waste (Cui et al., 2018). This method offers dual advantages. Firstly, it minimizes waste generation across various businesses, and secondly, it provides economic benefits to waste resource utilization enterprises. For instance, if a chemical company opts to utilize another company’s wastewater, it can receive financial benefits or tax reductions. However, in situations where waste can only be reused by a single company, it must be provided free of charge to maintain a balance in the interests of resource utilization companies (Park et al., 2008).

B.1.2. Reduce costs

The second economic criteria that has not been included in this research is the criteria of reducing costs by joining an IS water network. Reducing costs is one of the most important objectives for the stakeholders within the chemical park. IS could bring considerable financial benefits in raw material substitution and transportation cost savings for stakeholders within the chemical park (Yu et al., 2015). Moreover, government financial incentives are used to build byproduct treatment equipment, pipe networks, and other installations for IS which could reduce the initial investment the stakeholders would have to make by building IS water connections. However, however decisions regarding industrial symbiosis always require investment, which results in stakeholders knowing they will not be able to reduce costs.

B.2. Environmental criteria

In this research, one environmental criteria has been included, the internal sustainability policy. Two other criteria, reducing freshwater intake and reducing water pollution, have been found as other possible criteria that could influence stakeholders’ decisions to join an IS system within industrial parks, but have not been included in this research. The two criteria will be discussed below.

B.2.1. Reduce freshwater intake

The first environmental criteria that has not been included in this research is the criteria gor reducing the freshwater intake by joining an IS water system. The water scarcity is growing globally, as has been explained in Chapter 1. Therefore, companies become more conscious of the amount of freshwater they are using, and the public perception towards great freshwater using enterprises is shifting. This is why stakeholders within industrial parks are already busy with reducing their water usage, mainly by internal efficiency measures within the industrial processes. But by joining an IS water network, the freshwater intake can be reduced even further because wastewater of other chemical facotries can be used. This criteria has not been included in this reseach as it could already be an apsect of the internal sustainability policy.

B.2.2. Reduce water pollution

The second environmental criteria thas has not been included in this research is the criteria of reducing water pollution by joining an IS water system. Several emissions are seen as pollution and play an important role in the industrial sector because of their negative effects on the environment. For chemical factories, the values of several chemicals within the wastewater are one of the most important aspects which they monitor (Eslamizadeh et al., 2022). By discharging wastewater with too high values of certain chemicals, could have a polluting effect on the surrounding environment or water basins. Although this is an important aspect for chemical factories, by joining an IS water system, the water is not polluted less. Only less polluted water is discharged into nature.

B.3. Social criteria

In Chapter 3, most of the decision criteria that were identified were socially oriented. Six different social decision criteria were identified of which trust and awareness were used in this research. All the other criteria, community spirit, information sharing, dependency and job creation will be discussed below.

B.3.1. Community Spirit

Community spirit is a social criteria that has been identified in a literature study performed by Park et al. (2008) as the third most essential criteria for collaboration between industrial actors in an IS system. According to Eslamizadeh et al. (2022) mentions, whereas collaborative water usage and demand management are not known to be part of established IS communities, it briefly hints that ’community spirit’ is the potential, influential factor for a successful IS establishment. By community spirit, firms tent to participate more actively, ensuring continutiy and networking (Tudor et al., 2007). This criteria has often been mentioned together with trust, therefore only one of these criteria have been included in this research.

B.3.2. Importance of security

The second social criteria that has not been included in this research is the criteria for the important of information sharing (mostly about water usage) with other stakeholders on an industrial park. Information sharing is seen as the degree of not being interested in sharing the information on your company’s water consumption with others. The lack of sufficient information sharing among stakeholders has emerged as a significant challenge for smart industrial parks in achieving sustainable cooperation, despite the rapid advancement of intelligent technologies. While there has been some progress in information sharing, not all stakeholders possess the necessary knowledge or enthusiasm for effective collaboration. Therefore, adopting a collaborative approach centered around information sharing can foster the sustainable development of smart industrial parks (Tudor et al., 2007). This criteria has not been included in this research as it is interrelated with trust and community spirit.

B.3.3. Dependence

One of the primary limitations in the development of EIPs is the potential vulnerability of the system. When an industrial network is small, the departure or diversion of one of the main enterprises for its materials or products can disrupt the entire chain. The Guitang Group, a sugar refinery in China (Zhu and Cote, 2004), addressed this issue by operating their plants as an interconnected system, where one plant could compensate for the problems faced by another. Another suggested strategy by Korhonen (2001) is to diversify the system in terms of suppliers and resources, enabling it to adapt to change and recover more efficiently. However, excessive diversity can lead to conflicting preferences, values, interests, and higher transaction costs in establishing relationships (Korhonen and Sankin, 2005). The key lies in fostering cooperation among all major stakeholders involved (Korhonen, 2001). Consequently, the connectivity of the IS water system also amplifies the risk of failures, which serves as a crucial point of criticism and a barrier for industrial plants considering integration into an EIP.

According to the interview with Mrs. van Oord, program manager at Chemelot, currently the different factories are already dependent of each other in a way that they all treat their water by the IAZI, the central treatment center. If one company sends wrong polluted water to the IAZI, all other factories are the loser of the fine or the polluted wastewater it sends to the Maas as well. But she states, this dependence becomes much higher with IS. She is insecure how the attitudes towards dependence of the factories will change and develop.

Job creation

The last social criteria that has not been included in this research is the criteria of the creation of jobs when joining an IS water system. This social criteria is often mentioned in literature and is also used for measuring the social performance of an IS system, as explained in Chapter 2. IS development in enterprises can improve business visibility and social identity as well as reflect the moral culture and social responsibility of enterprises (Yu et al., 2015). It does often not create jobs within the chemical factories, however it could create jobs for other businesses located near the chemical park. This is the main reason why this criteria has not been included in this research, as only the local symbiosis partners are included as stakeholders in the scope of this research.

B.4. Technological criteria

Lastly, technological criteria have also been identified as being influential for stakeholders located on chemical parks for deciding to join an IS water network. Technological feasibility has been included in this research and technological reliability has not, but will be discussed below.

B.4.1. Technological reliability

The quality of the water is a very important aspect within chemical parks. Chemical factories require water of a specific quality for their processes. All processes are adjusted to a specific water quality and work optimally with this water quality. If chemical factories have to choose to use wastewater that is firstly treated by a treatment facility, and afterwards used by them, they have to rely the quality of the water is right (Tudor et al., 2007). The treatment facility should consist of treatment technologies that could upgrade the water to a specific quality. Therefore technological reliability is a criteria that stakeholders could consider for joining an IS water network.

C

Additional steps incorporated in the technical optimization model

The appendix complements the information given in Chapter 5 and 6. In Chapter 5, Figure 4.2 shows all steps the entire designed model consists of. The most important steps have been discussed in more detail in Chapter 5 and 6. These steps often contain simplifications that have an impact on the system, which need to be discussed. Some other steps have been discussed less elaborately in these chapters and will be discussed in this appendix according to the summary tables.

C.1. Additional steps and included simplifications

All steps that have not been discussed or shortly discussed in Chapters 5 and 6 will be discussed below. However, the reason for not discussing these steps in the report was that these steps do not contain important simplifications that needed to be discussed or are just very straightforward. Therefore, the discussion of several steps below is kept very short.

C.1.1. Step 2

In this step, all possible edges within the network are defined according to the provided input information of the water quality demand and supply of the chemical factories and treatment facilities. It is assumed that the source can provide any water quality and the sink can receive all different water qualities. Furthermore, nothing important needs to be mentioned for this step.

Step 2	Task	Simplification	Alternative	Computation time
Define all possible edges	Add edges to the network according to in and out water quality of nodes			Very short

Table C.1: Overview of the task, simplifications, alternative, and computation time of step 2 in the designed technical optimization model

C.1.2. Step 3a and 3b

Step 3a and 3b have been discussed in Chapter 5, only the overview tables have not been included in this chapter. Therefore, these overview tables are attached below.

C.1.3. Step 4a and 4c

Step 4c has not been discussed in Chapter 5. Step 4c is specially constructed to reduce the computation time for the optimization function in step 6. As discussed in Chapter 7, experiments are performed each time according to new input variables. If the only change between these different sets of input parameters is the number of involved nodes, the data from the previous run with fewer nodes could be used. The data will be added to the additional data of the new run that involve the analyzed routes of the newly

Step 3a	Task	Simplification	Alternative	Computation time
Step 3a Define the directed inner network	Generate a graph without source and sink			Very short

Table C.2: Overview of the task, simplifications, alternative, and computation time of step 3a in the designed technical optimization model

Step3b	Task	Simplification	Alternative	Computation time
Define the complete network	Add source and sink to the network with only one direction edge and set the attributes	All chemical factories are already connected, No edge from source to treatment facility		Very short

Table C.3: Overview of the task, simplifications, alternative, and computation time of step 3b in the designed technical optimization model

added nodes to the network. This reduces the set of possible routes that need to be analyzed further in the model.

Step 4c	Task	Simplification	Alternative	Computation time
Only analyze the new routes	Check which routes contain the nodes that are new in this network	Only run the model for the routes that contain the newly added nodes and edges	Run the model with every possible route	Very short

Table C.4: Overview of the task, simplifications, alternative, and computation time of step 4c in the designed technical optimization model

C.1.4. Step 5

Step 5 has been deleted from the model, as is illustrated by the red cross in Figure 4.2. This step is included in the high-over scheme of the model as it illustrates the optimization that has been made to reduce the computation time. Usually, step 5 would be an essential step, as it checks if a generated route from a subnetwork is connected. If the route is not connected from source to sink, no water can flow through the network. A new directed graph had to be constructed which checks the connectedness, this step would take long. However, this step did not have to be executed anymore, as the model assumes every chemical factory is already connected to a source and each treatment facility is already connected to a sink. Therefore, every route is already connected.

C.1.5. Step 8b

Step 8b	Task	Simplification	Alternative	Computation time
Register involved stakeholders and the sum of all water demands	Per route analyze which stakeholders are involved and sum up all their water demands to know the sum of all water demands with which the optimization will be performed			Short

Table C.5: Overview of the task, simplifications, alternative, and computation time of step 10 in the designed technical optimization model

C.1.6. Step 9

Step 9 is just a replica of step 6. Because it needs to be performed per scenario, it needed to be illustrated within the blue dotted line in Figure 4.2. This is why is has been illustrated as a separate step, but just works the same as step 6, but then for new networks with fewer stakeholders joining.

C.1.7. Step 10

Step 10 is the last step within the designed model. It is the step in which all data of all scenarios is gathered and merged into a single overview file with which further analysis can be performed.

Step 10	Task	Simplification	Alternative	Computation time
Setup overview file with all data for each experiment	Gather all data for the initial network and the new network per scenario after the social analysis has been performed	Generate overview file for only the added routes	Generate overview file of all routes per experiment	Medium

Table C.6: Overview of the task, simplifications, alternative, and computation time of step 10 in the designed technical optimization model

D

Interviews

During this thesis research, several interviews have been conducted to get a better contextual understanding and to get better understanding of which social criteria play more important roles than other social criteria for the social analysis part of the model. Several employees of chemical factories have been interviewed. Moreover, other experts within the water and wastewater sector or within the chemical sector have been interviewed. Summaries of the different interviews are enlisted below.

Interview	Company	Company type	Employee's position
Interview 1	1	Chemical company producing paints	Global Director Environment
Interview 2	2	Chemical company for health, nutrition and materials	Plant Improvement Engineer facility
Interview 3	Coalition 3	Coalition for defining sustainability goals for the industry in the Netherlands	Manager Water Sustainability
Interview 4	4	IT consultant	Utilities Manager specialized in Water
Interview 5	1	Chemical company producing paints	Technology Lead
Interview 6	5	Research institution for sustainability in chemical industry	Program Manager Circularity Chemelot

Table D.1: Overview of the different social scenarios

D.1. Summaries of interviews for decision criteria

D.1.1. Interview 1

Goal of the interview: The interview aimed to understand the current state and plans for circular water usage at Company 1, as well as the motives and concerns at the management level regarding sustainability and the environment. The goal was also to identify differences in behaviour between sites in top-down regulated countries and bottom-up regulated countries, and to verify technical input variables and social factors.

The interviewee, the Global Director of Environment at Company 1, is responsible for the environmental aspects of the company's operations, focusing on People, Planet, and Paint. His role involves safeguarding and improving the environmental footprint of all factories. Specific targets are defined for carbon footprint, waste, VOC emissions, and water usage based on material assessments conducted across the factories.

Initially, Company 1 aimed for 100% circular water usage by 2030, as stated in their sustainability statements. However, the interviewee later revised this statement, considering the relatively low water consumption of the factories compared to other industries. The cost-benefit analysis did not justify the significant investment required to achieve full circularity for all sites. Instead, the focus shifted to achieving 100% circular water usage only at water-intensive sites.

The interviewee manages the environmental footprint of all sites based on factors such as fines imposed on Company 1 (the most important factor), the adherence of individual sites to internal policies and procedures, and the overall relevance to the company. In terms of wastewater management, each plant is individually responsible for complying with regional and national regulations, which can vary significantly. The risk of fines related to polluted wastewater is relatively low within the painting and coating chemical processes.

Social factors, such as trust and awareness, play a significant role in decision-making. The interviewee stated that the investment in joining an Environmental Industrial Program (EIP) would depend on the specific context. However, if joining such a program could significantly reduce the costs associated with wastewater outflow, it could be considered.

D.1.2. Interview 2

During the interview, I spoke with a plant chemist working at the Company 2 plant near Basel, Switzerland. His responsibilities include managing security and quality related to chemical tasks, specifically for the central water treatment center at the plant and one of the chemical factories that produces intermediates for vitamin A. The site consists of five different chemical factories owned by Company 2, along with a central treatment center. All the wastewater generated by these factories is combined and sent through a large pipe to the treatment center, where it is treated regardless of its type or quality.

At the treatment center, approximately 93% of waste particles are removed from the water. The center, which is as large as a football field, utilizes various processes to achieve this. First, different parameters such as pH, chloride levels, and temperature are measured. Then, solvents are extracted from the water. The subsequent operations must be performed consistently to optimize the process, as they involve biological steps. The water enters a gas reactor where organic particles are broken down, and then flows into two large pools with oxygen supplied from the bottom. At this stage, the water reaches a quality level that allows it to be discharged into nearby rivers. However, Company 2 takes additional steps. Nitrite in the water is diverted, and the water passes through three filters to remove suspended solids. The entire process takes around two days.

The water that leaves the treatment center is still considered ”polluted water” by industry standards, although 93% of waste particles have been removed. The quality requirements for the incoming water at each chemical factory vary based on the certificates they hold. For instance, if a factory requires water with a ”pharma” certificate, it must be 100% clean. On the other hand, a ”food” certificate allows for 98% clean water, although this requirement is shifting towards 100%. If the polluted water from the treatment center is not further treated before being used in a factory, it cannot meet the necessary quality standards. Notably, Company 2 is currently constructing a new factory at the site, which will have its own treatment center for pre-treatment.

Several factors influence Company 2’s decision to recycle more wastewater, including economic considerations, support from the local government, the company’s license to operate, and its internal sustainability policy. Company 2 has a progressive approach to sustainability and is willing to invest significant funds if the desired impact can be demonstrated. Additionally, bundling the central treatment center with other factories on the site, even those not owned by Company 2, may be beneficial, even if it increases dependency or compromises security to some extent.

D.1.3. Interview 3

Coalition 3 is a CEO led coalition of eight Dutch companies: AkzoNobel, Company 2, Friesland Campina, Heineken, KLM, Philips, Shell and Unilever, chaired by Jan Peter Balkenende. These companies advocate sustainable growth in business and contribute to the UN Sustainable Development Goals SDGs.

The coalition seeks ways to scale purpose driven business models; to share sustainability practices and knowledge and to help shape the policy framework that enables and incentivises sustainable business, in order to regenerate our earth systems while also tackling major global environmental and social challenges concluded in the SDGs.

As Lead Facilitator the interviewee is responsible for driving execution of the Coalition 3 strategy as formulated by the Coalition 3 Chairman and Liaisons. She is responsible for organizing joint events, setting-up concrete initiatives and the overall program deliverables. The interviewee collaborates with CEOs from each company, collectively shaping the strategy and managing the decision-making processes. VNO-NCW provides substantive support to the coalition. The coalition meets every six weeks and discusses another topic chosen by the interviewee. Therefore she has a big influence on this coalition. A few subjects have been focused on and seen as most important since the start, social equality, three different emissions and circular economy. The coalition visited Brightland Chemelot campus recently to talk about circularity possibilities and future.

While some topics are predetermined annually (such as circular economy, which has been a focus since the coalition's inception), upcoming discussions will revolve around measuring circularity. The issue of plastics holds relevance across all member companies, emphasizing the shared interest in circular economy approaches.

Water-related matters have been discussed multiple times, although not all companies fully support this focus area. Heineken places high importance on water management, considering public perception as an important factor. The interviewee emphasizes the need for increased measurement and assessment to create more support in each company. The interviewee makes the comparison with the CO2 reduction progress stimulated by harsh measurements. Moreover, the interviewee stresses that stricter legislation and economic advantages as important drivers for progress within the water-related circularity.

The connection between circularity and the SDGs is explored, highlighting the comparatively lower emphasis on measuring and integrating water-related goals into legislation. While progress on CO2 reduction is driven by external pressure, clear targets, upcoming CO2 taxes, trading platforms, and regulations, water-related aspects receive less attention and measurement. Each company within the coalition has its own goals and initiatives related to water sustainability. AkzoNobel aims for 100% water waste reuse at water-intensive sites. Company 2 focuses on responsible care, aiming to reduce water consumption by 4.3 relative to 2017 and improve water intake efficiency. FrieslandCampina targets a 25% reduction in water use by 2030 compared to 2015. Shell aims to manage water use and discharges while developing relevant technologies. Unilever seeks to halve water use in consumer-related products, reaching 2008 levels by 2020, and aims to make water biodegradable.

D.1.4. Interview 4

The interviewee helps water, waste, electricity and gas utilities deliver on the promise of technology and human ingenuity. Together with his team he delivers value and contributes to sustainable development goals. On behalf of Company 4 he is proud to lead the Dutch water waste utility sector and to manage the global Company 4 water community of practice.

The urgency for good treatment of water becomes higher and higher, seen the PFAS scandal in Antwerpen and Zeeland. Fish from the river Schelde is not allowed to be eaten anymore and men in this area have a lower fertility. The problem is much and much bigger than we know/expected.

New regulations and laws will be introduced regarding the treatment of water and the quality of water. Currently only 1% of the industrial companies complies to the Water Directive while in 2027 every company has to comply to this policy. Actors that treat water have to comply with this regulation and to several others. Therefore the urgency for centralized water treatment centers becomes higher as actors do not want to be responsible for the treatment of their wastewater. They could get higher fines if they discharge water of wrong quality. The interviewee stresses the importance of the difference between central treatment facilities and separate treatment facilities.

With the new regulatory stimulus to treat the wastewater within industrial parks more centrally, the interviewee stresses the importance for companies trusting each other. This becomes a new dimension attached to the circularity case. The factor of trusting others should outweight the factor for being responsible for treating their own wastewater.

According to the interviewee does the question remain if the trade-off between the difficulty and costs of centralized treatment centers for all qualities is higher versus decentralized treatment centers specifically for the water quality/ies of one chemical factory. This trade-off should be researched. This also interrelates with the willingness for paying the costs.

D.1.5. Interview 5

The interviewee is working at Company 1 since 2013 and is responsible for the end-of-line systems, like robotic systems or automated guide vehicles that are doing waste handling, wastewater recycling, treatment, solvent recovery, process etc. The first thing he explained is how the process goes for deciding what kind of treatment facility needs to be developed at a certain location. First, the guidelines of that specific region or country are requested and analyzed. There are legal guidelines per country for the quantities of how much of a specific chemical the wastewater may contain. The local engineers of Company 1 analyze these requirements. After the analysis, the team has meetings to discuss how they are going to meet these requirements. According to the requirements they define and decide which components the treatment facility needs to have. Following by decisions on what kind of extra technologies are implemented in the treatment facility. They decide this according to a decision matrix defined for global use.

As Company 1 mostly manufactures paint or latex materials, it is possible the wastewater contains hazardous material directly after the factory. For example, in a certain country, the max required level of COD in the water is 6000, while the water contains 20000 COD after it is used in the water paint factory and 20000 for the latex factory as well. This is why some wastewater needs to be pre-treated before it goes to the central treatment facility. The pre-treatment process goes as follows: The wastewater is screened, the ph level is corrected by acids and bases (chemicals), then salt is added and afterward a separation process happens in which sludge is separated from the effluent water stream. This stream goes to the central treatment facility. The wastewater of different factories often gets mixed together into one pipe before it flows into the central treatment facility.

After the wastewater has been treated in a pre-treatment process and afterward in the central treatment facility, Company 1 considers the water to be useful as ‘process water’. This means the treated water could be used in the green area within the park, for washing machines etc. Or it just flows into the sewer.

When I asked what he thinks important social factors are for Company 1 for considering trying to use more wastewater as input again for the factories in a park. Cenk directly mentioned they are busy with a project at the moment, called ‘zero waste’, in which the water is being treated extra with a biological treatment and bacteria treatment. Then the water can be reused again. However, Cenk mentions that this project is economically extremely difficult. The return of investments is more than 15 years for this project, while normally Company 1 strives to have a return on investment of 4 or 5 years. The investment of this project is around 800K. Therefore he states that for Company 1 to consider doing more of these projects, there needs to be a higher economic incentive. Moreover, he thinks there needs to be a regulatory rule or stick to intensify change.

Bundling with other factories of other companies in an industrial park to use the same central treatment facility would not be a problem for Company 1, if there would be some discharging rules. So some factories would need to pretreat their wastewater for example.

D.1.6. Interview 6

During the interview, the following topics were discussed: the current state of water circularity at Chemelot, perspectives on central versus decentralized water treatment centers, collaboration among stakeholders, verification and testing of input variables, and the influence of social factors.

Brightsite, in collaboration with TNO, the University of Maastricht, Company 5, and Chemelot, focuses on the sustainable development of Chemelot. The interviewee serves as the program manager for emissions reduction, with water being a key aspect for the past few years. Since 2020, the ”Process

Innovation" program has been initiated, aiming for full water circularity and zero water waste by 2050. Currently, Brightsite, together with an external consultant, has developed a roadmap to reduce water usage from the point of water leaving the factories, rather than focusing on internal processes within the factories themselves. The specific measures for reducing water usage are still under investigation, and scenario analysis will be conducted to explore different options. It is uncertain whether a central water treatment center or decentralized treatment centers at the factories would be more beneficial.

The existing central treatment facility, IAZI, is not designed for handling complex chemicals, resulting in the disposal of these chemicals into the water, which poses a problem. The possibility of constructing a new IAZI is being considered.

Chemelot and its site users comply with regulations, which reduces the urgency to further reduce water usage and promote circularity. Consequently, it is expected that implementation of circular water systems will take more than five years to materialize. Water is relatively inexpensive, so the business case for reducing water usage primarily focuses on reducing energy consumption associated with water usage. While water is increasingly considered in companies' sustainability visions, these visions are often developed globally, such as in Saudi Arabia, while the challenges and regulations are specific to the local context.

Several social factors play a role in driving circular water initiatives: Social factors that play a role:

- License to operate (given by Company 5)
- Mitigate risks (by becoming circular)
- Internal responsibility policies by companies and therefore awareness
- Revenue growth

Each company operates independently, with its own business case, ideas, hidden agendas, internal statements, and risk management practices. However, dependency already exists within the chemical plant, as all factories rely on the IAZI. If one company compromises water quality, it affects other companies dependent on the shared water source. The interviewee finds it interesting to observe how the relationships between the companies may evolve with the changing circularity plans, water stress, and regulations. It's worth noting that companies outside of Chemelot also depend on water usage at the Chemelot site. Lastly, the interviewee emphasized that in addition to the high costs associated with water construction and treatment, energy costs for water treatment significantly impact the business case.

D.2. Summary of the interview for the validation

An important aspect within this research is to validate the outcomes of the designed model. A check needs to be performed to see if the designed model gives outcomes that are representative of the real world. Most of the outcomes within this research or qualitative or cannot be validated by literature because no existing literature is present that applies to a chemical park. Therefore, a second interview has been conducted with the Program Manager Circularity at Chemelot of Company 5 to validate if certain outcomes from the model could be true relevant to the chemical park Chemelot. The summary is enlisted below.

Regarding the choice between in-house and separate water treatment facilities, the interviewee mentioned that she doesn't have precise information on the cost difference. However, she referred to a document that outlined the reasons and considerations behind the decision to build the large central separate treatment facility, known as 'IAZI 1.0,' in Chemelot. One of the main considerations was that the park was still under development, with existing and future chemical factories whose specific water demand and quality were uncertain. By constructing a central treatment facility capable of processing various water qualities, they aimed to cater to the future needs of the park. However, the extremely high construction costs of the large central facility were also a significant factor. Chemelot bore all the investment costs for the central facility, whereas with separate in-house treatment facilities, the costs would be more distributed among the chemical factories.

The goal of making Chemelot circular by 2050 involved investigating every aspect of circularity, including water. Five different possibilities were identified to achieve circularity in water at Chemelot, with each option building upon the previous one. One of these possibilities is recycling the water discharged from the central treatment facility. This option could be realized if many chemical factories were willing to participate and consider this discharged water as incoming water. The interviewee highlighted that the likelihood of recycling this discharged water is higher with the treatment facility at Chemelot, as it is separate from the chemical factories and capable of processing various water qualities. However, trust in the Chemelot governance and the other connected chemical factories was deemed crucial. Company 5 and Chemelot are considering the construction of a second IAZI treatment facility or adding additional treatment technologies to the existing one. Currently, complex chemicals cannot be completely removed from the water, which is vital for building trust among the chemical factories and enabling water recycling from IAZI.

Analyzing sensitivity and decision-making of stakeholders regarding participation in the IS water network at the chemical park proved challenging. The interviewee refrained from making definitive statements about the sensitivity of stakeholders' decisions or comparing them with a chemical park that predominantly uses in-house treatment facilities.

Lastly, the interviewee believes that the total amount of recycled water in Chemelot could be higher than the outcome predicted by the model. This is because many chemical companies can handle multiple water qualities, and there is already a high level of trust within the chemical park due to the presence of a single large central treatment facility.

After reviewing the results, the interviewee concluded that she and her company hold significant power through the ”license to operate.” It is crucial to tighten regulations related to wastewater quality, as she believes it is the most important incentive to encourage chemical factories in Chemelot to use water from other factories or treatment facilities.

E

Additional results

This appendix complements the information given in Chapter 8. Within this Chapter the most important results of this research are discussed. All other results and all graphs to which is referred in this chapter will be enlisted in this Appendix. The different results have been included per step. The graphs are illustrated in a large manner, otherwise, the graphs are not readable.

E.1. Additional results for step 2

The goal of step 2 has been discussed in Chapter 8. It contains all results for the scenario-based analysis. First the three graphs for the average performances per scenario will be shown in a larger extent. Afterwards, all boxplots per scenario and histograms will be shown.

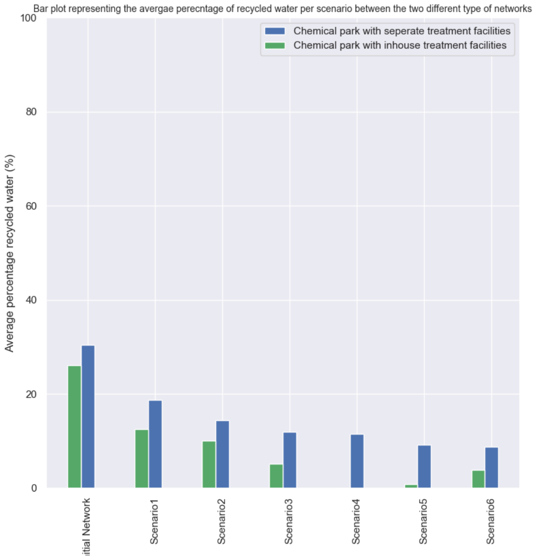


Figure E.1: Average performance per scenario of the environmental performance metric: amount of recycled water

E.2. Additional results for step 3

The goal of step 3 has been discussed in Chapter 8. It contains all results for the component-based analysis. First, the correlation matrices will be shown, and afterwards the graphs for the single and double components.

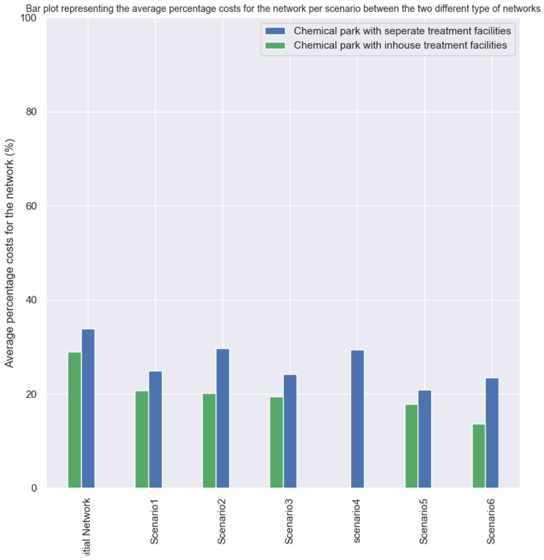


Figure E.2: Average performance per scenario of the economic performance metric: costs for the additional network

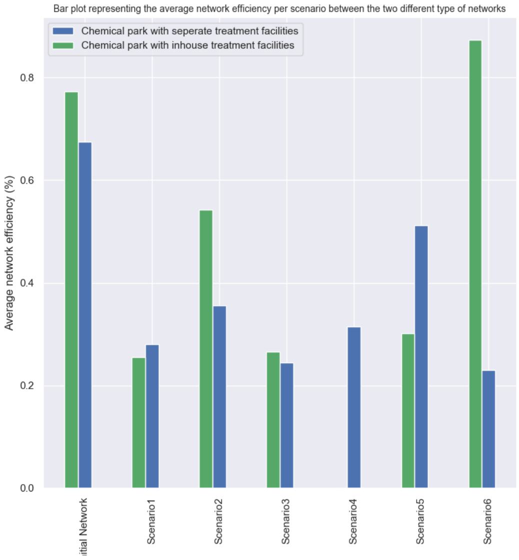


Figure E.3: Average performance per scenario of the social performance metric: the network efficiency of the water network

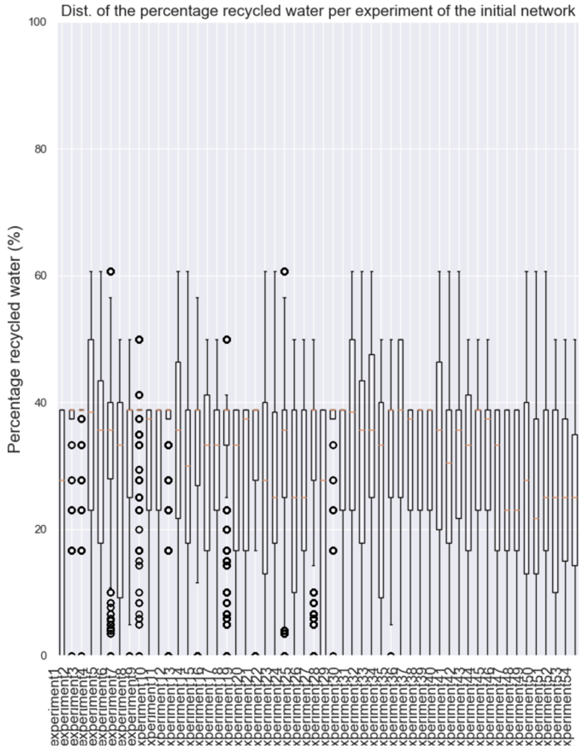


Figure E.4: Distribution of the % recycled water per different network structure for the initial scenario

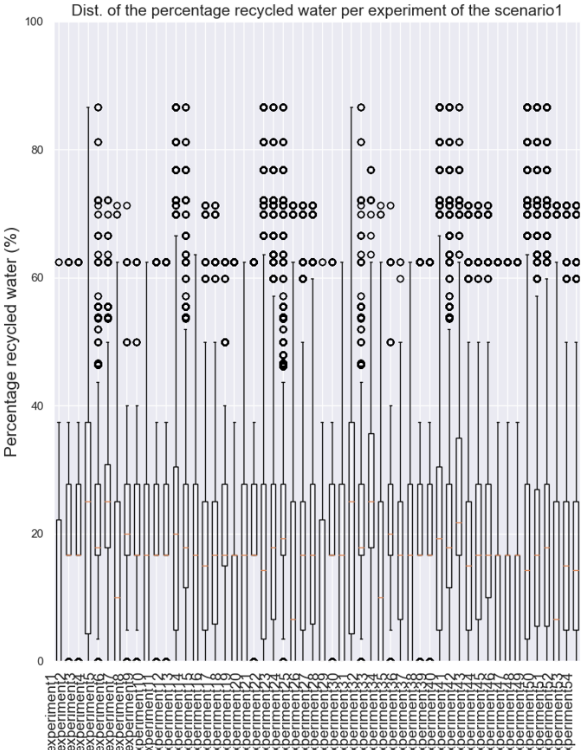


Figure E.5: Distribution of the % recycled water per different network structure for scenario 1

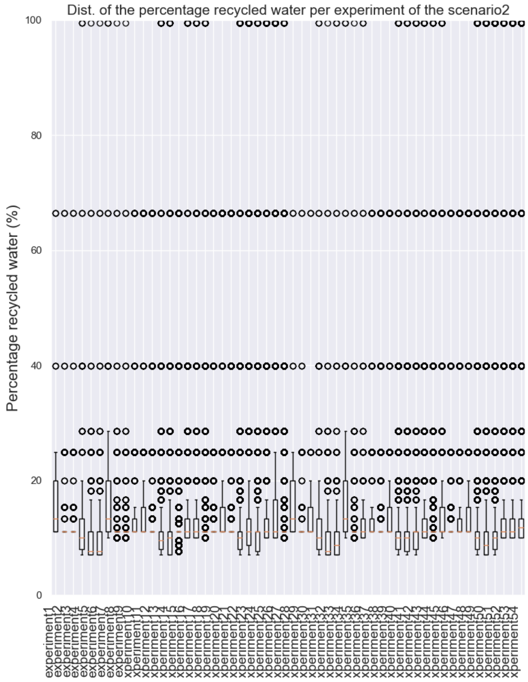


Figure E.6: Distribution of the % recycled water per different network structure for scenario 2

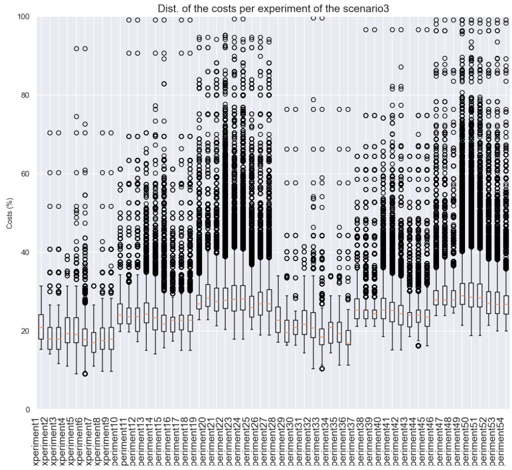


Figure E.7: Distribution of the % recycled water per different network structure for scenario 3

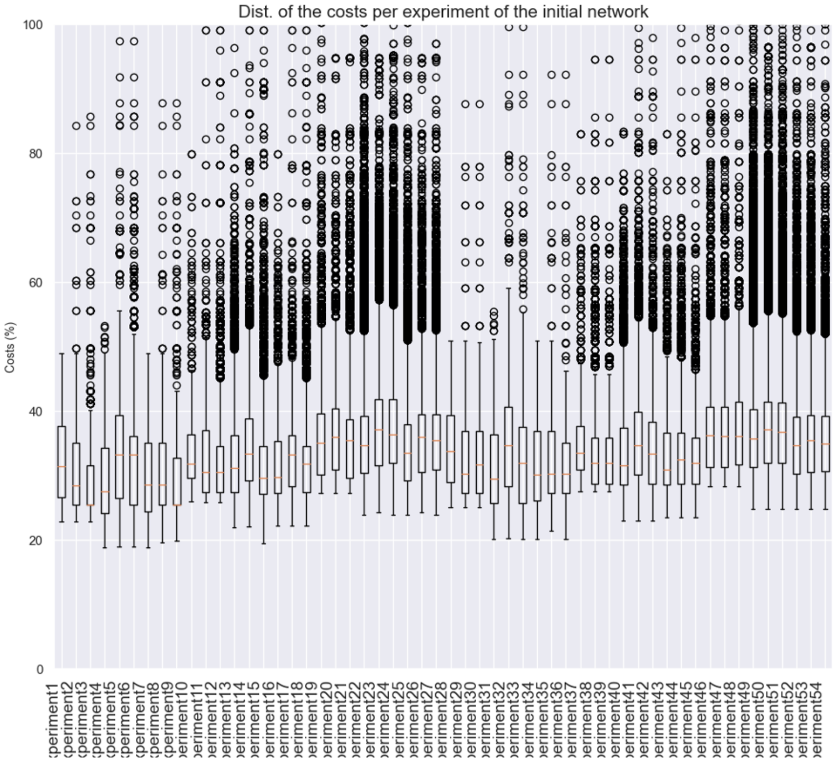


Figure E.8: Distribution of the % costs per different network structure for the initial scenario

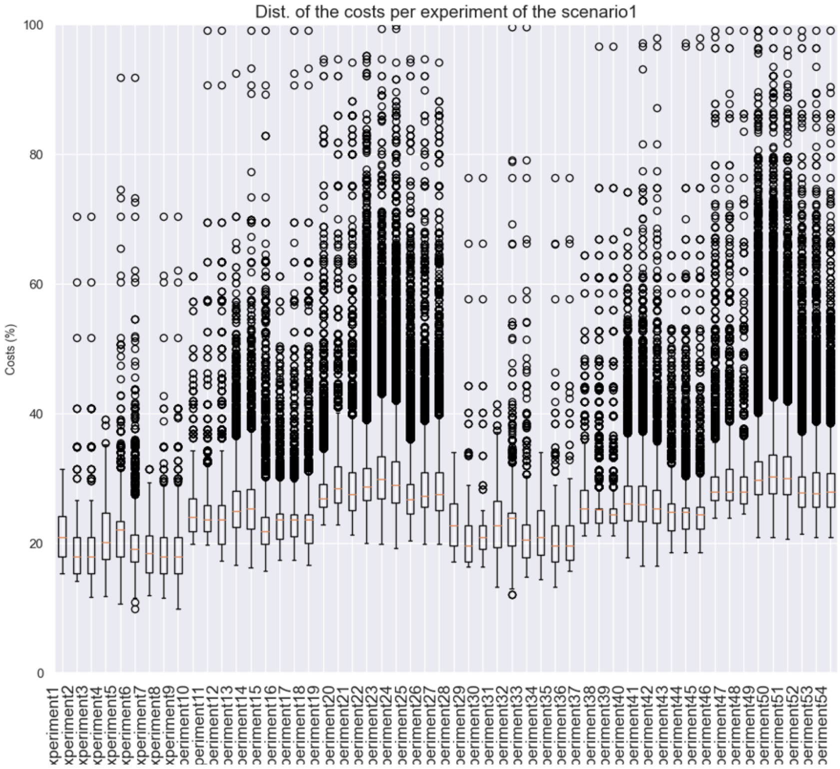


Figure E.9: Distribution of the % costs per different network structure for scenario 1

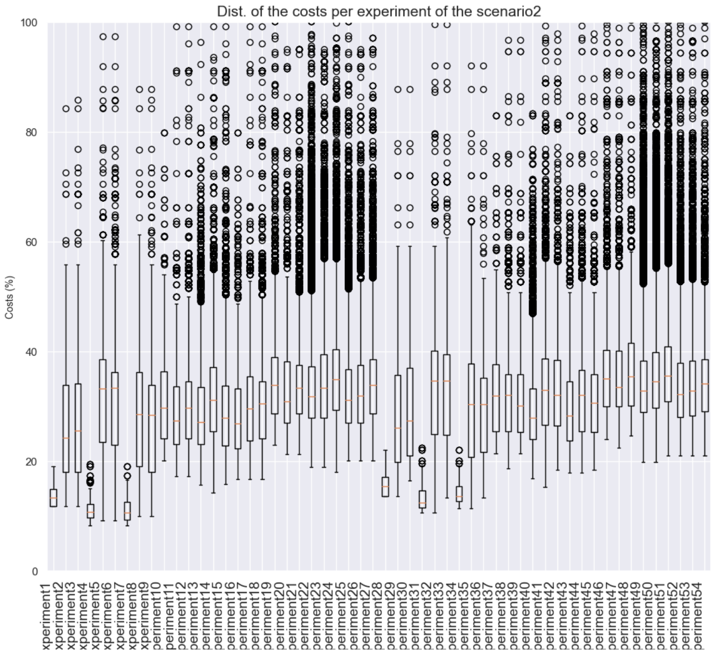


Figure E.10: Distribution of the % costs per different network structure for scenario 2

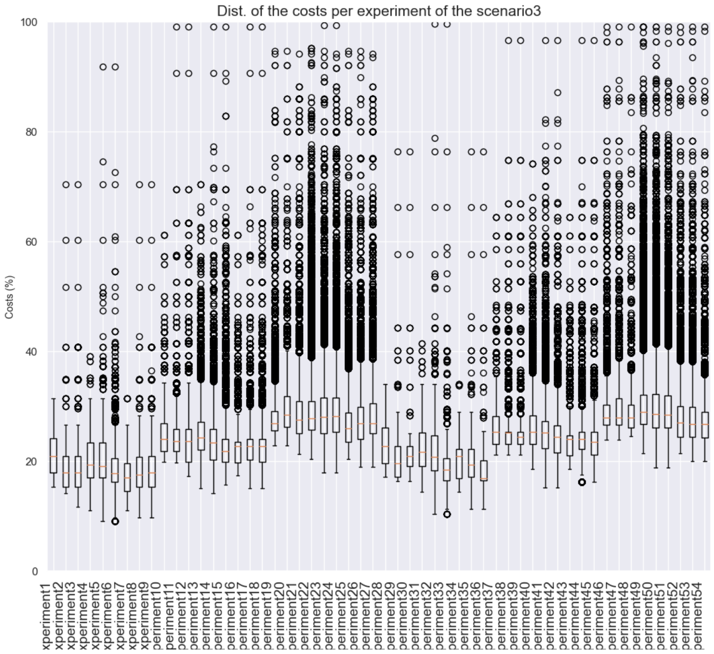
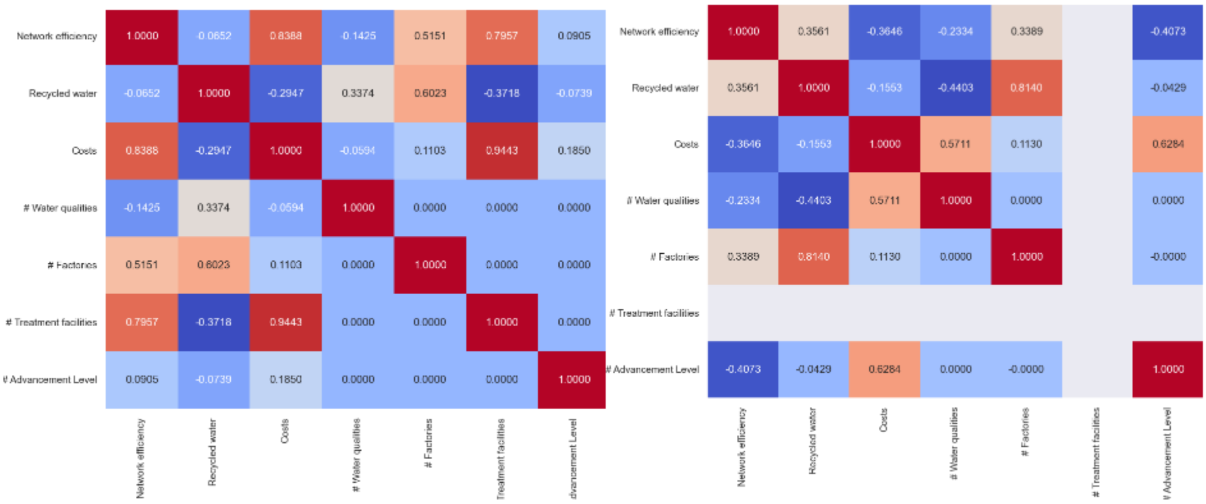


Figure E.11: Distribution of the % costs per different network structure for scenario 3



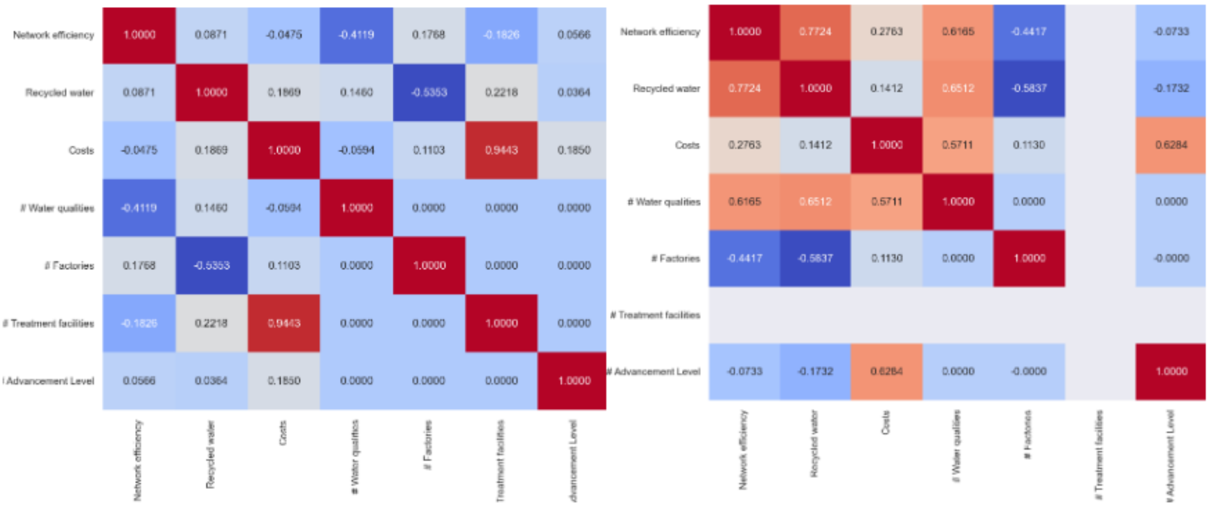
	Network efficiency	Recycled water	Costs	# Water qualities	# Factories	Treatment facilities	dvancement Level
Network efficiency	1.0000	-0.0652	0.8388	-0.1425	0.5151	0.7957	0.0905
Recycled water	-0.0652	1.0000	-0.2947	0.3374	0.6023	-0.3718	-0.0739
Costs	0.8388	-0.2947	1.0000	-0.0594	0.1103	0.9443	0.1850
# Water qualities	-0.1425	0.3374	-0.0594	1.0000	0.0000	0.0000	0.0000
# Factories	0.5151	0.6023	0.1103	0.0000	1.0000	0.0000	0.0000
# Treatment facilities	0.7957	-0.3718	0.9443	0.0000	0.0000	1.0000	0.0000
# Advancement Level	0.0905	-0.0739	0.1850	0.0000	0.0000	0.0000	1.0000

(a) Correlation for network with seperate treatment facilities

	Network efficiency	Recycled water	Costs	# Water qualities	# Factories	# Treatment facilities	# Advancement Level
Network efficiency	1.0000	0.3561	-0.3646	-0.2334	0.3389		-0.4073
Recycled water	0.3561	1.0000	-0.1553	-0.4403	0.8140		-0.0429
Costs	-0.3646	-0.1553	1.0000	0.5711	0.1130		0.6284
# Water qualities	-0.2334	-0.4403	0.5711	1.0000	0.0000		0.0000
# Factories	0.3389	0.8140	0.1130	0.0000	1.0000		-0.0000
# Treatment facilities							
# Advancement Level	-0.4073	-0.0429	0.6284	0.0000	-0.0000		1.0000

(b) Correlation for network with inhouse treatment facilities

Figure E.12: Difference in the correlation between the technical components and the performance metrics between scenario 1 of the different types of networks



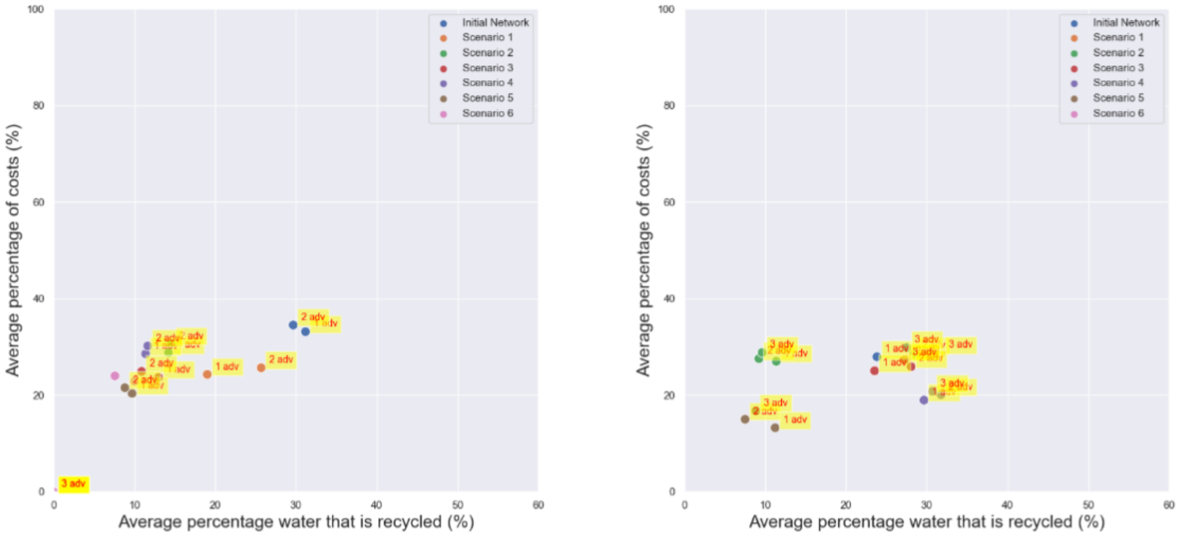
	Network efficiency	Recycled water	Costs	# Water qualities	# Factories	Treatment facilities	dvancement Level
Network efficiency	1.0000	0.0871	-0.0475	-0.4119	0.1768	-0.1826	0.0566
Recycled water	0.0871	1.0000	0.1869	0.1460	-0.5353	0.2218	0.0364
Costs	-0.0475	0.1869	1.0000	-0.0594	0.1103	0.9443	0.1850
# Water qualities	-0.4119	0.1460	-0.0594	1.0000	0.0000	0.0000	0.0000
# Factories	0.1768	-0.5353	0.1103	0.0000	1.0000	0.0000	0.0000
# Treatment facilities	-0.1826	0.2218	0.9443	0.0000	0.0000	1.0000	0.0000
Advancement Level	0.0566	0.0364	0.1850	0.0000	0.0000	0.0000	1.0000

(a) Correlation for network with seperate treatment facilities

	Network efficiency	Recycled water	Costs	# Water qualities	# Factories	# Treatment facilities	# Advancement Level
Network efficiency	1.0000	0.7724	0.2763	0.6165	-0.4417		-0.0733
Recycled water	0.7724	1.0000	0.1412	0.6512	-0.5837		-0.1732
Costs	0.2763	0.1412	1.0000	0.5711	0.1130		0.6284
# Water qualities	0.6165	0.6512	0.5711	1.0000	0.0000		0.0000
# Factories	-0.4417	-0.5837	0.1130	0.0000	1.0000		-0.0000
# Treatment facilities							
# Advancement Level	-0.0733	-0.1732	0.6284	0.0000	-0.0000		1.0000

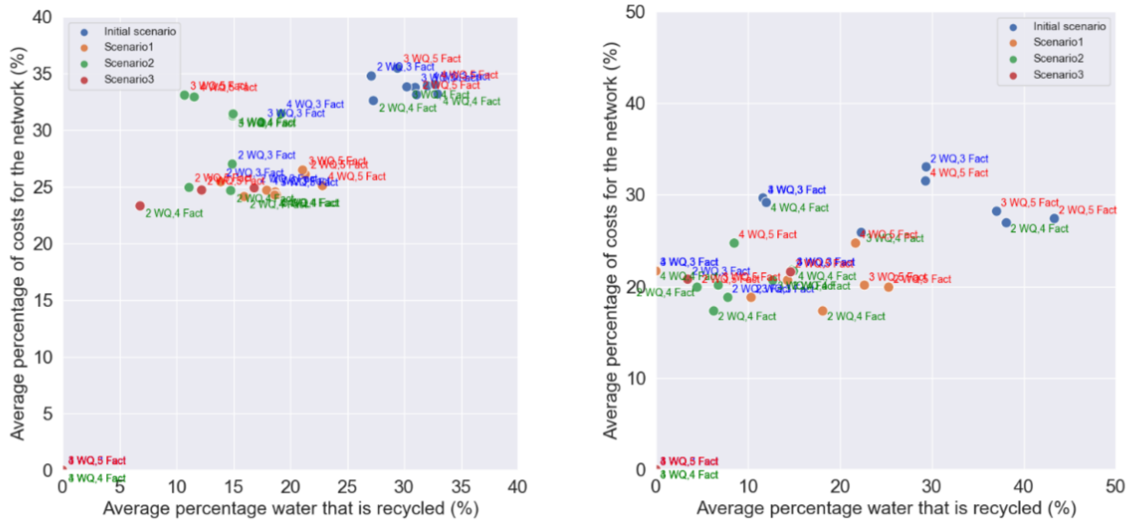
(b) Correlation for network with inhouse treatment facilities

Figure E.13: Difference in the correlation between the technical components and the performance metrics of scenario 2 between the different type of networks



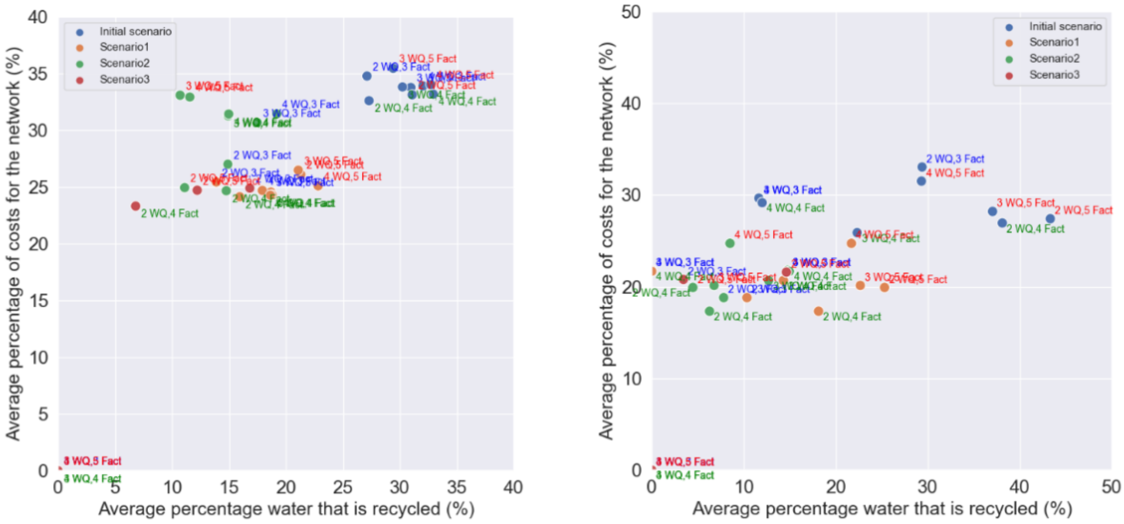
(a) Network with seperate treatment facilities (b) Network with inhouse treatment facilities

Figure E.14: Difference in the pareto optimum for the different network structures according to the advancement levels, between the different types of networks



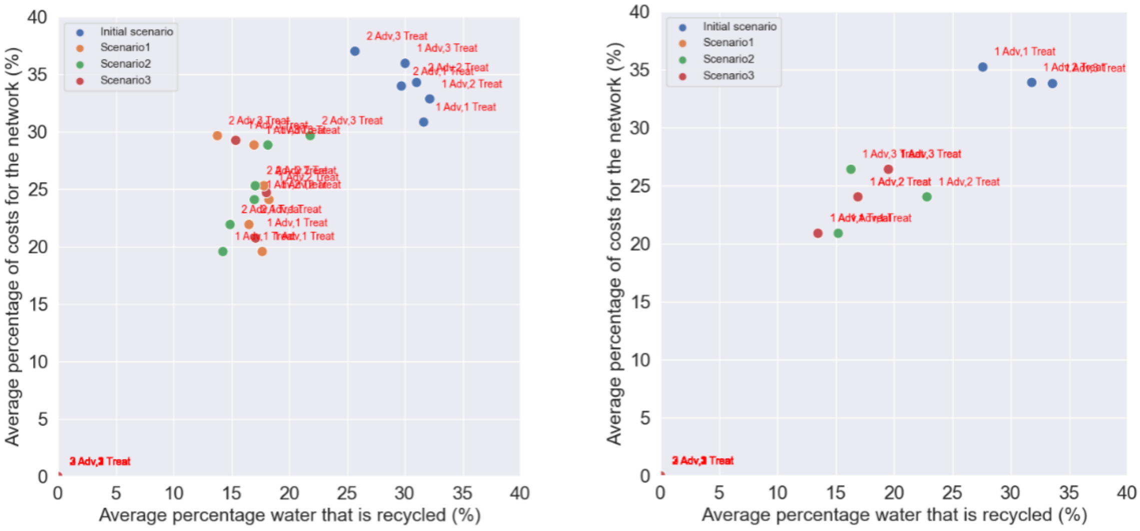
(a) Correlation matrix for experiments with original length routes for the initial scenario (b) Correlation matrix for experiments with original length routes for scenario 2

Figure E.15: Difference in the pareto optimum for the different network structures according to networks with specific components of chemical factories and water qualities, between the different scenarios, (*Red text applies to 5 factories, green text to 4 factories, blue text to 3 factories)*



(a) Correlation matrix for experiments with original length routes for the initial scenario (b) Correlation matrix for experiments with original length routes for scenario 2

Figure E.16: Difference in the pareto optimum for the different network structures according to networks with specific components of chemical factories and water qualities, between the different scenarios, Red text applies to 5 factories, green text to 4 factories, blue text to 3 factories



(a) Pareto optimum for the chemical park with separate treatment facilities regarding the treatment facilities and advancement level (b) Pareto optimum for the chemical park with inhouse treatment facilities regarding the treatment facilities and advancement level

Figure E.17: Difference in the pareto optimum for the different network structures according to networks with specific components of treatment facilities and advancement level