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Industrial network under water stress: exploring the use of industrial symbiosis and desalination alternatives

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Declaration

I declare that this document is an original work of my own authorship and that it fulfils all the requirements of the Code of Conduct and Good Practices of the Universidade de Lisboa.

Declaração

Declaro que o presente documento é um trabalho original da minha autoria e que cumpre todos os requisitos do Código de Conduta e Boas Práticas da Universidade de Lisboa.

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Abstract

Water scarcity is a pressing global issue, prompting industries to seek ways to reduce their reliance on freshwater. To tackle this challenge, this study introduces a MILP model that integrates three different water supply sources: public network (ground or surface water), industrial symbiosis (IS), and seawater desalination. The main goal is to design the optimal network connecting the potential sources to the recipient industries, by minimizing freshwater consumption, overall cost structure, and environmental impacts. The model is applied to a case study involving five Portuguese industries, analysing three scenarios: (1) current situation, where industries resort mostly to public network and self-reuse, (2) addition of IS and desalination as alternatives, (3) includes the three possible sources, but factors in the future freshwater availability limitation. Firstly, considering a single-objective optimization, the inclusion of IS and desalination as alternatives to the public water network leads to a considerable 33% reduction in freshwater consumption compared to the present situation. When factoring in limited freshwater availability, this reduction deepens to 64%, although counterbalanced by extremely elevated costs and environmental impacts. However, when the optimization is done simultaneously for the three objectives, the solution is much more well-balanced. Indeed, it achieves a 38% reduction in freshwater consumption, this time associated with a much lower increase in costs and environmental impacts of 26% and 120%, respectively. To enhance its robustness, this study includes stochastic programming to handle uncertainties in water demand for each business.

Keywords: Water scarcity; Freshwater consumption; Water industrial symbiosis; Desalination; Industrial network design; Multi-objective optimization.

Resumo

A escassez de água é uma questão global urgente, impulsionando as indústrias a procurar formas de reduzir a sua dependência da água doce. Para enfrentar este desafio, o presente estudo introduz um modelo MILP que integra três diferentes fontes de água: rede pública (água doce), simbiose industrial (SI) e dessalinização da água do mar. O principal objetivo é desenhar a rede ótima que conecta as potenciais fontes de água às indústrias recetoras., minimizando o consumo de água doce, a estrutura global de custos e os impactos ambientais. Para aumentar a sua robustez, a incerteza é abordada através de programação estocástica. O modelo é posteriormente aplicado a um caso de estudo que envolve cinco indústrias em Portugal, analisando três cenários: (1) a situação presente, em que as indústrias recorrem maioritariamente à rede pública, (2) acrescento da SI e dessalinização como alternativas, (3) considera as três fontes, mas contabiliza a limitação futura da disponibilidade de água. Inicialmente, otimizando um único objetivo, a inclusão da SI e dessalinização como alternativas à rede pública permite uma redução considerável de 33% no consumo de água doce quando comparado ao cenário atual. Contabilizando a limitação de água doce disponível, esta redução atinge os 64%, embora contrabalançada por custos e impactos ambientais extremamente elevados. No entanto, a otimização integrada dos três objetivos permite alcançar uma solução mais equilibrada. Obtém-se uma redução de 38% no consumo de água doce, desta vez associada a um aumento bastante mais razoável de 26% nos custos e 120% nos impactos ambientais.

Palavras-chave: Escassez de água; Consumo água doce; Simbiose industrial de água; Dessalinização; Otimização rede industrial; Otimização multiobjectivo.

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Acronyms

SDGs	Sustainable Development Goals
GHG	Greenhouse gas
IS	Industrial Symbiosis
EIPs	Eco-Industrial Parks
CO_2	Carbon Dioxide
RO	Reverse Osmosis
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non-Linear Programming
UWF	Uncoated Woodfree Paper
FP	Final Product
TS	Treatment Station
PVC	Polyvinyl Chloride
GW	Global warming
OD	Stratospheric ozone depletion
IR	Ionizing radiation
OFH	Ozone formation. Human health
PMF	Fine particulate matter formation
OFT	Ozone formation. Terrestrial ecosystems
TA	Terrestrial acidification
FET	Freshwater eutrophication
MET	Marine eutrophication
TE	Terrestrial ecotoxicity
FE	Freshwater ecotoxicity
ME	Marine ecotoxicity
HCT	Human carcinogenic toxicity
HNCT	Human non-carcinogenic toxicity
LU	Land use

MRS	Mineral resource scarcity
FRS	Fossil resource scarcity
WC	Water consumption
GAMS	General Algebraic Modelling System

1. Introduction

This chapter introduces the context and outlining of the dissertation. The first section offers an insight into the significance and context of the issue under investigation. Subsequently, Section 1.2 delineates the goals of this study along with the adopted methodology. Lastly, Section 1.3 provides an overview of the dissertation's outline.

1.1 Problem context and relevance

In recent years, the worsening of climate change, exponential population growth and aggravation of water scarcity have revealed the imperative necessity to preserve natural resources (Allaoui et al., 2019). In light of this, the concept of sustainability has become crucial, and organizations have been pressured to balance economic efficiency with environmental and social considerations (Koberg & Longoni, 2019).

As a response, the United Nations established a set of 17 interconnected global objectives, designated by Sustainable Development Goals (SDGs), to achieve a more sustainable and equitable world by 2030 (United Nations, 2015). These goals cover many of the current issues, such as poverty and climate change, but, for this dissertation, the focus has been given to one of the most pressing concerns: water scarcity. Indeed, this has become one of the most urgent global issues as studies reveal that by 2025 it is possible that half of the world's population will reside in regions with very limited water supplies and the ecosystems across the globe are set to face even greater damage in the future (Hundertmark et al., 2020; Unicef, 2021; United Nations, 2018a). Hence, there is an urgent need to enhance the management and utilization of water resources, with the Sustainable Development Goals (SDGs) undertaking an important role in this action. In fact, goals 12 and 14, regarding responsible consumption patterns and conservation of the life below water, respectively, already give an indication of the aggravated situation and possible metrics to alleviate the pressure on water sources. Nonetheless, the main focus is given in goal 6, that aims to guarantee the availability and sustainable management of water on a global level. Indeed, this goal encompasses two rather important targets that underscore the relevance of this dissertation, namely targets 6.4 and 6.a. The first one states that by the year of 2030, there should be an improvement in water-use efficiency, establishing dependable and sustainable methods for withdrawing and supplying freshwater to combat water scarcity. The second one explores the need for cooperation and expanded capacity regarding water initiatives, such as desalination, wastewater treatment and the implementation of recycling and reuse technologies (United Nations, 2015).

Understanding the distribution of water consumption by sector is also crucial to understand the relevance of this work. According to the 2021 UN Water Development Report, freshwater withdrawals are divided into three major sectors. Agriculture stands out as the largest consumer, responsible for approximately 70% of global water withdrawals, primarily for irrigation purposes. Industries follow closely, accounting for nearly 20% of freshwater withdrawals. Domestic use represents the remaining 10% (Unesco, 2021). This data reveals that the agricultural and industrial sectors together account for 90% of freshwater withdrawals globally. Given their substantial water usage, it becomes imperative to prioritize the improvement in water use and management practices especially in these sectors, particularly when facing water shortage challenges.

This way, given the context of water scarcity and the relevance of pursuing the SDGs, two solutions emerge as possible and viable responses to address large freshwater withdrawals by the agriculture and industrial sectors: water industrial symbiosis and seawater desalination. Industrial symbiosis is a collaborative approach that enables the by-products from an industry to become raw materials for another (Yu et al., 2023). This way, it is possible to minimise material consumption and reduce waste creation by encouraging resource exchange between various industries, which is aligned with the objective of achieving sustainability (Herczeg et al., 2018). In the context of water scarcity, the focus is given to water industrial symbiosis, which consists in the exchange of treated wastewater between different industries (Chin et al., 2021).

On the other hand, desalination allows the transformation of seawater into potable water. Indeed, by removing salts and minerals, desalination provides a suitable water for industrial use and even human consumption. This process effectively addresses water challenges, helping to reduce pressure on freshwater reserves, and contributing to improved water management in regions that face significant water stress (Asadollahi et al., 2017).

Thus, studying water industrial symbiosis and desalination as freshwater alternatives becomes highly relevant in the context of sustainable development. By exploring their capacity to alleviate pressure on freshwater resources and facilitate the adaptation of agriculture and industries to the urgent water scarcity situation, this study aims to contribute to effective water management strategies and sustainable practices, aligning with the sixth SDG.

1.2 Objectives and methodology

The aim of this dissertation is to explore alternative water sourcing approaches for the agricultural and industrial sectors to address and adapt to the decrease of freshwater availability. To achieve this, an optimization model is developed, facilitating the establishment of connections between industries in the form of water industrial symbiosis and desalination. The model provides a generic but comprehensive framework, enabling its adaptation in accordance with each case. This way, this work answers to significant gaps in the existing literature, mainly by combining three potential water sources: public network, water industrial symbiosis and desalination.

The multi-objective model intends to reduce water consumption, while still minimizing economic and environmental impacts. Firstly, the minimization of water intake concerns the extraction of water from nature, in the form of both freshwater and seawater. By minimizing the intake of both these two potential sources, the objective function allows the model to maximize the quantity of reused water circulating between industries, therefore alleviating the pressure of withdrawing water from nature. Secondly, the economic aspects are taken into account through the minimization of costs, while still accounting for the potential revenues resulting from the exchange of treated wastewater between industries. Thirdly, the environmental impacts regarding the type of water supplied and infrastructures necessary are also minimized, that way accounting for other environmental concerns other than freshwater scarcity.

To reach the present goal the developed research methodology includes seven main steps that are present in Figure 1.

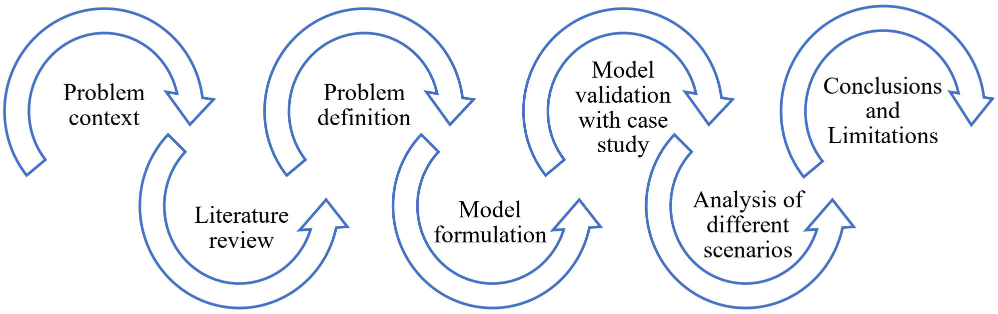


Figure 1 - General methodology

- Problem Context: The initial phase highlights the urgency of industries to adapt to a water scarcity environment. It outlines the challenges related with freshwater consumption, indicating two alternatives that can address these problems.
- Literature Review: An extensive investigation into the concepts relevant to the topic discussed, and existing optimization models is conducted. The literature review provides a comprehensive overview of existing research, highlighting gaps that guide the study's direction and potential contributions to the field.
- Problem Definition: The problem and its specifications are precisely defined, establishing the groundwork for developing the optimization model.
- Model Formulation: Building upon the defined problem, a mathematical optimization model is developed to address the dissertation's objective.
- Model Validation with Case Study: The generic model undergoes validation through a real-world case study. Extensive data collection ensures the case study accurately represents the practical context.
- Analysis of Different Scenarios: The model is tested under various scenarios, investigating the viability and implications of each alternative. It considers significant parameter variations and uncertainties, allowing the identification of critical aspects.
- Conclusions and Limitations: Based on the results, the research questions are addressed, and the suitability of considered alternatives is determined. The analysis also reveals major limitations of the model and case study application.

1.3 Structure of Dissertation

The dissertation is organized into six main chapters, as follows:

Chapter 1: This chapter provides a concise overview of the water scarcity context, introducing the urgency and relevance of finding other alternatives to freshwater withdrawals. It outlines the primary objectives of the study and introduces the dissertation's structure.

Chapter 2: The second chapter explores the theoretical foundation of the dissertation, contemplating literature on industrial symbiosis and desalination concepts and existing optimization models regarding industrial freshwater consumption. By identifying gaps in the literature, this chapter establishes how the dissertation can contribute to this problem, supporting the relevance of the study.

Chapter 3: This chapter presents the problem in study and outlines the generic model to be developed. Additionally, the mathematical formulation of the previously defined model is detailed.

Chapter 4: This chapter introduces the case study where the developed model will be applied. It offers a comprehensive description of the case study, including relevant data, as well as presenting the different scenarios to be analysed.

Chapter 5: In this chapter, the results obtained from the model application to each scenario from Chapter 4 are analysed. Both single and multi-objective optimizations are performed, revealing critical points and efficient sets of results for the problem under study.

Chapter 6: The final chapter summarizes the most important findings and conclusions. Limitations of the study are addressed, and potential areas for future development are suggested.

2. State of Art

This chapter is structured into four sections. Section 2.1 discusses further research on water context sustainability. Sections 2.2 and 2.3 explore the concepts and impacts of water industrial symbiosis and desalination, respectively. In Section 2.4, the research on optimization models and their application for these two alternatives is presented. Finally, this information is consolidated to understand the existing literature, identifying potential gaps for further exploration.

2.1 Water context

As outlined, climate change and population growth have significantly heightened the need for a more sustainable world (Kirby & Mainuddin, 2022). Specifically, these factors reinforce the urgent issue of water availability. According to the United Nations, “Water is at the core of sustainable development and is critical for socio-economic development, healthy ecosystems and for human survival itself.” (United Nations, 2018b). Despite the planet's abundance of water, only a small fraction is accessible for purposes such as domestic, industrial, or agricultural use (Klop et al., 2008). This limited freshwater supply is rapidly approaching a critical threshold, making it increasingly challenging to maintain water consumption at sustainable levels, particularly in the face of climate change, population growth, and changing consumer patterns (Rockström et al., 2009; Vörösmarty, 2000; Wada et al., 2011). According to Gude (2016), this shortage of freshwater availability is a highly potential obstacle of sustainable development, where “Water scarcity hinders economic development, detriments human health, leads to environmental degradation and promotes political and social instability”.

As time goes on, the negative predictions are starting to materialize, with the World Resources Institute stating that “[in 2021] 17 countries, home to a quarter of the world's population, are experiencing extreme water stress” (Mulhern, 2022). Water stress results from water demand exceeding availability, either through withdrawals or consumption, leading to challenges in accessing this vital resource and causing environmental impacts (Kummu et al., 2016).

More specifically, the scarcity of water significantly impacts industries, disrupting their operations and supply chains. Indeed, stricter regulations, including elevated water prices, reduced allocations, and mandatory water-saving measures, contribute to this impact. Additionally, there are reputational concerns as public awareness of unsustainable water practices grows (Hoekstra, 2014). The consequences of water over-exploitation extend beyond environmental worries, affecting economies and governments' policy objectives. While the impact is more evident on water-intensive industries in their direct operations, the supply chain also presents considerable challenges, particularly for businesses reliant on agriculture or extractive industries. Even regions with ample water resources face vulnerability due to global supply chains, potentially leading to business disruptions or closures (Schmidt & Seiz, 2011).

Economically, water scarcity causes changes in consumption patterns, resulting in increased costs to secure water from alternative sources or engage in different activities (Dolan et al., 2021).

Moreover, water holds vital importance for life. Its social significance contrasts with its role in various production processes, where it carries economic value. The physical, regulatory, and reputational risks are interconnected: as water scarcity worsens, regulations tend to tighten, and the public becomes more concerned about a company's water-related practices when communities lack sufficient access to water for basic needs (Schmidt & Seiz, 2011).

Thus, considering the current context of water stress, its impacts, and the predictions of global population growth in the near future, it is important to invest and develop alternative water supplies that can meet this increasing demand, in light of sustainable development (Gude, 2016). At the same time, it is crucial to consider not only economic aspects but also social and environmental dimensions. Finding a balance between these elements is essential for sustainable water management in the attempt of deaccelerating the worsening of climate change and water scarcity’s impacts.

It is important to acknowledge that concerns about sustainability emerged long ago, where the World Commission on Environment and Development defined it as “Development that meets the needs of the present without compromising the ability of future generations to meet their own needs” (WCED, 1987). Despite the unanimous agreement on this definition, it was still rather difficult to pursue the concept without concrete objectives and targets. With the aggravating of the situation, and as a response, the United Nations formulated the Sustainable Development Goals (SDGs) in 2015, as a representation of a systems approach to sustainable economic development (Barbier & Burgess, 2017). By encompassing the three-bottom line, regarding economic, environmental and social aspects, the SDGs become the best set of actions for industries to adapt and resist to the water scarcity context.

Even though the SDGs’ objectives represent an intergovernmental commitment, the engagement of multiple stakeholders from the public, private, and civil society sectors is highlighted as fundamental to achieving global sustainability progress (Johnsson et al., 2020). This way, it is clear that businesses are important players in driving sustainability and are facing increasing demands from external entities, such as governments, to improve their overall sustainability performance and meet specific sustainable standards. This includes looking at their supply chain to enhance sustainability practices, commit to and report on their sustainability initiatives (Koplin et al., 2007; Labuschagne et al., 2005). Nevertheless, it is still necessary to establish indicators for the measurement of industries' impacts regarding the triple bottom line encompassed by the SDGs, namely economic, environmental and social aspects. Generally, the most frequently used metrics are concerning costs (material, operating), greenhouse gas (GHG) emissions and customer satisfaction, respectively. However, with the escalating concern about water-related issues, metrics pertaining to water have gained significance, such as water consumption, industrial water reuse ratio, wastewater, amongst others (Ahi & Searcy, 2015; Mengistu & Panizzolo, 2023).

Indeed, in light of these metrics, industries have been making efforts to improve their water efficiency, by decreasing their water consumption and wastewater generation. In fact, water management approaches can be related with both demand mitigation and supply enhancement strategies. Demand mitigation involves implementing water conservation practices through technological, process or chemical innovations (Hussain & Wahab, 2018). Additionally, mechanisms can be enforced to influence user-responsible behaviour, such as implementing higher water prices, for example. On the other hand, supply enhancement is achieved by employing methods for water reclamation, reuse, and recycle (Gude, 2017). For instance, for longer-term solutions in supply enhancement, industries mostly opt to resort to reuse treated wastewater, or brackish groundwater and seawater suitable for desalination. Although these solutions provide alternatives to direct freshwater intake, their affordability becomes a challenge (Gude, 2017).

In the end, various technologies are available to produce high-quality and safe drinking water or water suitable for other beneficial uses. This allows seawater and wastewater to be treated to a satisfactory quality for industrial use, serving as possible alternatives to freshwater consumption and a solution to its decreasing availability (Gude, 2017).

2.2 Industrial Symbiosis

Industrial symbiosis (IS) plays a crucial role in promoting sustainable development through its focus on managing residues generated during production processes. It operates as a collaborative supply chain management approach, facilitating the exchange of resources, materials, energy, water, and by-products among traditionally separate industries (Neves et al., 2020). By embracing industrial symbiosis, businesses can collectively gather benefits, enhance competitive advantage, and optimize material and energy consumption. The essence of industrial symbiosis lies in the utilization of by-products from one industry as valuable raw materials for others, leading to a reduction in waste disposal and minimizing resource loss (Yang et al., 2023). This interconnected system allows what was determined as inevitable production residues from one industry to be transformed into valuable assets for another. This approach not only promotes industrial growth and economic prosperity but also contributes to the pursuit of a more sustainable world (Herczeg et al., 2018).

The pioneering case of industrial symbiosis can be traced back to the Eco-Industrial Park (EIP) in Kalundborg, Denmark (Chertow, 2008; Ehrenfeld et al., 1997). Note that the IS concept is often associated with EIPs, since these include a close group of industries that share resources to achieve collective benefits. Kalundborg's remarkable success in implementing industrial symbiosis has served as an incentive for numerous projects worldwide, transcending borders and economies (Neves et al., 2020). By effectively utilizing by-products from one company as valuable resources for others, the park achieved reduced waste disposal and optimized resource consumption (Domenech & Davies, 2011; Ehrenfeld et al., 1997). As a result, a diverse number of case studies has emerged, showcasing the versatility of industrial symbiosis across various industries and by-products exchange, solidifying its significance in advancing environmental, economic, and societal goals (Ehrenfeld et al., 1997; Jacobsen, 2008; Neves et al., 2020).

According to Neves et al. (2020), industrial symbiosis encompasses a wide variety of materials that can be exchanged, including water. Several successful examples demonstrate the effectiveness of such symbiotic relationships involving water. In fact, in the EIP Kalundborg example, freshwater scarcity prompted the implementation of water reuse schemes. An oil refinery pipes cooling water to a coal power plant, where it is purified and used as boiler feed-water. Additionally, the refinery provides treated wastewater to the power plant for cleaning purposes, resulting in a significant reduction of about 25% in freshwater consumption (Domenech & Davies, 2011; Ehrenfeld et al., 1997). Another noteworthy case is in Tianjin, China, where various businesses engage in a synergy of water and wastewater exchanges (Shi et al., 2010). In Texas, a case study indicated an impressive 83% reduction in freshwater consumption and a 73% reduction in wastewater generation (Aviso, 2014). These examples demonstrate how industrial symbiosis plays a crucial role in waste minimization and, more importantly, alleviates pressure on essential raw materials, such as water.

Industrial Symbiosis offers a multitude of benefits across economic, environmental, and social dimensions. Economically, it provides resource conservation and cost-effectiveness by transforming by-products into valuable raw materials. These secondary resources are often more affordable to procure than virgin materials, while also reducing disposal expenses and generating additional revenue through by-product sales (Ehrenfeld et al., 1997; Jacobsen, 2008). Nonetheless, establishing a symbiotic network often requires substantial investments, for instance regarding treatment and transportation (Herczeg et al., 2018). Regardless, in the long-term, it is expected a total economic surplus (Neves et al., 2020).

One of the strongest driving forces behind the adoption of industrial symbiosis is its environmental benefits. By reusing materials, the negative impacts of creating new resources are averted. This not only eases the strain on natural resources and waste disposal but also results in reduced emissions into the air, water, and soil (Herczeg et al., 2018). These gains manifest in various ways. For instance, measurable reductions in CO2 emissions, along with lower instances of landfill and methane emissions (Wadström et al., 2021). Equally important is its role in conserving freshwater, as evidenced in the earlier examples focusing on water-based symbiosis. In the end, this approach contributes to lower energy consumption, reduced waste production, lower wastewater generation, and an overall decrease in emissions (Neves et al., 2020). However, the tendency of industries to prioritize economic aspects might sometimes overshadow the full potential of realizing these substantial environmental advantages (Herczeg et al., 2018). In the case of water industrial symbiosis, there are even some additional challenges regarding “water governance, health risks, regulatory aspects, and public perception” (Gude, 2017).

From a social perspective, one of the main benefits considered is the relationships and network established between industries, authorities and the local communities affected by the industries’ operations. The share of knowledge and practical insights between industries regarding waste management practices, allows for a collective achievement of sustainable development (Cecelja et al., 2015; Simatupang et al., 2002). By reducing their environmental impact mainly regarding emissions, industries contribute to the quality of air and water, benefiting the communities (Herczeg et al., 2018; Neves et al., 2020). There is also the question of improving life quality through the creation of jobs, also improving local economies (Baldassarre et al., 2019; Khan et al., 2023). However, there are some challenges regarding the social component as well. Although communities can benefit from IS, at start it can be difficult to build this relationship of trust and aligning interests amongst stakeholders (Faria et al., 2021).

This way, the variety of benefits associated with Industrial Symbiosis ranges from resource efficiency and cost savings to environmental responsibility and societal progress. By maximizing the utilization of resources and promote interdependence, IS offers economic viability, environmental integrity, and social advancement, which is in accordance with the SDGs.

2.3 Desalination

Desalination is a process that converts seawater into freshwater by extracting dissolved solids, leaving behind a concentrated solution designated as brine. This method employs either thermal evaporation or membrane separation, with the latter being more prevalent due to its lower energy demands (Gude, 2017).

While this process has been in use for some time, its energy-intensive nature and associated costs have limited its adoption. Nevertheless, the population growth and increasing industrialization aligned with the worsening of climate change and water scarcity, have led to an exponential shift towards this approach. Indeed, the global installed capacity of desalination facilities rose by approximately 105% between 2007 and 2015, highlighting its growing significance as an alternative freshwater source (Gude, 2016).

In 2015, desalination facilities globally supplied approximately 87 million cubic meters of water per day, with nearly half of this capacity concentrated in the Middle East and North African (MENA) countries (Gude, 2017). This region has been at the forefront of seawater desalination due to its critical scarcity of freshwater resources, attributed to the absence of rivers. Consequently, countries in the MENA region heavily rely on desalination as their primary water source (El Saliby et al., 2009; Van Hoop et al., 1999). Saudi Arabia stands out as an important example, where the Saline Water Conversion Corporation established one of the world's largest desalination stations in 2014, having a capacity of nearly one million cubic meters per day. Additionally, Australia, struggling with the impacts of climate change and water scarcity, has increasingly embraced desalination as a solution. Within the efforts to implement water reuse and recycling strategies, desalination has had significant developments in the country (Gude, 2017). A noteworthy instance occurred in 2008 when a renewable energy-powered desalination plant supplied 17% of Perth's water needs (El Saliby et al., 2009). These cases exemplify the global necessity of finding alternative solutions to freshwater, being possible to rely on desalination as a solution.

Several aspects shape the economic implications of desalination. These encompass the availability and quality of the water source, the technological methods used to convert seawater into freshwater, and the energy source powering the desalination plant, particularly whether it is a renewable option or not (Gude, 2016). The latter two factors are particularly significant due to the considerable energy requirements historically associated with desalination. In fact, these energy demands have been reported to be as much as "9 times higher than those for traditional groundwater sources" (Gude, 2016). However, it is worth noting that recent developments have led to a decrease in these requirements and the associated costs, mainly due to the increased production of desalted water, which benefits from economies of scale, and the continuous improvement of technologies, resulting in higher energy efficiency. Hence, the choice of desalination technology is rather important, as it directly impacts various aspects of the cost structure, namely energy consumption. For instance, the Reverse Osmosis (RO) treatment process has become one of the most opted method due to its comparative low costs and complementary simplicity (Neves et al., 2020). Moreover, operational costs, including maintenance and labour expenses, are also relevant contributors to the economic aspect of desalination (Gude, 2016).

The geographic positioning is also as a critical in the economic structure. The proximity of the desalination plant's installation site to its target area significantly affects costs (Gude, 2016). Shorter distances translate to lower transportation expenses and reduced need for associated infrastructure. This geographical aspect highlights the importance of strategic plant placement to optimize economic efficiency. Naturally, adequate financial resources are essential to ensure the successful implementation and operation of desalination projects (Gude, 2016). Therefore, securing appropriate funding is a key factor in determining the viability and economic sustainability of desalination initiatives.

Despite being one of the more energy-efficient methods for obtaining freshwater, the seawater Reverse Osmosis process still requires a substantial amount of energy, leading to significant greenhouse gas (GHG) emissions that have adverse effects on both human health and the environment, particularly in terms of climate change (Amy et al., 2017; Gude, 2016). There are multiple environmental concerns linked to this method as an alternative water source. Apart from the emission of air pollutants, a key challenge arises from the resulting byproduct of the process: brine. This concentrated brine solution has high salt levels, posing difficulties for a proper disposal. Discharging it into surface waters or sewers can elevate salinity levels, impacting existing water supplies. On the other hand, releasing it into marine ecosystems can pose serious risks to marine life, altering water quality, ecology, and even temperatures (Gude, 2016, 2017; Manju & Sagar, 2017). Moreover, the use of chemicals in the treatment process and their subsequent discharge also raises valid environmental concerns (Amy et al., 2017; Gude, 2016). Another aspect is the impact of land and materials usage, as well as the effect of invading marine organisms caused by the extraction and intake of seawater (Amy et al., 2017; Manju & Sagar, 2017).

Nonetheless, the increasing interest in seawater desalination has incentivised the development of sustainable solutions to mitigate these adverse impacts (Amy et al., 2017). One major focus has been on reducing air pollution linked to fossil fuels by transitioning to renewable energy sources or cleaner alternatives like natural gas. This shift can significantly decrease GHG emissions, thereby contributing to global warming mitigation and the overall well-being of ecosystems and human lives (Gude, 2016). Addressing the issue of brine disposal, it is possible to dilute the salt concentration in seawater before discharge, which reduces the brine's salt intensity. This step enables a reduction of the negative impacts on water supply quality and marine ecosystems (Gude, 2016). While these solution examples signify steps toward a more sustainable desalination process, further efforts are necessary to substantially minimize the environmental footprints associated with this alternative water source (Amy et al., 2017; Gude, 2016).

The establishment and operation of desalination plants can have significant social implications, both during their construction phase and in their ongoing operation. This alternative can have a range of effects on society, including concerns related to noise pollution, dust generation, and alterations to the landscape (Gude, 2016). Indeed, there is a possibility of altering areas that might otherwise have been assigned for future residential or industrial development, and also of disrupting properties situated along the path of pipelines, impacting the daily lives of these communities. The introduction of such changes can also raise doubts about the water provider's reliability, water quality, and overall safety (Gude, 2016).

Nonetheless, promoting sustainable behaviours and practices can significantly enhance the success of desalination plants. This involves not only ensuring responsible usage of water resources but also careful maintenance of the desalination facilities. These practices hold particular significance in safeguarding the well-being and viability of smaller communities. Demonstrating respect towards water resources and the infrastructure that supports them ensures that desalination initiatives have a more lasting, positive impact on social sustainability (Gude, 2016).

In the end, regardless of the economic, environmental and social impacts desalination might have, in the global context of water scarcity, this alternative can be considered as a solution for sustainable development (Manju & Sagar, 2017).

2.4 Industrial Symbiosis and Desalination

As previously discussed in Section 2.1, the aggravation of climate change, rapid industrialization, and projected population growth are collectively intensifying the strain on water resources, worsening the issue of water scarcity. In this context, there is a pressing need to explore alternative water sources beyond the conventional ground and surface water options (Tzanakakis et al., 2020). Sections 2.2 and 2.3 elucidate two such sources – treated wastewater reuse, particularly within the framework of water industrial symbiosis, and seawater desalination – both holding the potential to meet future water demands while alleviating the load on freshwater resources (Ghaffour et al., 2013).

While desalination and water reuse share similarities regarding technology, they present quite some differences in their respective processes (Gude et al., 2010). As outlined in Section 2.3, desalination is associated with high costs and environmentally adverse impacts. Indeed, even though wastewater treatment also requires significant initial investment, it ends up by offering greater cost efficiency and notably less harmful environmental effects (Gude, 2017; Gude et al., 2010). However, the downside of water reuse is that it is inherently linked to the quantity of wastewater produced, which is not unlimited, especially considering the natural water losses during the reuse process and transportation (Gude, 2016).

Hence, combining the strategies of water industrial symbiosis with desalination could yield substantial benefits by mitigating the individual drawbacks of each approach. Water industrial symbiosis, which faces quantitative water limitations, could be supplemented by desalination to fulfil the remaining water needs (Gude, 2016). Similarly, desalination's negative environmental impacts could be reduced by resorting to water reuse simultaneously, allowing businesses to rely less on desalination and thus avoiding its unnecessary adverse effects (Ghaffour et al., 2013). By combining the advantages of these two water sources, it becomes possible to address water scarcity effectively and pursue sustainable development (Ghaffour et al., 2013).

Incorporating water industrial symbiosis and desalination as alternatives to conventional water supply sources necessitates a thorough understanding of the extent to which industries can rely on each of these sources. Specifically, it is necessary to determine the optimal allocation and combination of water resources from the different sources. To address this challenge, numerous studies have integrated optimization models, which identify the most balanced solution environmentally and economically.

2.5 Mathematical optimization models

This section is organized as follows. Sections 2.5.1 and 2.5.2 provide a literature review of mathematical models integrating water industrial symbiosis and desalination, respectively. Section 2.5.3 explores model formulations that combine both of these water sources, concluding with a summary table of the discussed papers and respective models.

It is important to emphasize that these two alternatives have undergone extensive research, resulting in a considerable number of optimization models. However, to ensure reliability and relevance, the focus is given to the most recent papers, highlighting the latest updates and advancements in the field. In addition, the papers chosen for discussion were selected based on their innovative contributions to the existing literature. Specifically, preference was given to papers that enhanced the overall research field, by extending the applicability of models or exploring novel objective functions, for example.

2.5.1 Models including industrial symbiosis as water source

Until the development of Kolluri et al.'s (2016) work, various optimization models aimed at improving the economic viability of EIPs existed. However, these previous studies failed to account for potential miscommunications among interconnected industries within EIPs, disregarding the potential future impacts on established networks. Kolluri et al. (2016) addressed this gap by introducing different future scenarios and offering a multi-objective mathematical model. The aim is to minimize freshwater consumption and regenerated water flowrate, encouraging the use of reuse networks to conserve this resource. Despite this advancement, the paper disregarded economic impacts. To address this, Maillé & Frayret (2016) developed a model optimizing by-product synergies and network configuration, minimizing costs related to waste procurement, storage, and disposal. Applied to the water synergies of Kalundborg EIP's case study, this model analysed the trade-off between economic benefits and freshwater conservation across multiple time periods. Importantly, this versatile model is applicable not only to EIPs but also to larger-scale options. Tiu & Cruz (2017) took yet another step by incorporating environmental impacts and water quality differentiation. Utilizing goal programming, they minimized the costs of piping, operating, and treatment costs, as well as of fresh and wastewater, while simultaneously minimizing environmental impacts. In contrast, Taheri (2021) introduced an improved framework for synthesizing water and wastewater flows within EIP networks. This paper aimed to fill the literature gap by optimizing economic and environmental impacts, while still acknowledging the necessity of incorporating flexibility to adapt to uncertainty. This was a crucial aspect often overlooked in previous research. However, the limitation of this work remains with its restrictive applicability on EIPs. Lastly, Espinoza Pérez et al. (2023) contributed to the field by designing a sustainable and robust network, focused on reusing treated wastewater in agriculture. Their approach factored in uncertainty in the resource's demand while achieving a balance between economic and environmental optimization.

2.5.2 Models with desalination as water source

Seawater desalination optimization models have a quite extensive literature, primarily focusing on economic aspects from around 2005 to the present. Noteworthy examples from this period include Lu et al. (2006) and Skiborowski et al. (2012), concentrating on enhancing cost-effectiveness within desalination plant technologies. Addressing this research gap, Shahabi et al. (2017) introduced a comprehensive mathematical optimization model encompassing both environmental and economic objectives. It explores the optimal desalination station locations, infrastructure considerations, and life cycle impacts, from construction to operation. Taking a step further, Hipólito-Valencia et al. (2021) extended desalination's scope by incorporating it as an agricultural water source. Their multi-objective model aimed to minimize annual costs and groundwater consumption and enabled significant freshwater savings when applied to a case study. Futhermore, Kizhisseri et al. (2022) offered an economic evaluation of water supply options in arid regions. Their mathematical model includes residential, industrial, and agricultural demands supplied by groundwater or desalinated water, presenting a versatile solution applicable across various contexts.

2.5.3 Models including various water sources

When it comes to mathematical formulations integrating both wastewater reuse and desalination as water sources, the available research is rather limited. Despite extensive exploration, only a couple of noteworthy papers emerge from a while back, namely Kondili et al. (2010) and Liu et al. (2011). However, these sources might contain outdated content. On the other hand, a more recent contribution comes from Abdulbaki et al. (2017). This work presents a unique model designed for optimizing the allocation of water resources. The objective is to minimize overall water costs, and what sets this study apart is its consideration of geographically distant water supply and demand nodes, diverse water sources (freshwater, seawater, and wastewater), and various demand types including industrial and agricultural, all while accounting for water quality aspects.

Table 1 groups the most pertinent optimization studies to comprehend their respective focal areas. The table features five primary columns. The initial column pertains to the water source addressed in each study, encompassing public water network (groundwater and surface water), water industrial symbiosis (reuse of treated wastewater), or seawater desalination. In the subsequent column, the nature of the objective function is assessed, distinguishing between minimizing water consumption, cost reduction (or other economic considerations), and minimizing environmental impacts. When considering the economic component, most of the articles opt by minimizing costs. These mainly include expenses incurred in the investment, construction and maintenance of infrastructures such as pipelines and treatment facilities, in water treatment and the price of consuming each type of water. On the other hand, the environmental impacts are measured by the volume or quality of water discharged by an industry, the amount of desalted water supplied or by the impacts of building a water transportation infrastructure. The third segment concerns the study's scope, whether it is intended solely for Eco-Industrial Parks (EIPs), broader networks (including distant industries), or for agricultural applications. The fourth column assesses the model type formulated, while the final column indicates whether the model incorporates uncertainty or not. In the cases where uncertainty was considered, it was mainly focused on the demand of wastewater for reuse purposes.

Table 1 - Literature Review mathematical models' contribution summary

Article	Water Source			Objective Function			Application Level			Model	Unc
	Public	IS	Desal	Water intake	Costs	Env Imp	EIP	Large scale	Agri		
(Kolluri et al., 2016)	x	x	-	x	-	-	x	-	-	MILP	-
(Maill, 2016)	x	x	-	x	x	-	x	x	-	MILP	-
(Tiu & Cruz, 2017)	x	x	-	-	x	x	x	-	-	MILP	-
(Taheri, 2021)	x	x	-	x	x	-	x	-	-	MINLP	x
(Perez et al., 2023)	x	x	-	-	x	x	x	-	x	MILP	x
(Sahabi et al., 2017)	-	-	x	-	x	x	-	x	-	MILP	-
(Hipólito-Valencia et al., 2021)	x	-	x	x	x	-	-	-	x	MINLP	-
(Kizhisseri et al., 2022)	x	-	x	-	x	-	x	x	x	MILP	-
(Abdulbaki et al., 2017)	x	x	x	-	x	-	x	x	x	MILP	-
This work	x	x	x	x	x	x	x	x	x	MILP	x

The reviewed articles reveal several notable gaps in the existing literature. Despite the chosen articles' substantial contributions, a predominant pattern emerged where optimization models for industrial symbiosis are mainly applicable to EIPs. Thus, there is a lack of models applicable to larger scales or agricultural settings. Among the researched models, the primary emphasis remains on economic considerations, with some extending to address water consumption and environmental impacts. However, the integration of all three objectives remains unexplored in the current literature. Additionally, while some models did address uncertainty, this factor has not been given enough attention.

Regarding desalination models, a similar trend occurs with a clear focus on economic factors. However, there is a distinct lack of models that effectively balance cost reduction with the simultaneous goals of minimizing environmental impacts and freshwater usage. Additionally, the aspect of incorporating uncertainty has been essentially overlooked, as no identified recent and relevant article has yet integrated this dimension into its model.

Furthermore, locating articles that incorporate all three potential water sources, that is, freshwater, treated wastewater, and seawater, proved to be quite challenging. Consequently, another critical gap lies in the scarcity of models capable of effectively allocating different water resources to attain both economic and environmental sustainability, while simultaneously minimizing freshwater consumption.

In order to respond to the identified gaps in the existing literature, this current work develops an optimization model that integrates the three potential water supply sources. The model aims to simultaneously minimize freshwater consumption, overall cost structure, and environmental impacts, while accounting for uncertainty of demand. By considering water quality available from each source as well as quality requirements for the recipient entities, the model extends its applicability to various contexts, including EIPs, larger scale scenarios, and agricultural settings.

3. Problem Definition and formulation

In light of the previous research and identified gaps in the literature, this chapter aims to define the problem addressed in this dissertation, specifically focusing on alternatives to freshwater consumption in the industrial and agricultural sectors. Section 3.1 presents the problem statement, highlighting its key features. In addition, section 3.2 presents the mathematical formulation developed to address the identified problem.

3.1 Problem Statement

Water scarcity is a pressing global issue that requires immediate attention. With the population growth rate on the rise and projected to increase further, the demand for water is also escalating, putting significant pressure on available water sources. Therefore, industries are bound to adapt to this challenge by reducing water losses, minimize water requirements, and explore alternative approaches that alleviate the pressure on natural resources. Despite this global concern, there are still some gaps in the existing literature, which this study aims to address. Firstly, there is a lack of research that comprehensively considers desalination and water industrial symbiosis as alternatives to freshwater consumption. Secondly, the integration of multi-objective network design encompassing water consumption, costs, and environmental impact within the context of industrial symbiosis requires further exploration. Lastly, there is also a lack of studies examining water symbiosis on a larger scale, encompassing industries located in separate regions. Thus, two research questions are addressed in this paper:

1) How can Water Industrial Symbiosis and Desalination serve as alternatives to freshwater consumption in a water scarcity context?
2) What are the implications of such alternatives regarding water consumption, economic and environmental factors?

To answer these questions, the problem to be defined aims to design an industrial water network, minimizing fresh and seawater intake, network costs and environmental impacts.

The first step involves developing a mathematical model to optimize water consumption in each industry which considers the costs and environmental impacts associated with designing the network. While the model is not based on any specific existing model, it draws on insights and details from various models discussed in the literature review. The model is then constructed considering a generic network that enables the exchanges illustrated in Figure 2. To validate the effectiveness of the model, a real-world case study will be conducted, providing practical application and valuable insights into actual water usage. Lastly, the analysis of the results obtained from implementing the model in the case study will provide understanding insights into addressing the research objectives and questions.

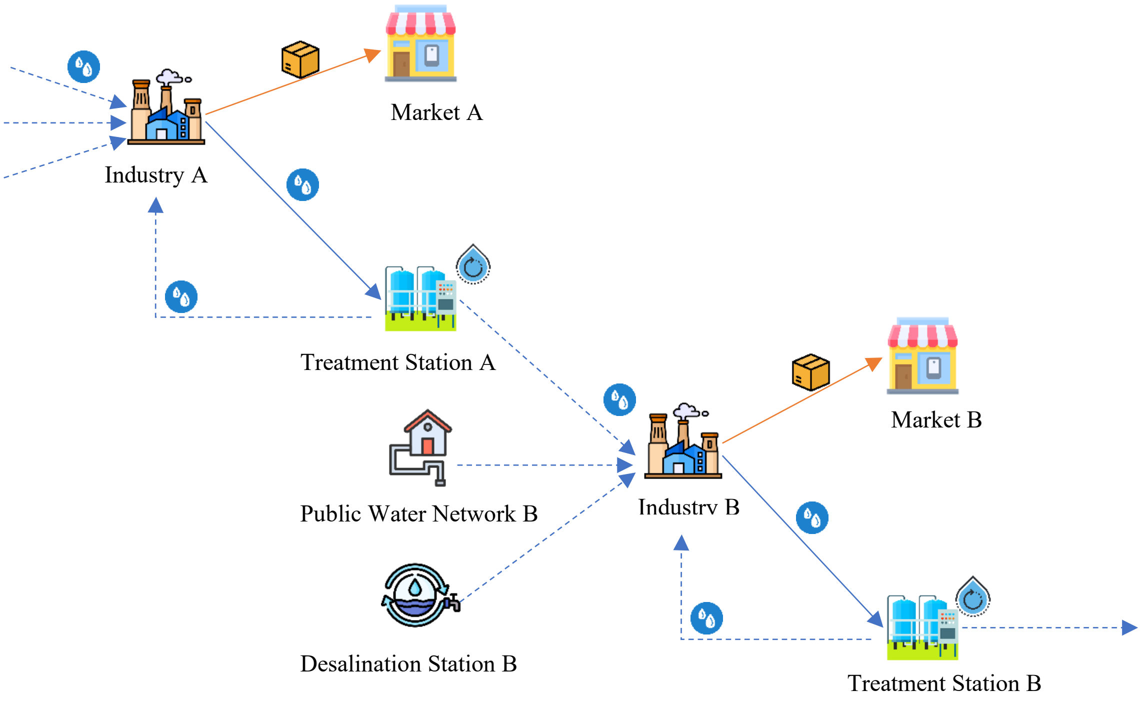


Figure 2 - Generic exchanges between entities

Figure 2 depicts the interactions between various entities involved in the problem, including:

- Markets: These entities receive the final products required to meet external demand. Each market is associated with an industry responsible for producing the specific final product.
- Industries: These entities are responsible for manufacturing and supplying the final products to the respective markets. For this, a certain amount of water is required, which can be sourced from three options: public network, water industrial symbiosis and desalination.
- Treatment stations: These stations receive wastewater from industries and utilize advanced technology to treat it for potential reuse.
- Public Water Network: This network provides conventional freshwater distribution, supplying the required water to industries.
- Desalination Stations: These entities extract seawater and process it to meet drinking water standards.

Furthermore, the model focuses on the exchanges between entities during each time period to fulfil the market demand. These exchanges are illustrated in Figure 2 and can be:

- Final product exchanges: Between industries and markets, where the firsts have to satisfy the demand of each market by supplying the final products. These interactions are represented in figure 2 by orange arrows.
- Water exchanges: From treatment stations, public water network, desalination stations to industries. Each industry decides which water source alternative is more useful to satisfy its water needs. In Figure 2, these exchanges are depicted by blue arrows. Solid blue arrows represent

confirmed flows, indicating that the exchange is certain to occur. This is the case for the resultant wastewater of each industry, as water as to undergo certain treatments either for discharge or reuse. Dotted blue arrows, on the other hand, represent potential exchanges, indicating that there is a possibility for flow to occur between the entities.

Acknowledging these entities and the potential exchanges between them, the flow of Figure 2 can be analysed as follows. Two markets, Market A and Market B, have specific demands that must be met. In order to meet the demand of Market A, Industry A requires water for the production of its final product. This water can be sourced from three different options, indicated by the blue dotted arrows. Additionally, the production process generates wastewater, which is then directed to Treatment Station A for treatment. The treated water can be reused within Industry A (self-reuse) or shared with other industries (symbiotic approach). Similarly, Industry B aims to fulfil the demand of Market B and can choose to source water from Treatment Station A, the public network, or the desalination station, or a combination of these sources. Wastewater generated by Industry B is directed to Treatment Station B for further treatment. Once more, after this, the treated water can be reused within Industry B (self-reuse) or shared with other industries (symbiotic approach). Figure 2 provides only a partial representation of the network, as there are more entities to be included. The problem can involve multiple interactions, with water flowing in short loops or among various industries. Indeed, industries can receive water from diverse sources and supply water to numerous other industries.

For the purpose of this study, certain aspects of the product's manufacturing and distribution process were simplified. Specifically, considerations such as the geographical locations of markets, distances to industries, and inventory levels were deemed irrelevant to the paper's objectives since the focus is water flows, which would not be affected by any of these factors, hence not impacting the decision-making process or the conclusions drawn. Additionally, in the model, the concept of water demand is approached by considering its disaggregation based on quality requirements. When companies report their water demand, it encompasses various water qualities necessary for different applications, as certain processes require higher water quality than others. Aggregating all demands into a single value is impractical because water of lower quality cannot meet the requirements of applications with higher quality standards. To address this, the model separates the demands based on quality to ensure that water of lower quality can only fulfil the needs of applications with lower quality requirements. Conversely, water of higher quality serves as a virtual substitute for fresh water and can fully satisfy the entire water demand of a factory. Moreover, each treatment station is assumed to have only one installed technology, even though it may be capable of producing multiple water qualities. At the same time, there can only be one type of quality exchanged between two industries. These two simplifications are done to avoid mixing different water qualities and ensure clarity in the exchange process between industries. Additionally, having a single treatment technology in each station simplifies the management and operation of the treatment process, reduces complexity, and facilitates decision-making regarding the water quality to be exchanged between industries.

The problem statement is summarized as follows:

Given:

- Location of industries
- Distance between entities
- Maximum flow capacity for public water supply, treatment, and desalination stations (in volume per time units)
- Maximum capacity of water flow between entities (in volume per time units)
- Maximum production capacity of each final product in each industry (in material per time units)
- Cost of building a water transportation structure (in currency units)
- Cost of using a certain treatment technology to treat wastewater (in currency units per volume units)
- Cost of the desalination process (in currency units per volume units)
- Cost of building a treatment station (in currency units)
- Cost of building a desalination station (in currency units)
- Price of fresh, desalted and treated water with a certain quality (in currency units per volume units)
- Market demand (in material units)
- Quantity of final product exported from each industry to each market (in material per time units)
- Amount of water necessary for each industry (in volume per time units)
- Bill of materials that expresses the quantity of wastewater generated per each unit of final product produced (in volume units per material units)
- Bill of materials that expresses the quantity of water necessary to produce each unit of final product (in volume units per material units)
- Minimal necessary quantity to accept a symbiotic partner (in volume units)
- Environmental impact characterization factors associated with the water flow transported (in distance units)
- Environmental impact characterization factors associated with the volume and type of water produced (in volume units)

Determine:

- Flow of water between public network, treatment stations, desalination stations and industries (in volume per time units)
- Connection between entities with water transfer of a certain quality
- Location of public water network supply
- Location of treatment station and technology installed
- Location of desalination station

So as to:

- Minimize unused water intake, as in fresh and sea water
- Minimize the network's costs
- Minimize the network's environmental impacts

3.2 Mathematical Formulation

3.2.1 Indices and sets

$i, j, d \in I$ Entities $I = I_{ind} \cup I_{mkt} \cup I_{pub} \cup I_{ts}$

	I_e	Industries
	I_{mk}	Markets
	I_p	Public Water Network
	I_{ts}	Treatment stations
	I_d	Desalination
$m, l \, \epsilon \, M$	Products$M = M_{ww} \cup M_{tw} \cup M_{pw} \cup M_{fp} \cup M_{inw}$	
	M_{ww}	Wastewater
	M_{tw}	Treated Water
	M_{pw}	Public Water
	M_{dw}	Desalted Water
	M_{fp}	Final products
	M_{inw}	Water entering an entity
$k \, \epsilon \, K$	Treatment technologies	
$q, c \, \epsilon \, Q$	Quality of the water	
$t \epsilon \, T$	Time periods	
$g \, \epsilon \, G$	Environmental midpoint categories	

U Allowed entity-entity connections $U = \{(i, j): i, j \, \epsilon \, I\}$

For the description of this subset please consider the following:

U^{em}	Connection between industry and market
U^{et}	Connection between industry and treatment station
U^{te}	Connection between treatment station and industry
U^{pe}	Connection between public water network industry
U^{de}	Connection between desalination station and industry

V Allowed product-entity connections $V = \{(m, i): m \, \epsilon \, M \ \wedge \ i \, \epsilon \, I\}$

For the description of this subset please consider the following:

V^{fpmk}	Connection between final product and market
V^{fpe}	Connection between final product and industry

V^{wwts}	Connection between wastewater and treatment station
V^{inwe}	Connection between water entering an industry

R Allowed water quality-entity connections $R = \{(q,i): q \in Q \ \wedge \ i \in I\}$

R^{eq}	Connection between industry and wastewater quality

B Allowed entity-technology connections $B = \{(i,k): i \in I \ \wedge \ k \in K\}$

H Allowed technology-quality connections $H = \{(k,q): k \in K \ \wedge \ q \in Q\}$

F Allowed flows of materials between entities connection $F = \{(m,i,j): (m,i) \in V \wedge (i,j) \in U\}$

For the description of this subset please consider the following:

F^{fpINmk}	Final product that enters a market coming from an industry
F^{fpOUTe}	Final product that comes from an industry and enters a market
F^{wwOUTe}	Wastewater that comes from an entity into a treatment station
F^{wwINts}	Wastewater entering a treatment station coming from an industry
F^{twINe}	Treated water that enters an industry from a treatment station
F^{pwINe}	Public water that enters an industry from the public network
F^{dwINe}	Desalted water that enters an industry from a desalination station

A Allowed flows of water qualities between entities connection $A = \{(q,i,j): (q,i) \in G \wedge (i,j) \in U\}$

For the description of this subset please consider the following:

$A^{qOUTtsINe}$	Quality of the water leaving the treatment station and entering an industry, if matched with its quality requirement
$A^{qOUTpINe}$	Quality of the water leaving the public network and entering an industry, if matched with its quality requirement
$A^{qOUTdINe}$	Quality of the water leaving the desalination station and entering an industry, if fit with its quality requirement
A^{qConv}	Quality conversion from water quality entering the treatment station and water quality leaving treatment station, and matching with water quality requirements from receiving industry

N Allowed qualities in entities and technologies

$N = \{(q,i,k): (q,i) \in G \wedge (k,q) \in H\}$

For the description of this subset please consider the following:

$N^{qStaTech}$	Quality of the water entering the treatment station and appropriate technology to treat such quality

S	Allowed

$$S = \{(q,k,i,j): (k,i)\epsilon B \wedge (k,q)\epsilon\ H \wedge (q,i,j)\ \epsilon\ A\}$$

For the description of this subset please consider the following:

$S^{qOUTTech}$	Quality resultant from treatment with technology installed in a treatment station with possible transfer to an industry, if matching quality requirements

3.2.2 Parameters

Distances

$dist_{i,j}$	Distance between entities i and j (km)

Capacities

$capEnt_{i,t}^{max}$	Maximum flow capacity for entity i in period t (volume per time units)
$capTransp_{i,j,t}^{max}$	Maximum capacity of transport between entities i and j in period t (volume per time units)
$capProd_{m,i,t}^{max}$	Maximum production capacity of final product m in each entity i in period t (material per time units)

Costs

$cPipe$	Cost of building a pipeline (per km) (currency units)
$cTech_k$	Cost of using technology k to treat wastewater (per material units) (currency units)
$cDesal_i$	Cost of desalting water in desalination station i (per material units) (currency units)
$cBldTreat_i$	Cost of building a treatment station i (currency units)
$cBldDesal_i$	Cost of building a desalination station i (currency units)

Prices

$priceFresh_{q,t}$	Price of freshwater with quality q on period t (currency per time units)
$priceDesal_{q,t}$	Price of desalted water with quality q on period t (currency per time units)
$priceTreat_{q,t}$	Price of treated water with quality q on period t (currency per time units)

Product Related

$dmd_{m,i,t}$	Demand of product m from market i in period t (material per time units)
$Qfp_{m,i,j,t}$	Amount of final product m exported from industry i to market j in time period t (material per time units)
$WaterDmd_{m,i,t}$	Amount of water m entering entity i in time period t (volume per time units)
$WaterDmdQlt_{m,i,q,t}$	Water demand of entity i of quality q in time period t (volume per time units)
$BOM_{m,l}^{ww}$	Bill of materials that expresses the quantity of wastewater generated per each unit of final product produced
$BOM_{m,l}^{wfp}$	Bill of materials that expresses the quantity of water necessary to produce each unit of final product
$BOM_{m,l}^{wq}$	Bill of materials that expresses the quantity of water of quality q necessary to produce each unit of final product
$BOM_{q,c,k}^{conv}$	Bill of materials that expresses the conversion of water from quality q to quality c with technology k
$MinQty_{i,j,t}$	Minimum quantity of treated water for which industry j accepts a symbiotic industry partner I (volume per time units)

Environmental

$envTranspInf_g$	Characterization factor (per km) for environmental impact of transportation infrastructure in midpoint category g
$envWaterProdEnt_{g,i}$	Characterization factor (per m3) for environmental impact of water production in entity i in midpoint category g
$NormFactor_g$	Normalization factor for each midpoint category

3.2.3 Decision variables

Continuous non-negative variables

$x_{m,i,j,q,t}$	Flow of water m from entity i to entity j with quality q in time period t (volume per time units)

Binary variables

$y_{i,j,q}$	Defines if entity i is connected with entity j with transfer of water with quality q
$z_{k,i,j,q}$	Defines if entity i is connected with entity j with transfer of water with quality q treated with technology k

$Open_i$	Defines if treatment station i is installed
$Desal_i$	Defines if desalination station i is installed

Auxiliary variables at objective functions

$WaterPureIntake$	Total amount of pure/unused water sourced (fresh and salted water)
$WaterPublic$	Total amount of water obtained from public water network
$WaterDesal$	Total amount of water obtained from desalination
$TotalCostNetwork$	Total cost of the complete network
$CostSender_i$	Costs incurred by each sender entity
$CostReceiver_i$	Costs incurred by each receiving entity
$BldCost_i$	Total Cost of building each wastewater Treatment Station
$BldCostDesal_i$	Total Cost of building each Desalination Station
$TreatCostIS_{i,j}$	Total Cost of treatment each treatment station incurs in
$TreatCostDesal_{i,j}$	Total Cost of treatment each desalination station incurs in
$TranspCostIS_{i,j}$	Total Transportation Costs between entities i and j in IS context
$TranspCostDesal_{i,j}$	Total Transportation Costs between entities i and j in desalination context
$TranspCostPublic_{i,j}$	Total Transportation Costs between entities i and j in public network context
$soldReuse_i$	Financial gain from selling treated water
$BuyReuse_i$	Cost of buying treated water
$BuyFresh_i$	Cost of buying public water
$BuyDesal_i$	Cost of buying desalted water
$TotalEnvImp$	Final environmental impact indicator
$EnvImpTranspInf_g$	Environmental impact of transport by midpoint category
$EnvImpWaterProdEnt_{g,i}$	Environmental impact of producing water resorting to entity i by midpoint category
$EnvImpPerCateg_g$	Environmental impact of the final network by midpoint category

3.2.4 Constraints

Auxiliary equations: Defining parameters based on other parameters

Demand and final products' quantity: This equation defines that the quantity of final product produced in all industries is equal to the demand of each market, in each time period.

$$\sum_{i:(m,i,j)\in F^{fpINmk}} Qfp_{m,i,j,t} = dmd_{m,j,t} \quad \forall\, t \in T, (m,j) \in V^{fpmk} \tag{A}$$

Water Demand in total and per quality: These equations define the total quantity of water *m* necessary by each industry *i* in each time period *t* to guarantee the production of final product *l*. Equation C separates this total water demand by qualities, since not all water can be used for the same applications. The separation of these two parameters is justified by linearization aspects concerning the GAMS software. Their application is clarified in constraints 13 and 14.

$$\sum_{(l,j):(l,i,j)\in F^{fpOUTe}} Qfp_{l,i,j,t} * BOM_{m,l}^{wfp} = WaterDmd_{m,i,t} \quad \forall\, t \in T, (m,i) \in V^{inwe} \tag{B}$$

$$\sum_{(l,j):(l,i,j)\in F^{fpOUTe}} Qfp_{l,i,j,t} * BOM_{m,l}^{wq} = WaterDmdQlt_{m,i,q,t} \quad \forall\, t \in T, (m,i) \in V^{inwe}, q \in Q \tag{C}$$

Water Related Constraints

Wastewater generation: Using the bill of materials that quantifies wastewater generation for each final product, this constraint helps calculate the volume of wastewater *m* with a specific quality *q* generated during the production of the final product *l*.

$$\sum_{(l,d):(l,i,d)\in F^{fpOUTe}} Qfp_{l,i,d,t} * BOM_{m,l}^{ww} = x_{m,i,j,q,t} \quad \forall\, t \in T, (m,i,j) \in F^{wwOUTe}, (q,i) \in R^{eq} \tag{1}$$

Conversion of wastewater to treated water: This constraint expresses the conversion of water from quality *q* into quality *c*. It shows that the total amount of treated water *l* from quality *c* originated in treatment station *i* that follows to industries *j* has to be lower or equal than the total amount of wastewater *m* of quality *q* coming into that treatment station resultant from all industries *d*.

$$\sum_{(l,j):(l,i,j)\in F^{twINe}} \sum_{c:(q,c,i,j)\in A^{qConv}} x_{l,i,j,c,t} * BOM_{q,c,k}^{conv} \le \sum_{d:(m,d,i)\in F^{wwINts}} x_{m,d,i,q,t}$$

$$\forall\, t \in T, (i,q,k) \in N^{qStaTech}, (m,i) \in V^{wwts} \tag{2}$$

Threshold of water exchange: This constraint ensures that the quantity of water transferred between entities *i* and *j* respects the minimum quantity for which entity *j* accepts establishing a symbiotic relationship.

$$x_{m,i,j,q,t} \ge MinQty_{i,j,t} * y_{i,j,q} \quad \forall\, t \in T, (q,i,j) \in A^{qOUTtsINe}, (m,i,j) \in F^{twINe} \tag{3}$$

General Constraints

Limiting technologies: This constraint guarantees there is at most one technology *k* installed in each treatment station *i*, regardless of the number of industries it is connected with.

$$\sum_{(q,k):(q,k,i,j)\in S^{qOUTTech}} z_{k,i,j,q} \le 1 \quad \forall\, t \in T, (i,j) \in U^{te} \tag{4}$$

Limiting quality: These constraints assure there is at most only one quality water transfer between entities i an j.

$$\sum_{(q):(q,i,j)\in A^{qOUTtsINe}} y_{i,j,q} \leq 1 \quad \forall\, t \in T, (i,j) \in U^{te} \quad (5)$$

$$\sum_{(q):(q,i,j)\in A^{qOUTpINe}} y_{i,j,q} \leq 1 \quad \forall\, t \in T, (i,j) \in U^{pe} \quad (6)$$

$$\sum_{(q):(q,i,j)\in A^{qOUTdINe}} y_{i,j,q} \leq 1 \quad \forall\, t \in T, (i,j) \in U^{de} \quad (7)$$

Binary variables relationship: These constraints guarantee each binary variable assumes the correct value allowed by the relationship with other variables defined. That is, guarantee the interdependencies that exist in the problem domain are captured.

$$\sum_{k:(q,k,i,j)\in S^{qOUTTech}} z_{k,i,j,q} \leq y_{i,j,q} \quad \forall\, (q,i,j) \in A^{qOUTtsINe} \quad (8)$$

$$\sum_{k:(q,k,i,j)\in S^{qOUTTech}} z_{k,i,j,q} \geq y_{i,j,q} \quad \forall\, (q,i,j) \in A^{qOUTtsINe} \quad (9)$$

$$Open_i \leq \sum_{(q,k,j):(q,k,i,j)\in S^{qOUTTech}} z_{k,i,j,q} \;\forall\, i \in I_{ts} \quad (10)$$

$$Desal_i \leq \sum_{(j,q):(i,j,q)\in A^{qOUTdINe}} y_{i,j,q} \;\forall\, i \in I_d \quad (11)$$

$$y_{i,j,q} \leq x_{m,i,j,q,t} \quad \forall\, t \in T, (m,i,j) \in F^{pwINe}, (q,i,j) \in A^{qOUTpINe} \qquad (12)$$

Satisfying the necessity of water, in total and by quality: Constraint 13, in accordance with equation B, assures all water flows *l* entering industry *j* are the necessary amount to satisfy the water demand *m* of that industry. While constraint 14 establishes that the amount of water that enters each industry *j* must be lower or equal to the demand for its quality q. The combination of these constraints ensures that there is no excess of water entering industry *j*, even though the sum of both quality demands leads to an inflated value that exceeds the actual demand. This because the higher quality water can meet the totality of the demand, and the lower water quality can only address a portion of it. Consequently, the industry will either meet its entire demand, resorting only to high quality water that can be used for all applications, or solely satisfy the demand for low quality water using water of lower quality, while relying on higher quality water for the remaining demand. Therefore, the conjugation of both constraints is essential to ensure the exact satisfaction of the water demand.

$$\sum_{(l):(l,i,j)\in F^{twINe}} \sum_{(q,i):(q,i,j)\in A^{qOUTtsINe}} x_{l,i,j,q,t} + \sum_{(l,d):(l,d,j)\in F^{pwINe}} \sum_{(q):(q,d,j)\in A^{qOUTpINe}} x_{l,d,j,q,t}$$

$$+ \sum_{(l,d):(l,d,j)\in F^{dwINe}} \sum_{(q):(q,d,j)\in A^{qOUTdINe}} x_{l,d,j,q,t} = WaterDmd_{m,j,t} \quad \forall\, t \in T, (m,j) \in V^{inwe} \qquad (13)$$

$$\sum_{(l):(l,i,j)\in F^{twINe}} \sum_{(i):(q,i,j)\in A^{qOUTtsINe}} x_{l,i,j,q,t} + \sum_{(l,d):(l,d,j)\in F^{pwINe}} x_{l,d,j,q,t} + \sum_{(l,d):(l,d,j)\in F^{dwINe}} x_{l,d,j,q,t}$$

$$\leq WaterDmdQlt_{m,j,q,t} \quad \forall\, t \in T, (m,j) \in V^{inwe}, q \in Q \qquad (14)$$

Capacity Constraints

Entity capacity: These constraints guarantee that if a treatment station/public water network/desalination station is being used as a source of water, then the volume that is supplied by the facility cannot exceed its maximum capacity for each time period.

$$\sum_{(m,j):(m,i,j)\in F^{twINe}} \sum_{q:(q,i,j)\in A^{qOUTtsINe}} x_{m,i,j,q,t} \leq capEnt_{i,t}^{max} * Open_i \forall\, t \in T, i \in I_{ts} \qquad (15)$$

$$\sum_{(m,j):(m,i,j)\in F^{pwINe}} \sum_{q:(q,i,j)\in A^{qOUTpINe}} x_{m,i,j,q,t} \leq capEnt_{i,t}^{max} * y_{i,j,q} \quad \forall\, t \in T, i \in I_p \qquad (16)$$

$$\sum_{(m,j):(m,i,j)\in F^{dwINe}} \sum_{q:(q,i,j)\in A^{qOUTdINe}} x_{m,i,j,q,t} \leq capEnt_{i,t}^{max} * Desal_i \quad \forall\, t \in T, i \in I_d \qquad (17)$$

Pipeline volume capacity: These constraints define that the amount of water *m* of quality *q* transported between entities *i* and *j* in period *t* must be lower or equal than the maximum transport capacity allowed. Constraint 18 regards the transportation between treatment station *i* and the receiving industry *j*, constraint 19 for the flow sourced from the public network, and constraint 20 from the desalination stations.

$$x_{m,i,j,q,t} \leq capTransp_{i,j,t}^{max} * y_{i,j,q} \quad \forall\, t \in T, (q,i,j) \in A^{qOUTtsINe}, (m,i,j) \in F^{twINe} \qquad (18)$$

$$x_{m,i,j,q,t} \leq capTransp_{i,j,t}^{max} * y_{i,j,q} \quad \forall\, t \in T, (q,i,j) \in A^{qOUTpINe}, (m,i,j) \in F^{pwINe} \qquad (19)$$

$$x_{m,i,j,q,t} \leq capTransp_{i,j,t}^{max} * y_{i,j,q} \quad \forall\, t \in T, (q,i,j) \in A^{qOUTdINe}, (m,i,j) \in F^{dwINe} \qquad (20)$$

Production capacity: This constraint ensures that the total amount of final product produced in each industry *i* does not exceed the production capacity of that same entity.

$$\sum_{(l,j):(l,i,j)\in F^{fpOUTe}} Qfp_{l,i,j,t} \leq \sum_{l:(l,i)\in V^{fpmk}} capProd_{l,i,t}^{max} \quad \forall\, t \in T, i \in I_e \qquad (21)$$

3.2.5 Objective Functions

Freshwater and Seawater Intake Objective Function

The main objective of the problem is to minimize water consumption, namely concerning the extraction of raw water from nature, in the form of fresh and sea water. By minimizing the sum of these two potential sources, the objective function allows the model to maximize the quantity of reused water circulating between industries, therefore alleviating the pressure of extracting water from nature. Constraint 22 shows the minimization of this sum, being complemented by equations 23 and 24 that provide a definition for each of the individual components of said summation.

$$\min Freshwater\ and\ Seawater\ Intake = WaterPublic + WaterDesal \qquad (22)$$

Public Water Definition: Given by the sum of all water sourced from the public water network.

$$\sum_{(m,i,j):(m,i,j)\in F^{pwINe}} \sum_{q:(q,i,j)\in A^{qOUTpINe}} \sum_{t\in T} x_{m,i,j,q,t} = WaterPublic \quad (23)$$

Desalted Water Definition: Given by the sum of all water sourced from a desalination plant.

$$\sum_{(m,i,j):(m,i,j)\in F^{dwINe}} \sum_{q:(q,i,j)\in A^{qOUTdINe}} \sum_{t\in T} x_{m,i,j,q,t} = WaterDesal \quad (24)$$

Total Costs Objective Function

To capture the economic impact of the network, the costs were minimized. As mentioned in section 2.5, most of the articles reviewed in the existing literature also adopt this strategy, focusing on costs related with infrastructure, treatment and the price of water itself. However, this work takes an additional step by introducing a cost allocation structure, where all the entities involved in a water exchange divide the costs associated with it, categorizing the formulation into ‘sender’ and ‘receiver’ costs. This is relevant because the study includes industrial symbiosis, where there is a mutually benefit when industries engage in an exchange. This differentiation proves especially significant in the context of industrial symbiosis, where mutual benefits arise through a water exchange. In the same way as benefits are shared between the participating entities, the incurred costs should also be fairly distributed. Due to linearization considerations, the building costs were not incorporated directly into this division structure, rather they were added separately to the overall amount.

The cost minimization can be seen in constraint 25, followed by equations 26 to 38 that detail each cost component.

$$\min TotalCostNetwork = \sum_{i \in I_{ts}} CostSender_i + \sum_{j \in I_e} CostReceiver_j$$

$$+ \sum_{i \in I_{ts}} BldCost_i + \sum_{i \in I_d} BldCostDesal_i \qquad (25)$$

Costs incurred by the sender: The sender is seen as the entity where water is sourced from. If there is a symbiotic relationship between entities, the expenses of establishing that connection must be equally divided between the sender industry and the receiving industry, since both parties have gains and costs. In this case, the cost structure is composed by half the treatment and transportation costs, only when regarding industrial symbiosis. For the public network and desalination, the structure is often different since the role of the ‘sender entity’ does not fall under the industries’ responsibility, they are only perceived as receivers. In the case of the public network, the responsibility for ensuring the general water supply for the various domestic or industrial purposes falls upon governmental bodies or state-owned companies. Consequently, they assume the role of sender entities, while industries function solely as recipients. Similarly, in desalination projects, the majority of facilities are established through government investments or by private enterprises, not often by industrial entities. Once again, industries predominantly assume the role of recipients, not senders. For these reasons, it is not pertinent to separate costs associated with the public network and desalination into 'sender' and 'receiver' categories since the focus of this study is exclusively the costs incurred by industries, which are attributed entirely to the receiver's portion of costs.

Moreover, since it is an economic gain, the parcel that represents the revenue obtained by the sender when selling treated water to another industry is subtracted from the formula.

$$CostSender_i = \sum_{(m,j):(m,i,j) \in F^{twINe}} (TreatCostIS_{i,j} + TranspCostIS_{i,j})/2 \; - \; soldReuse_i \quad \forall \; i \in I_{ts} \qquad (26)$$

- Treatment Costs for Industrial Symbiosis: The treatment costs for this alternative are calculated multiplying the water volume exchanged between each treatment station *i* and industry *j* by the operational cost of using technology *k* to treat wastewater.

$$TreatCostIS_{i,j} = \sum_{k:(q,k)\in S^{qOUTTech}} \sum_{m:(m,i,j)\in F^{twINe}} \sum_{t\in T} cTech_k * x_{m,i,j,q,t} \quad \forall\, (i,j) \in U^{te} \quad (27)$$

- Transportation Costs for Industrial Symbiosis: These transportation costs are calculated by multiplying the cost of building the pipeline structure between treatment station *i* and industry *j* by the distance between those entities, if there is a connection between them.

$$TranspCostIS_{i,j} = \sum_{q:(q,i,j)\in A^{qOUTpINe}} cPipe * dist_{i,j} * y_{i,j,q} \; \forall\, (i,j) \in U^{te} \; (28)$$

- Financial gain from selling treated water: In the perspective of the sender, there are financial benefits of selling its treated wastewater to another industry. These gains depend on the price of such water and the quantity exchanged between the treatment station *i* and all industries *j*.

$$soldReuse_i = \sum_{(m):(m,i,j)\in F^{pwINe}} \sum_{(q,j):(q,i,j)\in A^{qOUTpINe}} \sum_{t\in T} x_{m,i,j,q,t} * priceTreat_{q,t} \quad \forall\, i \in I_{ts} \; (29)$$

Costs incurred by the receiver: These costs represent the counterpart of the costs incurred by the sender, as previously mentioned. They cover the costs of treatment and transportation. In the case of symbiosis, the costs are shared among the industries involved, while for desalination and the public network, the industries bear the costs individually. Furthermore, each industry is required to pay a fee to access water from either of these alternatives, represented by the three last parameters in the equation.

$$\begin{gathered} CostReceiver_i = \sum_{(m,i):(m,i,j)\in F^{twINe}} (TreatCostIS_{i,j} + TranspCostIS_{i,j})/2 \\ + \sum_{(m,i):(m,i,j)\in F^{dwINe}} (TreatCostDesal_{i,j} + TranspCostDesal_{i,j}) \\ + \sum_{(m,i):(m,i,j)\in F^{pwINe}} TranspCostPublic_{i,j} + BuyReuse_j + BuyFresh_j + BuyDesal_j \quad \forall\, j \in I_e \quad (30) \end{gathered}$$

- Treatment Costs for Desalination network: These costs are given by the product between the volume of water treated and the expense of treating salted water into admissible conditions.

$$TreatCostDesal_{i,j} = \sum_{(m):(m,i,j)\in F^{dwINe}} \sum_{q:(q,i,j)\in A^{qOUTdINe}} \sum_{t\in T} cDesal_i * x_{m,i,j,q,t} \quad \forall\, (i,j) \in U^{de} \; (31)$$

- Transportation Costs for Desalination network and Public network: These costs are calculated multiplying the cost of building the pipeline structure by the distance between entities, if there is a connection between those entities.

$$TranspCostDesal_{i,j} = \sum_{q:(q,i,j)\in A^{qOUTdINe}} cPipe * dist_{i,j} * y_{i,j,q} \; \forall\, (i,j) \in U^{de} \; (32)$$

$$TranspCostPublic_{i,j} = \sum_{q:(q,i,j)\in A^{qOUTpINe}} cPipe * dist_{i,j} * y_{i,j,q} \; \forall\, (i,j) \in U^{pe} \; (33)$$

- Cost of buying treated, desalted, and fresh water: These constraints establish the cost each entity has to incur in to access treated water, desalted water or fresh water, respectively.

$$BuyReuse_j = \sum_{(m):(m,i,j)\in F^{twINe}} \sum_{(q,i):(q,i,j)\in A^{qOUTtsINe}} \sum_{t\in T} x_{m,i,j,q,t} * priceTreat_{q,t} \quad \forall j \in I_e \; (34)$$

$$BuyDesal_j = \sum_{(m):(m,i,j)\in F^{dwINe}} \sum_{(q,i):(q,i,j)\in A^{qOUTdINe}} \sum_{t\in T} x_{m,i,j,q,t} * priceDesal_{q,t} \quad \forall j \in I_e \; (35)$$

$$BuyFresh_j = \sum_{(m):(m,i,j)\in F^{pwINe}} \sum_{(q,i):(q,i,j)\in A^{qOUTpINe}} \sum_{t\in T} x_{m,i,j,q,t} * priceFresh_{q,t} \quad \forall j \in I_e \; (36)$$

Building Costs: Costs of building treatment station and/or desalination plants, if installed, represented by the parameters $Open_i$ and $Desal_i$, respectively.

$$BldCost_i = cBldTreat_i * Open_i \quad \forall i \in I_{ts} \quad (37)$$

$$BldCostDesal_i = cBldDesal_i * Desal_i \quad \forall i \in I_d \quad (38)$$

Environmental Impact Objective Function

The environmental performance of the network is evaluated by minimizing the overall environmental impact associated with the activities conducted within the network, as presented in constraint 39. This is achieved by multiplying the normalization factor of each midpoint category by the environmental impact each alternative, which is specified in constraints 40 to 42.

$$\min TotalEnvImp = \sum_{g \in G} NormFactor_g * EnvImpPerCateg_g \quad (39)$$

Environmental Impact for each midpoint category: The midpoint category impact is divided into the impact of transportation and the impact of producing water by resorting to one of the alternatives.

$$EnvImpPerCateg_g = EnvImpTranspInf_g + \sum_{i \in I_p \cup I_{ts} \cup I_d} EnvImpWaterProdEnt_{g,i} \quad \forall g \in G \quad (40)$$

- Environmental impact of transport by midpoint category: The impact of transporting water through the whole water supply structure is obtained by multiplying the distance between entities *i* and *j* by the impact of the transportation infrastructure necessary to establish such connection.

$$EnvImpTranspInf_g = \sum_{(q,i,j):(q,i,j) \in A^{qOUTpINe} \cup A^{qOUTtsINe} \cup A^{qOUTdINe}} dist_{i,j} * y_{i,j,q} * envTranspInf_g \quad \forall g \in G \quad (41)$$

- Environmental impact of resorting to entity *i* by midpoint category: Incorporates the impact of all activities related with producing water by resorting to public network, industrial symbiosis and desalination options.

$$EnvImpWaterProdEnt_{g,i} = \sum_{(m,j):(m,i,j) \in F^{pwINe} \cup F^{twINe} \cup F^{dwINe}} \sum_{t \in T} \sum_{(q,i,j):(q,i,j) \in A^{qOUTpINe} \cup A^{qOUTtsINe} \cup A^{qOUTdINe}} x_{m,i,j,q,t} * envWaterProdEnt_{g,i}$$

$$\forall g \in G, i \in I_p \cup I_{ts} \cup I_d \quad (42)$$

4. Case Study Description

This chapter presents the case study conducted to validate and draw conclusions based on the developed model. The first section provides an overview of the current network. Subsequently, section 4.2 presents the different scenarios to be analysed in further sections.

4.1 Network characterization and data collection

This case study was particularly developed to create a practical application for the model developed, enabling the drawing of realistic conclusions that can answer to the research questions proposed. The study was conceived considering a tactical/strategic level, involving major industries with high water consumption, with the purpose of providing three different sources to satisfy their water necessity. This way, it refers to five different industries, with large water intakes: beverage industries, paper mills, refineries, breweries, and agriculture. For data collection purposes, five Portuguese companies were selected to represent each one of these businesses. The locations of their main plants were chosen to serve as proxies for their respective industry locations, based on the understanding that the main water demand and waste generation occur at these sites.

Nowadays, the water demand of these industries is primarily met through the use of the public water network. This choice is based on the source's high reliability and accessibility from multiple locations, making it the preferred water supply option. Indeed, there is an extensive network of freshwater supply stations distributed across the entire country, to the extent that both residences and industries can readily access a connection to the nearest supply station. This way, after checking the position of the existing freshwater supplies, the case study's public network locations selected were based on geographic proximity to each industry as to minimize costs and ensure the closest possible representation of real-world conditions.

However, the decreasing availability of freshwater has prompted industries to explore alternative sources, consequently, this case study presents two other alternatives: water industrial symbiosis and seawater desalination. Regarding the first option, the case study considers the need for a treatment station where the wastewater resultant from each industry can be treated for reuse. These stations were assumed to be located within each industry's plant in order to minimize logistical complexities and assure control and security. Additionally, the case study differentiates a treatment station for each industry instead of a centralized common station, in order to increase water recovery and assurance of the desired quality by preventing wastewater mixtures, which would complicate treatment and tracking of each industry's flow contribution (Li et al., 2022). With respect to the second option, the desalination station's location was considered in Portugal to align with the geographic scope of the companies involved in the case study. Currently, there is only an operational station in Portugal, but it is situated on an island, which is quite far from the companies under investigation. Nevertheless, there is a construction project in plan for a new station in the southern region of Portugal, specifically in Algarve, and is expected to initiate operations in a near future. While its exact location is not determined, for the purpose of this case study, it was assumed to be located near Lagos. Several prerequisites must be met when determining the location of a desalination station. These include proximity to seawater, closeness to both domestic and industrial users, consideration of the local topography, and even solar exposure, as many stations are adopting solar energy for sustainable operations (Dweiri et al., 2018). Therefore, while the selected location may appear distant from the industries in the case study, it has been studied by experts and considered strategically advantageous. However, it is worth noting that future work should incorporate an optimal approach for determining desalination station locations based on the specific industries involved and the requisite criteria.

This way, both the treatment stations and public network have five different locations, situated the closest possible to each industry, whilst the desalination station has a common position for all industries. The distribution of these entities is represented in Figure 3.

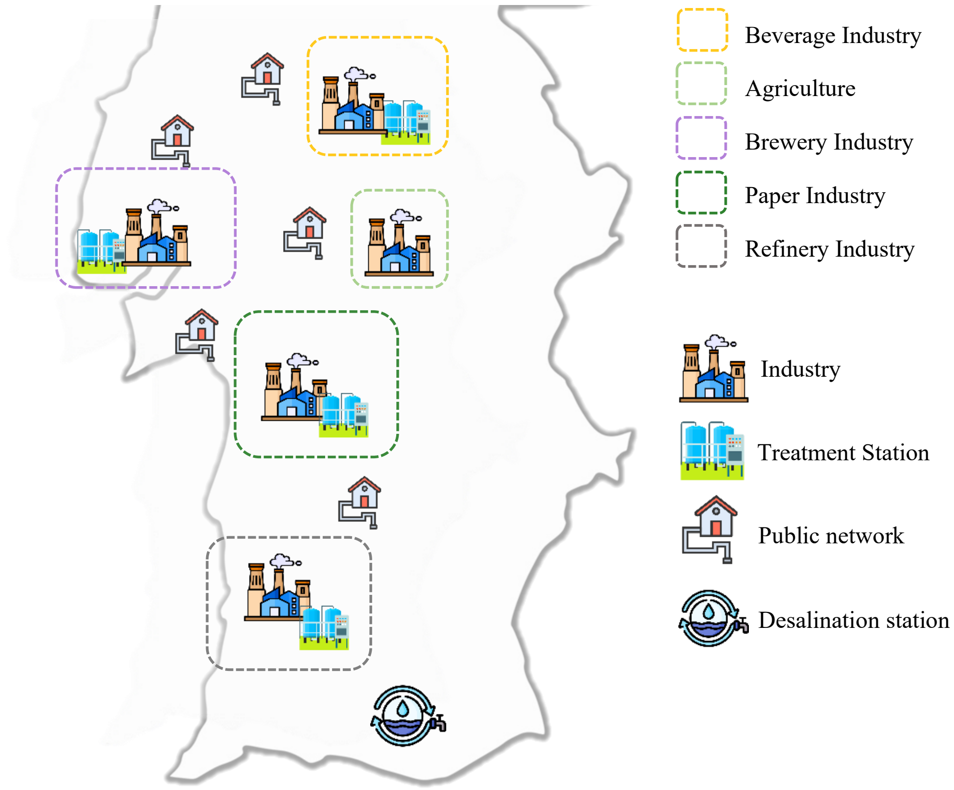


Figure 3 - Network configuration

4.1.1 Demand, Bills of Materials and Transportation

For each industry, there is a market with an external demand corresponding to their respective final products, namely Soft Drinks/Fruit Juice (measured in litres), Paper UWF (measured in tons), Oil (measured in barrels of oil equivalent), Beer (measured in hectolitres), and Rice (measured in tons), for the Beverage, Paper and Pulp Mill, Refinery, Brewery, and Rice cultivation industries. The data collected was derived from the demand observed during the years of 2019 to 2022. It considers a time span of ten years, with a recurring pattern that includes a 5% increase in demand every four years. This growth rate was determined based on the observed increase in demand for each industry between 2019 and 2022, which aligns with the average growth observed in the overall industrial sector. It is important to acknowledge that this approach has limitations as it includes the demand fluctuations caused by the pandemic and even though it accounts for demand increase, it still assumes a repeat of the same pattern, which is not likely. The 10-year time span allows a comprehensive assessment of the implemented network and its outcomes, providing sufficient duration to observe the long-term effects, dynamics and potential benefits.

All data utilised was gathered from publicly accessible online data, mostly from the companies' sustainability reports. However, despite efforts to select companies with accessible and reliable data, certain information remained challenging to obtain due to reasons of confidentiality. For example, there was a lack of reliable information regarding the market's demand for the rice cultivation, requiring calculations and estimations to obtain a representative value. On the other hand, the Soft Drink, Paper, Refinery and Brewery companies presented explicit information in their annual reports, resulting in values more trustworthy. The demand for each market and respective final product is presented in Table 2, together with the production capacity for each industries' plant. For the remaining time periods, the demand is presented in Table 30 of Appendix A.

Table 2 - Demand for each market in 2022 and production capacity of each industry

	Beverage	Paper	Refinery	Brewery	Agriculture
Market Demand	117 000 000	1 518 000	61 867 500	2 100 420	41 947
Production capacity	720 000 000	1 600 000	82 490 000	4 500 000	88 183
Units	L	ton	Barrel Oil Equivalent (BOE)	hL	ton

For each unit of product manufactured (FP), each factory requires a certain amount of water that can be represented by the bill of materials displayed in Table 3 concerning water necessity. On the other hand, there is also the generation of wastewater during the production of each final product, symbolized in the second half of Table 3. The corresponding volumes of water necessity and wastewater for the representative companies were extracted from their publicly accessible annual reports. Wastewater resultant from agricultural activities is not factored into this analysis, as it is not viable to collect and consequently treat for reuse. Therefore, this industry's role in a possible symbiotic relationship will always be as a receiver.

Table 3 - Bill of materials for total water necessity and wastewater generation

	FP Beverage	FP Paper	FP Refinery	FP Brewery	FP Agriculture	Units
Water Necessity	0.10134	0	0	0	0	m^3/L
	0	14.003	0	0	0	m^3/ton
	0	0	0.134	0	0	m^3/BOE
	0	0	0	0.31	0	m^3/hL
	0	0	0	0	410	m^3/ton
Wastewater generation	0.0335	0	0	0	-	m3/L
	0	11.7625	0	0	-	m3/ton
	0	0	0.0941	0	-	m3/BOE
	0	0	0	0.1088	-	m3/hL

As explained further in this chapter, the case study establishes a clear distinction between water of two qualities: Q5 and Q6. In a simplified matter, water of quality Q5 has the requisite purity to serve all industrial water needs effectively. On the other hand, quality Q6 denotes a lower standard, thereby limiting its suitability. In fact, water of this lower quality is only viable for approximately 60% of an industry's water applications, primarily those involving processes such as boiler feeds or cooling systems, where there is no direct contact with the final product (Al-Hazmi et al., 2023; Reddy et al., 2023). Therefore, the Q5 demand is the same as the one identified in Table 3, while the Q6 water demand accounts for 60% of those values.

To establish a meaningful and economically viable water exchange relationship between industries, a minimum threshold is set based on the water demand of each industry. For this study, it is assumed that in order for an industry to find it beneficial to receive water from another industry – thus sharing the costs associated with initiating the exchange – the received water must account for at least 5% of its total water demand. This value was an assumption with the intention of ensuring the water exchange is substantial enough to justify the costs associated with establishing and maintaining the symbiotic relationship between industries.

Alongside the establishment of industrial symbiosis, the case study also explores the potential for treating and reusing wastewater within individual industries. Although this concept is not technically included in the definition of industrial symbiosis, they are both concerning the reuse of water. Hence, for simplification purposes regarding model development and analysis, this case study aggregates self-reuse and water industrial symbiosis. Some industries have implemented treatment technologies to reuse their own wastewater, however, for most industries, it is not viable to solely rely on this water source. Therefore, to ensure a generic framework, the case study sets a limit on this self-reuse of water assuming that at most 40% of an industry's water necessities can be satisfied resorting to this source. This value is merely indicative, being necessary to explore it in future work. Nevertheless, this limitation can be explained by three reasons. First, in most cases the quantity of wastewater to be treated is not sufficient compared to an industry's water necessities. Secondly, not all industries have the necessary infrastructure and capabilities for self-reuse, and investing in such systems independently can be unaffordable. By allowing a significant portion of wastewater to be shared through symbiotic relationships, industries can share the costs associated with the treatment and transportation of the water to be reused between them, leading to a more reasonable situation. Moreover, the study aims to reduce freshwater intake across the country geographically. By restricting the quantity of self-reused water, it creates opportunities for larger symbiotic flows between industries and regions. This, in turn, promotes water exchange between regions with different levels of water scarcity. Industries located in regions with higher water stress can receive water from industries situated in regions with lower water stress, alleviating the extraction of freshwater from the more water-stressed regions. Overall, the case study's approach encourages water exchange and distribution, relieving freshwater withdrawals in high water stress regions.

To meet the water demand, it is necessary to assure a reliable transportation mode, especially when dealing with large quantities over long distances. The most used method for such transportation, and the one adopted for the case study, is pipeline, despite their high fixed cost. However, it is important to note that certain factors need to be carefully examined to determine the viability of this transportation mode within the specific case under consideration. The following simplifications have been made. Firstly, it is necessary to acknowledge that the study disregards the morphological and topographic characteristics of the terrain between the origin and destination points. Consequently, only the direct linear distance is considered, disregarding variations such as elevations, valleys, or bodies of water that may lie along the route. Secondly, the assessment focuses on basic materials and equipment commonly used for pipeline construction, being necessary to adapt and include other resources depending on the application. For example, adverse weather conditions may require protective coatings, and higher-pressure requisites may need water pumps. Similarly, the calculations pertaining to the flow rate and diameter of the pipes are approached in a simplified manner, focusing only on basic hydraulic formulas disregarding all the factors previously mentioned. By employing these formulas and considering standard pipeline measurements, such as a maximum velocity of 1.524 m/s and a diameter of 0.98m for PVC pipelines, the calculated flow capacity for each pipeline in the network amounts to 1.143 m^3 of water per second, equivalent to 35,812,800 m^3 per year (Bouhal et al., 2018; Westlake, 2021). The construction cost for these pipelines is estimated at 350,000€ per kilometre. The distances between the public network supply, the desalination and treatment stations to each industry are represented in Table 4.

Table 4 - Distance between each water possible source and receiving industry (km)

		Receiving Industries				
		Beverage	Paper	Refinery	Brewery	Agri
Public Network Supply for:	Beverage	8	-	-	-	-
	Paper	-	5	-	-	-
	Refinery	-	-	7.5	-	-
	Brewery	-	-	-	5	-
	Agriculture	-	-	-	-	17
Treatment Station of:	Beverage	-	83.32	141.4	53.04	29.91
	Paper	83.32	-	59.22	48.42	53.59
	Refinery	141.4	59.22	-	104.64	110
	Brewery	53.04	48.42	104.64	-	112
	Desalination Sta	236.32	154.92	95.77	202.44	204.55

4.1.2 Water treatment, quality and costs

Aside from the transportation, it is also necessary to evaluate the specifications related to each source alternative. Regarding the industrial symbiosis and water reuse alternative, there are many factors to consider. The study incorporates appropriate treatment methods for each wastewater type and considers the water quality achievable after treatment. The focus is on the viability of water industrial symbiosis at the tactical and strategic level, therefore water qualities are represented using the notation 'Q' followed by a number to indicate its type of quality, instead of detailing the chemical components and indicators present in each water. Wastewater qualities are represented from Q1 to Q4, corresponding to the origin of the wastewater from beverage, paper and pulp mill, refinery, and brewery industries, respectively. Again, there is no wastewater quality representation for agriculture since it cannot be collected for treatment and subsequent reuse. Each type of wastewater requires specific treatment processes to render it suitable for reuse and its potential applications depend on which treatment is undergone. The treatment typically follows a three-step sequence, encompassing primary treatment for the removal of suspended solids, secondary treatment to address dissolved organic matter, and tertiary treatment to purify water by eliminating remaining substances (Kesari et al., 2021). While these three steps form the foundation for water reuse across various industries, the differentiating factor lies primarily in the tertiary treatment phase. To simplify the incorporation of treatment techniques in the case study, only the final step is considered in terms of costs and produced water qualities. This simplification is also justified by the fact that most industries already undertake the necessary primary and secondary treatment steps before discharging their wastewater into the environment. Thus, the focus predominantly revolves around the tertiary treatment.

This way, the study considers the following technologies: Reverse Osmosis (K1), Nanofiltration with Reverse Osmosis (K2), Ultrafiltration followed by Reverse Osmosis (K3), Ultrafiltration (K4), and Activated Carbon along with Ion Exchange (K5). Intensive research has led to the conclusion that these techniques are not universally applicable for treating all types of wastewaters for the purpose of reuse, and each technology can generate varying water qualities (Eyvaz, 2019; Nidheesh et al., 2022; Sathya et al., 2022). In fact, some wastewaters can only achieve a certain level of purity after treated, while others can attain potable standards, depending on the treatment undergone. Consequently, the treated wastewater in this case study can assume two qualities, denoted as Q5 or Q6, depending on its intended reuse applications. Quality Q5 signifies water that practically meets potable standards and can be used essentially in all applications within the factory, the higher quality water previously mentioned. On the other hand, quality Q6 represents water suitable for limited applications, such as cooling systems and boiler feeds or other indirect-product related purposes, which do not demand such high-quality water. Notably, since Q5 represents water of higher quality that meets potable standards, it inherently includes the applications served by Q6. For instance, if water of Q6 quality can be utilized for cooling systems, Q5 water of superior quality can, naturally, also serve such purposes. However, the reverse is not true. This distinction becomes important when separating the water demand of each industry into Q5 and Q6 to ensure that the latter is not used in applications requiring higher water quality.

It is important to acknowledge that this case study is subject to several assumptions and simplifications. One of its limitations is the lack of specifications concerning the chemical considerations of water treatment and quality. Indeed, the combination of treatments and intended reuse applications will depend on various factors such as the characteristics of the wastewater, regulatory requirements, and water quality. This case study analysed this in a generic form, when for each specific case, a comprehensive analysis of the wastewater composition should be conducted as well as consultation with wastewater treatment experts to design an effective and accurate treatment system. This simplification can potentially affect the outcomes by implying that a particular wastewater type can be efficiently treated using a specific technology having a subsequent reuse application. However, in reality, the chemical composition of that wastewater might not align effectively with the chosen treatment technology, making it unsuitable for the designated reuse.

In summary, the wastewaters possible to treat with each treatment technology and resultant quality are represented in Table 5.

Table 5 - Treatment technology application to each industry and resulting water quality

Treatment Technology	Industries' Wastewater	Resultant Water Quality
K1	Beverage	Q6
	Brewery	Q5 or Q6
K2	Refinery	Q5 or Q6
	Beverage	Q5 or Q6
K3	Refinery	Q6
	Beverage	Q5 or Q6
K4	Paper	Q6
K5	Paper	Q6
	Refinery	Q6

As shown in Table 5, wastewater generated by the Paper industry can reach a maximum quality of Q6. This observation causes implications for the potential water cycle, since this quality can only be used to limited applications and can never meet the entire water demand of an industry, either itself or another. This because, at most, the Q6 quality can only be used in 60% of the water applications of each industry.

The wastewater treatment process is also subject to capacity limitations and associated costs. The determination of treatment station capacity is influenced by various factors and ultimately rests with the decision-maker. This way, the case study assumes a non-limiting capacity, adopting the same value as the previously determined transportation capacity, consequently adapting and calculating the infrastructure costs necessary to ensure this capacity.

The building costs of a treatment station are presented in Table 6. As mentioned earlier, most industries typically treat their wastewater before discharging it. However, for the sake of simplicity and to maintain a generic framework, this case study assumes that none of the five industries initially has treatment stations within their facilities. This approach aligns with common practices where wastewater treatment is often centralized and primarily designed for discharge purposes rather than direct reuse. It is also important to acknowledge that some industries may lack the infrastructure required for on-site treatment. Consequently, if the model's solution requires wastewater treatment, it is assumed that the respective industries will incur in those building costs.

Since only one technology can be installed per station, the costs are associated to each technology, even though they incorporate the average cost of the whole infrastructure construction of a treatment station. Seeing as there is few available information about the different costs of each technology, this value was assumed to be equivalent throughout all technology treatments.

Table 6 - Costs of treating wastewater with technology, station's building costs and capacity

	K1	K2	K3	K4	K5	Units
Treatment Cost	4.089	8.178	5.393	1.304	1.619	€/m^3
Building Cost	145 047 020	145 047 020	145 047 020	145 047 020	145 047 020	€
Capacity	35 812 800	35 812 800	35 812 800	35 812 800	35 812 800	m^3/year

The case study includes yet another possible water source: desalination. This option has been recognized as one of the oldest and most viable processes, being increasingly considered as an effective solution to meet the growing demand for high-quality freshwater (Gude, 2016). Given the relatively limited use of desalination as a water source in Portugal, the parameters for this process have been adapted from similar examples in Spain (Ortiz, 2022). The capacity of the desalination station is a key parameter, which serves as the basis for determining both the required infrastructure investment and the treatment cost. The treatment cost also takes into account factors such as energy consumption and associated costs. The values considered are showed in Table 7.

Table 7 - Cost of desalinating water, station's building costs and capacity

	Desalination Station	Units
Treatment Cost	1.12	€/ m^3
Building Cost	226 000 000	€
Capacity	80 000 000	m^3/year

The public network infrastructure is well-established and currently meeting the water demand of various users, including domestic and industrial consumers. Therefore, the infrastructure costs are neglected, as the network is already in place, and it is assumed there is no significant capacity limitations initially. This way, the primary cost component to account for in the public network is the price of freshwater for industrial users, which is presented in Table 8. This table also exhibits the water price for treated wastewater and desalted water, depending on the respective quality. Naturally, since water of quality Q5 is considered to be a suitable substitute for freshwater, it takes on a higher price.

Table 8 - Water pricing by quality for each water source alternative

	Quality Q5	Quality Q6	Units
Public Water Network	1.645	1.645	€/ m^3
Treated Wastewater	0.325	0.26	€/ m^3
Desalinated Water	0.475	0.475	€/ m^3

4.1.3 Environmental impacts

When considering the environmental impact of the three water source alternatives, it is important to identify the key activities that contribute to the overall environmental impact of the network. These activities include the producing and supply of water of a specific quality - including the extraction of seawater or freshwater, the energy, materials and infrastructure required for water treatment – and water transportation. The impact values were obtained using the Simapro software, resorting to the Ecoinvent library. The selection of references prioritized those specific to Europe, with a preference for references ending in "Cut-off, U" as they allow proper waste allocation. These references are depicted in Table 9.

Table 9 - References used for each alternative resorting to EcoInvent3 library in SimaPro

	EcoInvent Reference
Public	1 kg Tap water {Europe without Switzerland} | tap water production, conventional treatment | Cut-off, U 1 km Water supply network {GLO}| market for | Cut-off, U
Industrial Symbiosis	1 kg Tap water {Europe without Switzerland} | tap water production, ultrafiltration treatment | Cut-off, U 1 km Water supply network {GLO}| market for | Cut-off, U
Desalination	1 kg Tap water {GLO}| tap water production, seawater reverse osmosis, ultrafiltration pretreatment, enhance module, two stages | Cut-off, U 1 km Water supply network {GLO}| market for | Cut-off, U

After setting these references, the values for the environmental impact of each midpoint category were calculated using the ReCiPe2016 Midpoint (H) method, which is a globally recognized approach commonly used to assess environmental impacts across various midpoint categories (Huijbregts et al., 2017). For each alternative and for the most impacting activities, the values are presented in Table 10.

Table 10 - Midpoint impact category for producing and supplying water for each alternative (per m3) and for transporting water (per km)

Units	Impact category	Acronym	Public (per m^3)	IS (per m^3)	Desalination (per m^3)	Transport (per km)
kgCO2eq	Global warming	GW	2,7E-01	3,4E-01	2,4E+00	1,7E+05
kgCFC11eq	Stratospheric ozone depletion	OD	1,5E-07	3,1E-07	1,4E-05	6,3E-02
kBqCo-60eq	Ionizing radiation	IR	1,1E-01	1,0E-01	2,6E-01	5,3E+03
kgNOxeq	Ozone formation, Human health	OFH	5,6E-04	9,3E-04	4,9E-03	5,4E+02
kgPM2.5eq	Fine particulate matter formation	PMF	4,7E-04	6,0E-04	5,0E-03	3,4E+02
kgNOxeq	Ozone formation, Terrestrial ecosystems	OFT	5,6E-04	9,5E-04	5,0E-03	5,7E+02
kgSO2eq	Terrestrial acidification	TA	1,2E-03	1,5E-03	8,0E-03	5,5E+02
kgPeq	Freshwater eutrophication	FET	2,3E-04	2,3E-04	1,1E-03	6,2E+01
kgNeq	Marine eutrophication	MET	1,7E-05	1,7E-05	8,7E-05	1,4E+01
kg1,4-DCB	Terrestrial ecotoxicity	TE	6,6E-01	1,2E+00	4,4E+00	8,9E+05
kg1,4-DCB	Freshwater ecotoxicity	FE	1,6E-02	1,5E-02	1,5E-01	8,5E+03
kg1,4-DCB	Marine ecotoxicity	ME	2,1E-02	2,0E-02	1,8E-01	1,2E+04
kg1,4-DCB	Human carcinogenic toxicity	HCT	2,8E-02	1,8E-02	9,6E-02	1,6E+05
kg1,4-DCB	Human non-carcinogenic toxicity	HNCT	3,9E-01	5,2E-01	2,2E+00	2,1E+05
m2acropeq	Land use	LU	1,1E-02	1,0E-02	3,5E-02	2,6E+03
kgCueq	Mineral resource scarcity	MRS	1,8E-03	1,5E-03	4,3E-03	5,9E+03
kgoileq	Fossil resource scarcity	FRS	7,2E-02	9,5E-02	5,6E-01	4,2E+04
m3	Water consumption	WC	1,0E+00	1,0E+00	1,8E-02	6,3E+02

To ensure a comprehensive assessment of the overall environmental impact, it is important to standardize the values by using a normalization factor. This factor helps to bring all the impact values to a common unit of measurement, allowing for a meaningful comparison across different categories. In the SimaPro software, the normalization factor can be obtained specifically for the chosen assessment method, shown in Table 31 of Appendix A.

4.2 Scenarios under study

To analyse the case presented in section 4.1, three different scenarios were considered, each representing a different level of interaction between the entities involved. The scenarios are summarized in Figure 4.

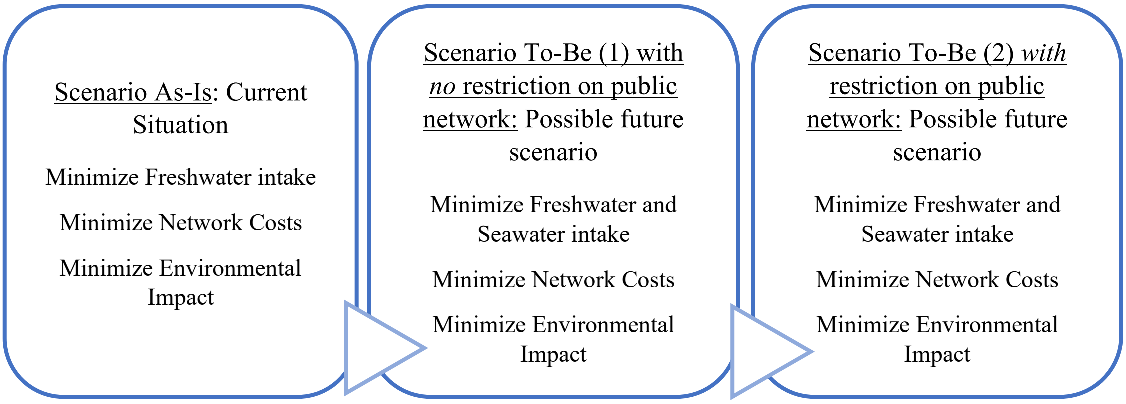


Figure 4 - Scenarios under analysis

The first scenario, known as the As-Is situation, focuses on evaluating the current network's functioning. In this scenario, the only available water sources are the public water network and the industry's self-reuse system.

The second scenario introduces two additional alternatives: industrial symbiosis and desalination. The objective in this scenario is to minimize the intake of pure water, which includes both freshwater from the public network and seawater from the desalination station.

The third scenario represents a realistic future network where industries have access to all three alternatives but face limitations on the public water network. This scenario accounts for potential water scarcity by considering a 40% reduction on the public network's capacity. The objective functions remain the same as in the second scenario, but the network needs to adapt to the reduced availability of freshwater due to the imposed restriction.

5. Case Study Results Analysis and Discussion

This chapter is structured as follows. In Section 5.1 the solution approach implementation is explained. Section 5.2 presents the results obtained from the model representing the current situation. Section 5.3 focuses on the results of the second scenario, which considers three different water source alternatives. In Section 5.3.1, the results of a sensitivity analysis to the critical parameters of the second scenario are presented to understand their impact on the established network. Section 5.4 analyses the results of a third scenario that includes capacity restrictions on the public water network supply, both in a single objective and multi-objective approach. Next, Section 5.5 examines the results of stochastic programming, specifically addressing demand uncertainty using a scenario-based approach. Finally, section 5.6 provides recommendations and an overview of the main takeaways of this chapter.

5.1 Solution implementation

The solution to the problem described in chapter 4 involved utilizing the mathematical model formulation presented in chapter 3 and implementing it using the GAMS software. The runs conducted throughout this dissertation were carried out using GAMS version 42.3 with CPLEX 20.1. running on an Intel (R) core (TM) i7-1260P CPU @ 2.10GHz with 16GB of RAM. The model developed in chapter 3 is a generic framework that requires adaptation for each specific scenario. For all scenarios examined, the model was tailored to each specific situation and executed using GAMS, considering all relevant entities, products, and connections within the network. Notably, for scenario 1 the model was simplified to exclude industrial symbiosis and desalination as possible water sources, as the main interest is to analyse the current situation.

For section 5.4, where the studied scenario includes a restriction to the public network capacity, it was necessary to integrate different individual objective functions and optimizing them simultaneously, which required the implementation of the method ϵ-constraint. In this study, a lexicographic approach is employed, in order to obtain a payoff table that represents the trade-offs between the different objectives (Mavrotas, 2009). To construct this table, the objective functions are optimised individually, starting with the prioritized objective function. Following that, the second objective is optimized while introducing a constraint to ensure the previously found optimal solution for the first objective is maintained. The process is repeated for the third objective function, where the optimal solution of the second objective is kept resorting to the addition of a constraint. This way, using the GAMS software, the results are obtained by iteratively optimizing each objective function individually and adding a constraint that preserves the previously obtained optimal solutions. This process is repeated for each objective function, resulting in a set of efficient solutions. From these solutions, it is possible to calculate the range between the maximum and minimum values for each objective. This range defines the interval within each intermediate solutions lies. The process is then repeated for each intermediate solution, where a constraint is added to preserve the value of the solution for the corresponding objective function while optimizing the remaining objectives. Finally, it is possible to obtain the set of Pareto solutions.

5.2 Scenario As-Is: Current Network

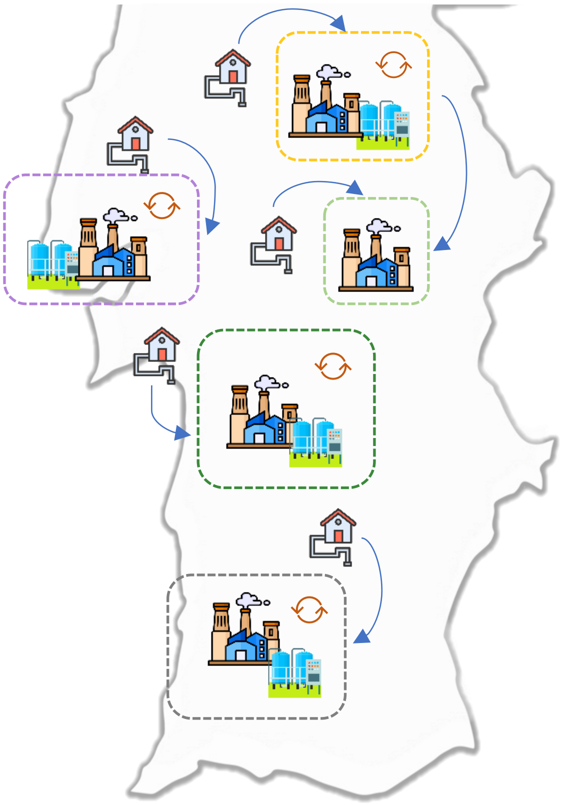
To establish a base scenario, the model previously described was adapted to exclude the industrial symbiosis and desalination alternatives. Furthermore, in the absence of symbiotic interactions between industries, the cost structure needs to be adjusted. In this case, the costs incurred by the sending and receiving industries are not separated, that is, there is no differentiation between these definitions since there is no industry sending water to another industry. The objective functions were all considered, as to facilitate the comparison with the more complex scenarios, with the necessary adjustments regarding the number of alternatives available. This way, the model was run three times: once to minimize freshwater intake, which consists of water supplied from the public network; another to minimize total costs; and a last one to minimize the environmental impacts associated with the production and usage of each water source type, as well as transportation. The results obtained for each objective function are presented in Table 11.

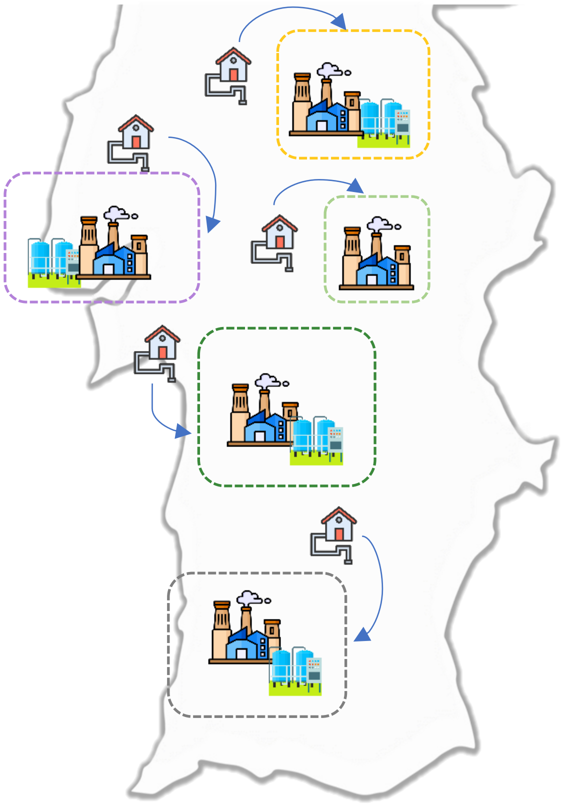
Table 11 - Results for current network with single objective

	Freshwater intake (m^3)	Total Cost (€)	Environmental Impact (Pts)
Case A: Minimize Freshwater Intake	**496 897 050**	1 616 294 773	33 974 186
Case B: Minimize Total Cost	608 638 081	**1 016 084 644**	34 286 447
Case C: Minimize Environmental Impact	496 897 050	1 616 294 773	**33 974 186**

The values situated in the diagonal of Table 11 show the best possible values, in this case the lowest, for each of the objective functions. Furthermore, the table reveals that the solution's values are consistent when minimizing freshwater intake and environmental impact (cases A and C). This aligns with expectations, as both objectives exhibit a similar trend: reducing freshwater consumption leads to a decrease in the environmental impacts associated with the network, and vice-versa. This finding is logical, since reusing water is environmentally preferable to extracting it from surface water sources, as there is less resource consumption.

Considering the priority of minimizing freshwater consumption in a water scarcity context, the solution presented in the first row of the table (Case A) will be the primary focus of the study. In Figure 5, the structure of the current network is presented for cases A and C, while case B is represented in Figure 6.





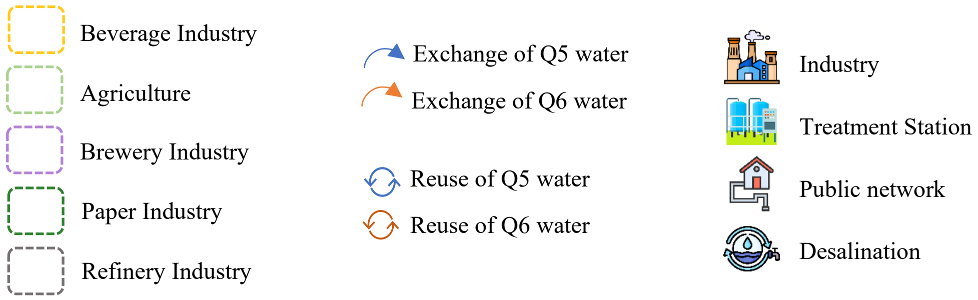


Figure 5 - Current network for Cases A and C

Figure 6 - Current network for Case B

In Figure 5, it can be observed that all industries are utilizing the public water network as their main source, which provides water of quality Q5. This is a logical choice as the public network is capable of meeting the water requirements for various applications within the industries. However, since the primary objective is to minimize freshwater intake, the industries are also treating and reusing their own water to supplement their water needs. This treated water is of the lower quality type, Q6, possibly due to the implementation of cost-effective treatment technologies. By relying on the public network for the majority of their water demand (Q5), the industries can allocate less expensive treatment technologies to meet the smaller portion of their water demand (Q6). This approach allows for a reduction in freshwater consumption while still satisfying the different water quality requirements within the industries.

The network design obtained in Figure 5, is exactly the same for the single objective of minimizing the environmental impact (Case C), which is again justified by the similar trend followed by both objectives. In contrast, the Case B network exhibits a slightly different pattern, as it can be observed in Figure 6. In this case, sourcing water solely from the public network is not only sufficient to meet the water demand but also the most cost-effective solution. Therefore, the model chooses to rely exclusively on the public network, disregarding the option of water reuse, resulting in no treatment station installation. This can be justified by the fact that the installation and operation of treatment stations, in order to obtain water for reuse purposes, naturally lead to cost incurrences. Since the main objective, in this case, is cost minimization, the model opts for the least expensive network, only sourcing water from the public network.

Regarding the cases A and C, Table 12 provides an overview of the water flow between entities in year 10, categorizing them based on their quality. It shows the amount of water reused by each industry, the water supplied by the public network, and the total water received by each industry. This last column represents the water necessity of each industry, therefore the values must correspond to the respective water demand, which must be fulfilled. The decision to focus on year 10 for presenting the flows is driven by the unique characteristics of the last scenario under consideration. By analysing the same time period across different scenarios, it allows for consistent and direct comparisons. Despite the variation of each period's water demand, and therefore water flow, the connections established between entities remain exactly the same throughout all time periods. This ensures that the flows exhibit similar patterns across different periods, with only varying values.

Table 12 - Flows of water (in m3) received by each industry from each possible source in year 10, in the current network, considering cases A and C. The colour range symbolises the sources responsible for sending more (green) or less (red) water to industries.

		From					
		Beverage	Paper	Refinery	Brewery	Public	Total Received
Beverage	Q5	-	-	-	-	1.27E+07	1.46E+07
	Q6	1.93E+06	-	-	-	-	
Paper	Q5	-	-	-	-	1.33E+07	2.00E+07
	Q6	-	6.72E+06	-	-		
Refinery	Q5	-	-	-	-	6.59E+06	9.16E+06
	Q6	-	-	2.57E+06	-		
Brewery	Q5	-	-	-	-	6.54E+05	7.61E+05
	Q6	-	-	-	1.07E+05		
Agriculture	Q5	-	-	-	-	1.90E+07	1.90E+07
Total Sent		1.93E+06	6.72E+06	2.57E+06	1.07E+05	5.21E+07	

Table 12 clearly illustrates the prominent role of the public network as the primary water supplier, being the entity with the highest amount of water sent. The paper industry stands out as the second largest water provider, justified by its substantial water consumption and subsequent wastewater generation that can be potentially reused. In contrast, the brewery industry, which requires and produces less water and wastewater, respectively, has lower opportunities for water reuse. Although the analysis focuses on year 10, when considering all time periods, the total water transferred from the public network to all industries amounts to 4.97E+08, which is 82% of the total water transfer. In contrast, the total amount of water reused by the industries is 1.12E+08 m^3, amounting to only 18%. This significant difference can be attributed to the model's restriction, which limits industries to reusing a maximum of 40% of their own wastewater. Consequently, the public network becomes the primary source for meeting the industries' significant water demand, highlighting the pressure on this water source.

In this case, only three treatment technologies are utilized: K1 (Reverse Osmosis), K4 (Ultrafiltration), and K5 (Activated Carbon with Ion Exchange). K1 is installed in both the beverage and brewery industries' treatment stations, producing water of quality Q6. The paper industry uses K4, while the refinery industry uses K5. The selection of these technologies is based on cost considerations, with industries choosing the most affordable options among the technologies allowed to treat their wastewater. In this case, since the desired treated water quality is Q6, the model had plenty of flexibility to choose from all available technologies possible, except for the brewery industry, which only has the option of using K1. Specifically, the beverage industry selects K1 as the cheapest technology among K1, K2 (Nanofiltration with Reverse Osmosis), and K3 (Ultrafiltration with Reverse Osmosis). The refinery industry, aiming for water of quality Q6, incurs lower costs by using K5 instead of K2 or K3. The paper industry has limited options but chooses the most cost-effective option, which is K4.

When considering the single objective of cost minimization (Case B), Table 13 displays the water flows observed in the current network. Comparing it to Table 11, which represents the other two single objectives, a notable difference is evident. Although the public network remains the primary water supplier, it also serves as the sole source in this case. Therefore, there is also no need to resort to treatment technologies.

Table 13 - Flows of water (in m3) received by each industry from each possible source in year 10, in the current network, considering Case B

			From					
			Beverage	Paper	Refinery	Brewery	Public	Total Received
To	Beverage	Q5	-	-	-	-	1.46E+07	1.46E+07
		Q6	-	-	-	-	-	
	Paper	Q5	-	-	-	-	2.00E+07	2.00E+07
		Q6	-	-	-	-		
	Refinery	Q5	-	-	-	-	9.16E+06	9.16E+06
		Q6	-	-	-	-		
	Brewery	Q5	-	-	-	-	7.61E+05	7.61E+05
		Q6	-	-	-	-		
	Agriculture	Q5	-	-	-	-	1.90E+07	1.90E+07
	Total Sent		-	-	-	-	6.35E+07	

In the current network, the cost structure is quite straightforward. Depending on the single objective, it can include the costs associated with building the treatment stations, the treatment processes using different technologies, and the transportation between entities. The cost distribution for each single objective is represented in Figure 7.

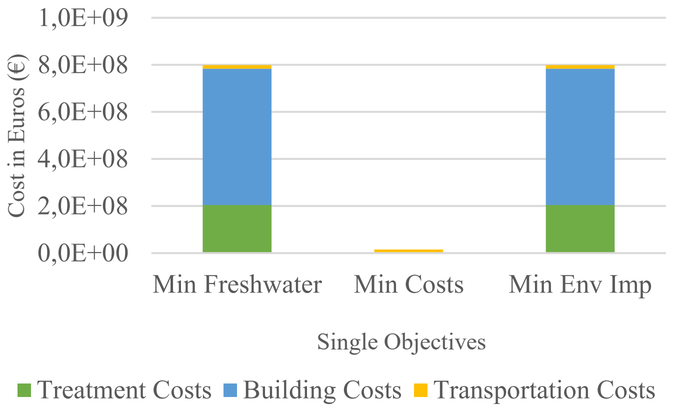


Figure 7 - Cost distribution for the current network scenario

Regarding the cases A and C, represented in the first and third column, Figure 7 demonstrates the significant impact of building costs on the overall costs of this scenario, as they account for 73% of the total cost structure, amounting to 580M €. While this may seem substantial, it is important to prioritize reducing freshwater consumption in the context of water scarcity, even if it implies incurring in higher costs. On the other hand, treatment costs are relatively lower as they depend on the quantity of water being treated. Since this amount represents only 18% of the total water exchanged between entities, it is reasonable that the associated costs are not very high. Regarding transportation costs, since the treatment stations are integrated within the industries' plants, this transportation is not considered, therefore model only accounts for the transfer of water from each public network entity to each industry. In case B, when the focus is minimizing costs, the only expenditures incurred in are these transportation costs, that amount to 15M €.

When considering the environmental impact for cases A and C, there are three significant components to account for in this scenario. First, there are the impacts associated with the water supply from treatment stations and the public network, which include material intakes and outputs, as well as energy consumption during the treatment processes. Second, there are the impacts related to the creation and operation of the transportation structure, that in this scenario only regards the public network. These impacts are represented in Figure 8 and categorized based on their midpoint impact categories.

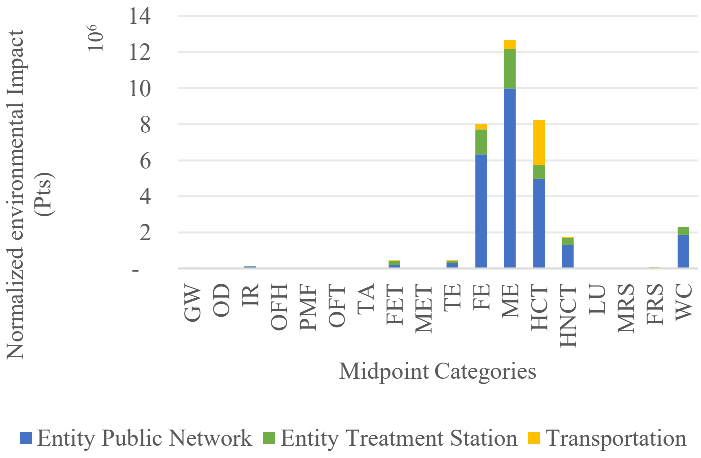


Figure 8 - Environmental impact (Pts) distribution by midpoint categories in current network for cases A and C

In Figure 8, it is evident that the public network has the highest impact in all categories. This is consistent with the cost structure, as the impact associated with the usage of an entity is directly proportional to the amount of water sourced from that entity. Since the majority of water in this scenario is supplied by the public network, it is expected to have the highest impacts. On the other hand, transportation has the lowest impact since it only involves the transfer of water between the public network and industries, which typically involves short distances. Among the midpoint categories, Marine Ecotoxicity (ME), Human carcinogenic toxicity (HCT), and Freshwater Ecotoxicity (FE) are found to have the highest impacts, in that order. The impacts on marine and freshwater ecosystems due to the extraction of freshwater for industrial use are understandable. The HCT category indicates that the exploration of water sources, such as freshwater reservoirs, can potentially have adverse effects on human health due to the materials and chemicals used and discharged into the environment. Therefore, the analysis of Figure 8 emphasizes the need for alternative water supplying practices to minimize the environmental impacts associated with water sourcing and usage in industrial processes.

In case B, the results are quite similar. The public network usage remains the most impactful component, with slightly higher values due to the larger amount of water supplied by this source. The transportation costs remain unchanged as the distances stay the same. However, there are no impacts related to treatment stations since they are not installed or used in this scenario. Additionally, the most impactful categories identified in cases A and C also hold true for case B. These findings are visually represented in Figure 9.

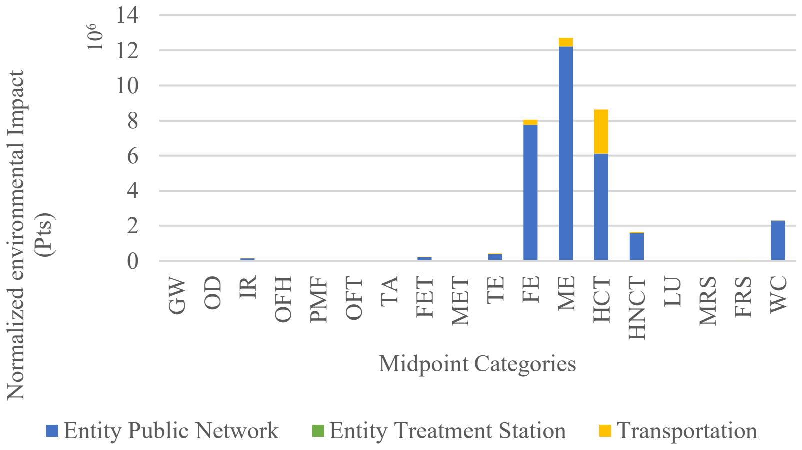


Figure 9 - Environmental impact distribution by midpoint categories in current network for case B

It is also relevant to assess the distribution of total water intake for each objective function during the whole 10 years. Table 14 provides a summary of those values when the main goal is to minimize freshwater consumption, costs and environmental impact, respectively.

Table 14 - Total water intake (in m3) distribution for the As-Is solution considering each different objective function

	Case A: Min Freshwater	Case B: Min Total Costs	Case C: Min Environmental Impact
Water Reused	1,12E+08	0,00E+00	1,12E+08
Freshwater	4,97E+08	6,09E+08	4,97E+08

As expected, the results are consistent with the data presented in tables 12 and 13. Indeed, the solutions for the first and third objective functions display the lowest freshwater intake. Once again, both objectives show a similar pattern. On the contrary, when the focus is on minimizing costs, the model opts to source water solely from the public network. Once again, this is explained by the fact that water reuse alone is insufficient to meet the total water demand, being necessary to resort to the use of the public network, in this scenario. This way, the model favours a single water source instead of utilizing both, thereby avoiding unnecessary building and water treatment costs.

5.3 Scenario To-Be (1): Possible situation with no constraint on public water network capacity

In a context of water scarcity, it is important to find alternatives to freshwater extraction. This scenario adds two different sources of water to the current network: industrial symbiosis and desalination. Nevertheless, it is relevant to note that the industries cannot rely solely on industrial symbiosis to meet their water demand due to capacity and circulation limitations imposed. As a result, there are several possible choices: relying solely on the public network; solely on desalination; a combination of industrial symbiosis with the public network; a combination of industrial symbiosis with desalination; or a combination of all three. Following the lexicographic approach, the payoff table values are presented in Table 15.

Table 15 - Results for Scenario To-Be (1) with single objective optimization

	Fresh and Seawater (m^3)	Total Costs (€)	Environmental Impact (Pts)
Case A: Min Fresh and Seawater Intake	330 588 670	1 724 227 425	52 153 554
Case B: Min Total Cost	608 638 080	1 016 084 644	34 286 447
Case C: Min Environmental Impact	496 897 050	1 616 294 792	33 974 186

Table 15 presents both similarities and differences when compared to Table 11 from the As-Is scenario. While the solutions for cases B and C remain unchanged, there are notable differences in the priority objective function, that is, case A. In light of this, Table 16 provides insights into the gains and losses between the two scenarios, highlighting the changes in the respective solutions.

Table 16 - Comparison between As-Is and To-Be (1) situations

	Fresh and Seawater intake	Total Costs	Environmental Impact
Case A: Min Fresh and Seawater Intake	-33%	+7%	+54%
Case B: Min Total Cost	0%	0%	0%
Case C: Min Environmental Impact	0%	0%	0%

As confirmed in Table 16, the only alterations between the two scenarios As-Is and To-Be are regarding case A, where fresh and seawater intake decreases, whilst costs and environmental impacts increase. Indeed, the introduction of industrial symbiosis as an option allows industries to utilize treated wastewaters from other industries. Thus, this alternative enables a reduction of 33% in the need for freshwater (public network) and seawater. Nevertheless, resorting to this option results in incurring in additional infrastructure and treatment costs, increasing the total cost by 7%. At the same time, the utilization of treatment stations, including energy and material intake and output, along with transportation between treatment stations and industries, results in a significant 54% increase in the overall environmental impact of the network.

In case B, as resorting to the public network is less expensive than resorting either to desalination or a combination of industrial symbiosis with one of these two alternatives, the model still chooses to rely solely on the public network in order to avoid building and water treatment costs associated with other options. Therefore, the same results as the As-Is scenario are obtained. In case C, the model continues to opt for sourcing water primarily from the public network and resorting to self-reuse. This is justified by the environmental advantage associated with self-reuse and by the impacts associated with transportation and entity-related factors. Indeed, resorting to desalination would increase impacts significantly, particularly due to the long distances between the station and industries, as well as the environmental effects of material and energy intake, along with the discharge of brine production. Between incurring in impacts of resorting to both industrial symbiosis and public network, or solely to public network and self-reuse, the most environmentally friendly option is the second one. The difference between opting for self-reuse instead of also engaging in industrial symbiosis relies with the higher amount of water that would need to be treated and transported, incurring in more environmental impacts. This strategy is the most beneficial in terms of lower environmental impacts, where industries gain by leveraging self-reuse and relying on the well-established and close infrastructure of the public network for the remaining water needs.

The network structure for case A is shown in Figure 10. In the case of scenarios B and C, their solutions and network configurations remain the same as in the As-Is scenario, already being represented in figures 6 and 5, respectively.

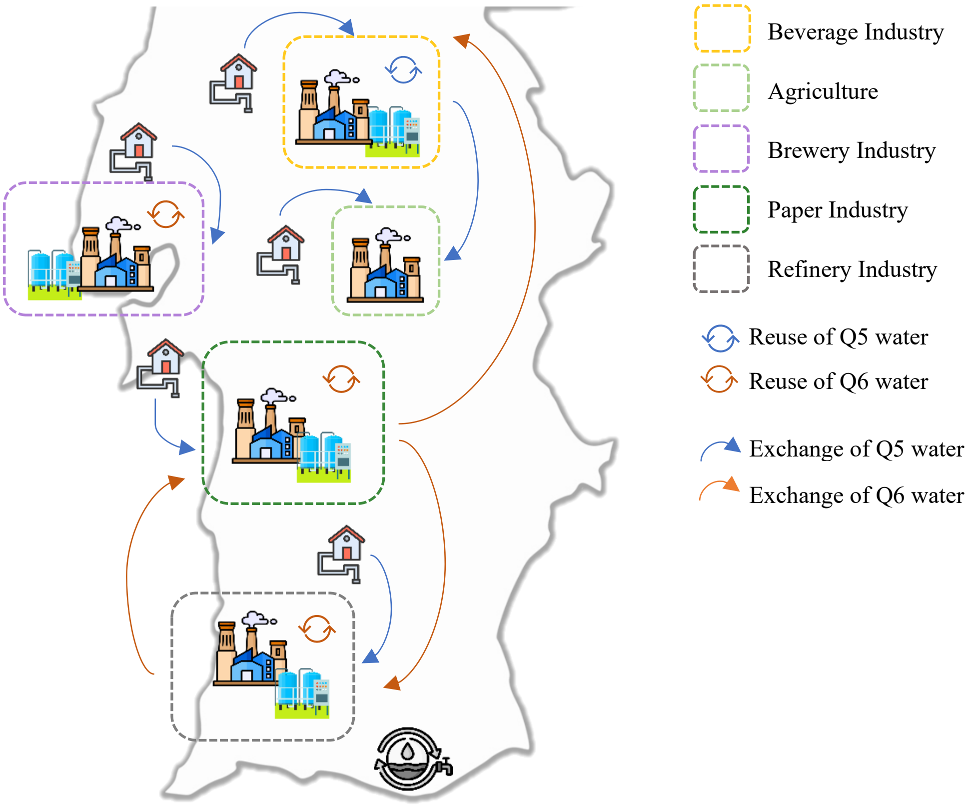


Figure 10 - To-Be network with no constraint on public water capacity for case A

Figure 10 confirms the network structure deduced from the analysis of the payoff table. The objective of minimizing fresh and seawater consumption leads to the maximization of water reuse options such as self-reuse, industrial symbiosis, or a combination of both. However, due to the limited capacity of these options, industries are compelled to additionally rely either on the public network or desalination to fulfil their remaining water demands. Given the higher costs and environmental impacts associated with desalination, the model favours the use of the public network, causing all industries to resort to this alternative. Consistent with the As-Is scenario, the public network supplies water of quality Q5 (high-quality) to ensure the fulfilment of this quality requirement, allowing industries to install more cost-effective technologies to produce water of quality Q6. Consequently, in Figure 10, it is evident that all industries reuse their treated wastewater of quality Q6, except for agriculture, which lacks this capability. Additionally, there are exchanges of Q6 water quality between the paper and refinery industries, as well as from the paper industry to the beverage industry. Furthermore, due to the restriction of agriculture to receive water of quality Q5, the symbiotic exchange that occurs between the beverage industry and agriculture is of this quality. This exchange is supported by the installation of technology K1 (Reverse Osmosis) in the beverage industry's treatment station, which has the capability to treat wastewater to Q5 quality. Since the beverage treatment station was already producing this quality for agricultural purposes, it is logical that for internal reuse purposes, the quality used was the same. Similarly to the As-Is scenario, the remaining technologies employed are also K1 in the brewery industry, K4 (Ultrafiltration) in the paper industry, and K5 (Activated Carbon with Ion Exchange) in the refinery industry. Once again, these technology choices are determined by cost considerations.

In order to better understand the flows of water considering self-reuse, industrial symbiosis, public network and desalination, Table 17 is presented for case A. Similarly to the network structure the cases B and C flows are already represented in Tables 13 and 12 in the As-Is scenario, respectively.

Table 17 - Flows of water (in m^3) received by each industry from each possible source in year 10, in Scenario To-Be with no constraint on the public network capacity for case A

		From						Total Received
To		Beverage	Paper	Refinery	Brewery	Public	Desalin.	
Beverage	Q5	7.29E+05	-	-	-	5.10E+06	-	1.46E+07
	Q6	-	8.75E+06	-	-	-	-	
Paper	Q5	-	-	-	-	9.43E+06	-	2.00E+07
	Q6	-	6.72E+06	3.85E+06	-	-	-	
Refinery	Q5	-	-	-	-	5.26E+06	-	9.16E+06
	Q6	-	1.33E+06	2.57E+06	-	-	-	
Brewery	Q5	-	-	-	-	6.54E+05	-	7.61E+05
	Q6	-	-	-	1.07E+05	-	-	
Agriculture	Q5	4.09E+06	-	-	-	1.49E+07	-	1.90E+07
Total Sent		4.82E+06	1.68E+07	6.42E+06	1.07E+05	3.53E+07	-	

Table 17 shows a substantial decrease in the supply of public water. As the primary objective is to minimize the intake of fresh and seawater, there is a prioritization of water reuse wherever possible, relying on the public network or desalination only to meet the remaining water demand. Since desalination is not chosen as an option, the 33% reduction in water intake directly corresponds to a decrease in the flow supplied by the public network. Conversely, the overall flow originating from the treatment stations of the beverage, paper, and refinery industries has experienced a significant increase of 150% due to the adoption of industrial symbiosis. However, the brewery industry is unable to provide water to other industries, as there exists a minimum threshold quantity required to establish a symbiotic relationship.

It is worth noting the interesting water exchange dynamics between the paper and refinery industries, which occur in both directions. This exchange is driven by the goal of maximizing water reuse, as industries with significant wastewater generation prefer to grant it for reuse than disposing of it. Since there are limitations on the amount of self-reuse that each industry can engage in, industries adapt by transferring as much water as possible to other industries. In the case of the refinery, the paper industry is the closest in proximity, making it a natural choice for establishing a symbiotic relationship. However, for the paper industry, despite its proximity to agriculture and the brewery industry, there is no water sent to these entities. This is because the paper industry can only generate water of Q6 quality, while agriculture requires water of Q5 quality. Furthermore, although the paper industry is closer to the brewery than the refinery, the amount of water it can send to the refinery (1.33E+06 m^3) surpasses the potential amount it could send to the brewery, which is determined by the volume of water demanded by the brewery industry that receives it from the public network (6.54E+05 m^3). This way, the double water flow exchange between the refinery and paper industry is justified by the prioritization of the minimization of fresh and seawater. In the end, despite the decrease, the public network remains the primary water provider, contributing to 54% of the total water circulation, while water reuse (self-reuse plus industrial symbiosis) accounts for 46%. In comparison, the corresponding values in the As-Is scenario were 82% and 18% respectively, highlighting the substantial shift in the significance of each supply source. This also means there is a reduction in wastewater disposed. Indeed, as more water is being treated for reuse, less water is being wasted and discharged into the environment.

In this scenario, the cost structure includes treatment costs only associated with self-reuse and industrial symbiosis, since there is no selection of desalination. It also accounts for the building costs associated with the installation of the treatment stations, and transportation costs between each provider (industries' treatment stations and the public network) and each industry.

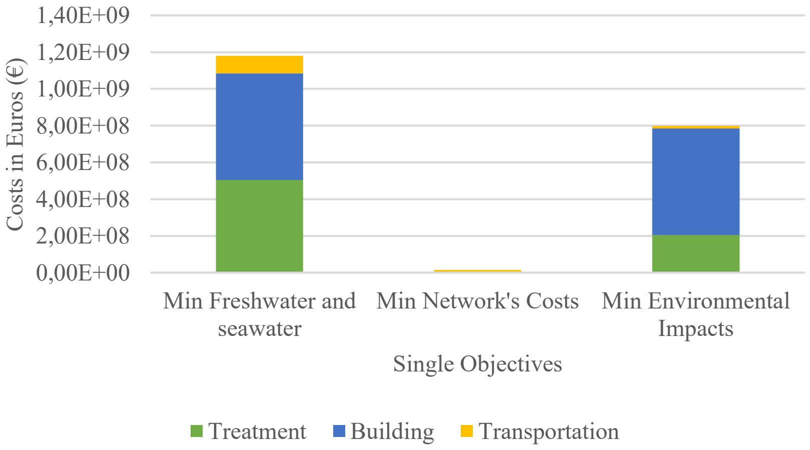


Figure 11 - Cost distribution for scenario To-Be (1)

Figure 11 allows for a direct comparison of the cost structure between this scenario and the As-Is solution. The figure confirms that costs have increased in this scenario, particularly in terms of treatment and transportation. This is expected since the introduction of industrial symbiosis as an alternative implies more water to be treated, resulting in higher treatment costs. The treatment costs now amount to 504M €, accounting for 43% of the total cost distribution in this scenario, whereas previously they accounted for only 26%. Similarly, transportation costs have increased from 2% to 8% due to the additional transportation of water between industries. Moreover, building costs remain at 580M € since all treatment stations are again installed. In the previous scenario, solely with the intent of self-reuse, whereas now due to industrial symbiosis as well. The difference is that the cost distribution is more balanced, with building costs now responsible for 49% instead of the previous 76% of the total costs in case A. Similarly to the As-Is situation, the only costs incurred in case B are regarding the transportation costs from the public network to each industry. For case C, in this scenario, the cost structure remains the same as the As-Is situation, with building costs accounting for 73% and treatment costs for 26% of the total costs.

In the end, due to the main objective of case B, the overall costs are the lowest compared with the other two scenarios. It is also possible to conclude the costs increase significantly by adding the alternative of industrial symbiosis, causing case A to be the most expensive situation.

Regarding environmental impacts, this scenario includes four different components: impacts associated with the usage of treatment stations and public network, in terms of materials and energy and impacts associated with the transportation structure for the public network and industrial symbiosis. Figure 12 presents the environmental impacts for each component by midpoint category in case A. Since cases B and C maintain the structure presented in the As-Is situation, the environment impacts by midpoint category were already presented in Figures 9 and 8, respectively.

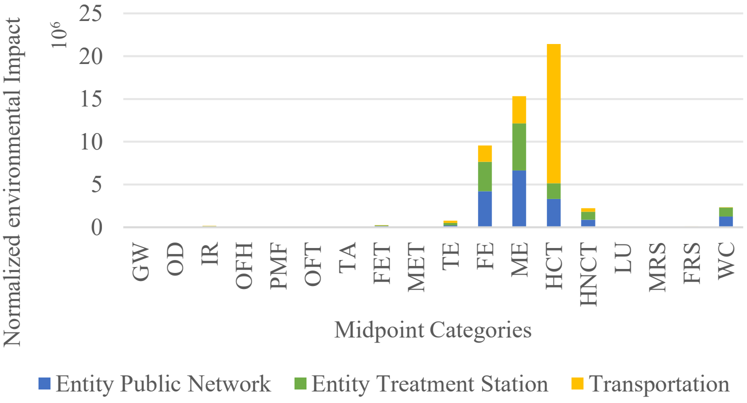


Figure 12 - Environmental impact distribution by midpoint categories in scenario To-Be (1) network for case A

Figure 12 indicates that transportation has the highest contribution to the overall environmental impact, particularly in the category of Human carcinogenic toxicity (HCT). In comparison to the As-Is scenario, there is a significant increase in this category's impact, primarily due to transportation. Indeed, the inclusion of industrial symbiosis in the network structure results in longer distances that require additional transportation infrastructure. It is important to note that the construction and use of these structures can potentially pose risks to human health, such as chemical exposure from materials and excavation processes.

Additionally, the categories of Marine Ecotoxicity (ME) and Freshwater Ecotoxicity (FE) remain highly impactful. These impacts are mainly attributed to the water production and supply of treatment stations and public network. The extraction and intake of raw surface water, along with the energy requirements and material discharge associated with these operations, contribute to the ecotoxicity of aquatic environments.

In order to better understand the type of water used, the total water consumption by alternative and by case is presented in Table 18.

Table 18 - Total water intake (in m3) distribution for the To-Be (1) solution considering each different objective function

	Min Freshwater and Seawater	Min Total Costs	Min Environmental Impact
Water Reused	2,78E+08	0,00E+00	1,12E+08
Freshwater	3,31E+08	6,09E+08	4,97E+08
Seawater	0,00E+00	0,00E+00	0,00E+00

Table 18 confirms that cases B and C remain unchanged from the As-Is solution, with no modifications to water reuse or freshwater consumption. However, in case A, there is a significant increase of 149% in water reuse and a decrease of 33% in freshwater consumption. This outcome aligns with the objective of minimizing freshwater usage by maximizing water reuse, which in turn helps to conserve this valuable resource. Nonetheless, although this case opens the possibility of desalination to be selected as an alternative, this option is not chosen due to its high costs and environmental impacts.

5.3.1 Sensitivity analysis

In this section, a sensitivity analysis is conducted to assess the robustness of the results and the impact of parameter variations, specifically in scenario To-Be (1) where it is crucial to study the influence of these changes. The centre of this type of analysis are critical parameters, characterized by their potential to significantly influence the final solution and often associated with high uncertainty, as they normally rely on estimates and assumptions. In this study, while optimizing the fresh and seawater intake, the focus is given to the following potential critical parameters: the capacity of the public water network, the bill of materials for wastewater generation and the cost parameters.

Capacity of the public water network

This study considers a projected 5% increase in demand for final products every four years, leading to a corresponding rise in water demand by industries. However, the availability of freshwater follows the opposite trend, where according to experts, its supply is estimated to be 40% shorter than its demand, in 2030 (Dsilva Winfred Rufuss et al., 2022). This estimated restriction to freshwater supply can greatly affect the network established in scenario To-Be (1), where the public water network was the major supply. Additionally, this capacity shortage is an estimation, therefore it carries inherent uncertainty. Thus, to understand the potential impact of this uncertainty on the network configuration, a sensitivity analysis was conducted on the parameter of public water capacity. The analysis involved varying this capacity from an unlimiting value of 100%, corresponding to scenario To-Be (1), to 60% based on the availability mentioned in the article (Dsilva Winfred Rufuss et al., 2022), and to 30% and 10% for more pessimistic perspectives.

This study results will serve as basis for the limiting capacity scenario in section 5.4. The results of this parameter variance, including its impact on freshwater and seawater intake, total network costs, and environmental impacts, are shown in Figure 13. Table 32 on Appendix B presents the data table with the detailed values of this analysis.

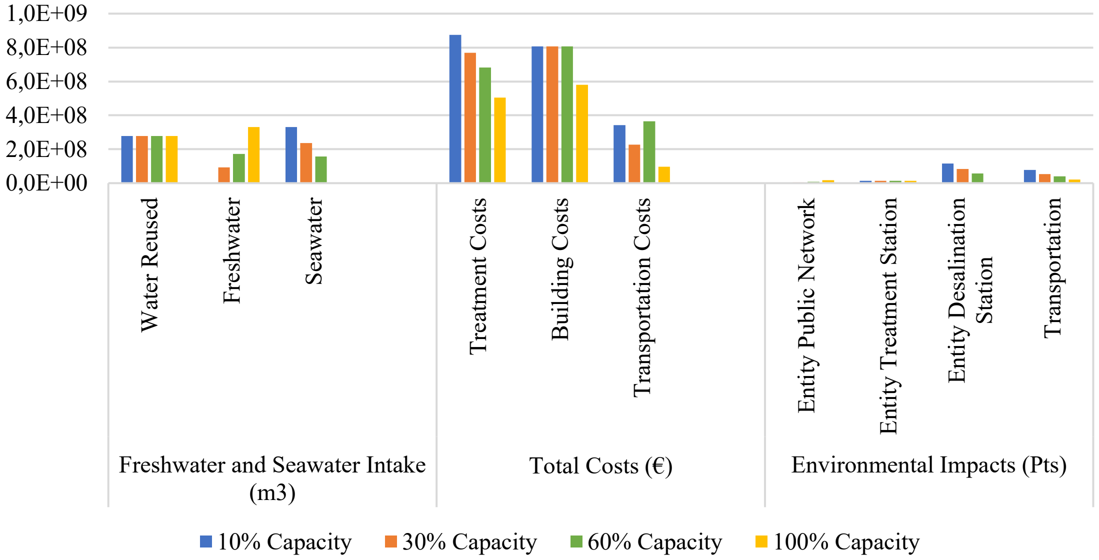


Figure 13 - Results for sensitivity analysis of the public network's capacity

Across all scenarios, the optimization model consistently maximizes water reuse, leading to the same amount of reused water. As the capacity of the public network decreases, there is a notable decrease in freshwater consumption, consequently increasing the seawater intake. This suggests that industries compensate for the shortage of freshwater by relying more on seawater and increasing their usage of desalination when the public network capacity is more limited. In the 10% capacity restriction scenario, no industry resorts to freshwater, meeting their demands solely through industrial symbiosis, self-reuse, and desalination, which leads to significant negative effects on the cost structure and environmental impacts. This way, the 10% capacity represents a turning point, where beyond this threshold, opting for the public network would only increase even more the costs and environmental impacts, as opposed to the previously chosen situations.

The total costs increase as less freshwater and more seawater are used. The resort to desalination drives this cost increase, as there is a need for more treatment of desalinated water, which becomes the major water source when freshwater availability decreases. Building costs also increase in the 60% capacity scenario due to the necessity of building the desalination station, but then they remain constant for the following capacities. This is due to the continuing adoption of water reuse and desalination by all industries, leading to a constant number of treatment and desalination stations installed. Important to note that the building costs are the only ones that act as fixed costs since they are independent from the amount of water flow or industries relying on the stations, that is, as long as they are installed these costs are incurred in. Transportation costs are significantly affected by the use of desalination, varying according to the industries connected to the desalination station. Indeed, while there is a considerable increase in transportation costs from the 100% capacity scenario to the other scenarios resulting from the choice of desalination, the difference between the costs of scenarios with capacities 60%, 30%, and 10% are relatively small, depending on the industries receiving water from the station and respective distance.

Likewise, the decrease in freshwater usage and increase in desalinated water contribute to an increase in environmental impacts. Less freshwater circulation results in decreased impacts associated with the operation and usage of the public network. Conversely, more desalted water circulation increases the impact associated with the water production in the desalination station. As the amount of reused water remains consistent, the impact from treatment stations remains stable as well. However, transportation shows an increase in impact as more industries resort to desalination. Considering that the station and most industries are separated by larger distances, this increasing impact is a direct consequence of the longer distances that need to be covered, resulting in the construction of more infrastructures and consequently increasing impacts.

To better understand the different network structure and connections established for each capacity restriction, Table 19 is presented.

Table 19 - Connections established for each case of public network capacity

		Beverage	Paper	Refinery	Brewery	Agriculture
100%	Self-reuse	x	x	x	x	
	IS Sender	x	x	x		
	IS Receiver	x	x	x		x
	Public Network Receiver	x	x	x	x	x
	Desalination Receiver					
60%	Self-reuse	x	x	x	x	
	IS Sender	x	x	x		
	IS Receiver	x	x	x	x	x
	Public Network Receiver	x	x	x		
	Desalination Receiver					x
30%	Self-reuse	x	x		x	
	IS Sender	x	x	x		
	IS Receiver	x	x	x	x	
	Public Network Receiver	x	x		x	
	Desalination Receiver			x		x
10%	Self-reuse	x	x		x	
	IS Sender	x	x	x		
	IS Receiver	x	x	x	x	x
	Public Network Receiver					
	Desalination Receiver	x	x	x		x

The connections established for the unlimiting capacity of 100% were already analysed in section 5.3 for the To-Be (1) scenario. However, as Table 19 indicated, there are indeed some changes when restricting more and more the capacity of the public network.

For the scenario where there is 60% of capacity, the connections established for the beverage, paper and refinery industries remain the same, resorting to self-reuse, industrial symbiosis both as senders and receivers, and to the public network. Nonetheless, this restriction causes the brewery industry and agriculture to exchange their dependencies on the public network by industrial symbiosis and desalination, respectively. Further reducing the capacity to 30% results in more changes. The beverage and paper industries maintain their previous connections, but the refinery industry no longer resorts to self-reuse and switches from the public network to desalination. On the other hand, the brewery industry returns to the public network, excluding desalination, and receives water from another industry through industrial symbiosis. Agriculture is now exclusively sourced from the desalination station.

Finally, in the scenario with a capacity of 10%, there is no circulation of freshwater, consequently no industry receives water from the public network. The refinery industry retains the same connections as in the previous scenario, while the beverage and paper industries exchange their dependency on the public network for desalination. The brewery industry and agriculture revert to the connections established in the 60% scenario, relying on self-reuse and industrial symbiosis, and industrial symbiosis and desalination, respectively. This relates to the supply capacity of each source. The restriction on access to the public network prompts industries to depend more on the other two sources. However, since these alternatives also have capacity limitations, the distribution of which industry utilizes each alternative is expected to shift as the network adapts to the limitations of the public network.

In conclusion, the sensitivity analysis demonstrates that there is an adjustment in the network configuration as a response to changes in freshwater availability by increasing seawater intake. While industries can adapt to water scarcity by reducing freshwater consumption, even achieving zero intake, this advantage comes with significant disadvantages in terms of increased costs and environmental impacts. Consequently, it emphasizes the necessity and importance for industries to proactively adapt to future freshwater restrictions by not only opting for alternatives to this resource, but also by improving the economic and environmental implications of these alternatives. This is crucial to ensure sustainability and resilience in the face of potential water scarcity challenges.

Bill of Materials for Wastewater

The bill of materials for wastewater expresses the amount of wastewater generated by each unit of final product produced. This parameter incorporates quite a level of uncertainty as it can strongly depend on industries water management systems and efficient water use. Additionally, it can influence the network established since the amount of wastewater generated determines the possible symbiotic relationships that can be established.

Although the demand for final products is expected to increase, it is also expected that, over time, the technology advancements, increased awareness of environmental issues, and the implementation of sustainable practices will lead to more efficient water usage and reduced waste in various industries. Indeed, from the industries' sustainability reports, it is possible to observe a pattern of reduction of the wastewater generated throughout the years. Therefore, to accommodate for these predictions, a sensitivity analysis was conducted on this parameter for each industry, decreasing its value 30% and 50%, while also considering a 30% increase to better understand the impacts. The results are shown in Figure 14. The detailed values are presented in Table 33 of Appendix B.

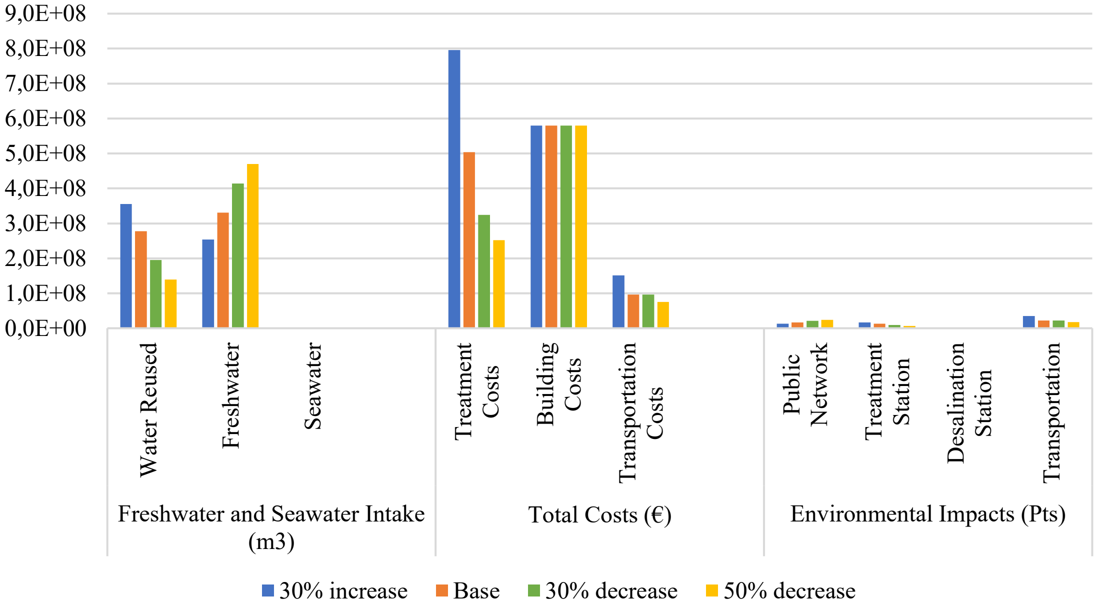


Figure 14 - Results of the sensitivity analysis for the bill of materials of wastewater generation

From Figure 14, it can be deduced that lower wastewater generation leads to an increased reliance on freshwater by industries. With reduced wastewater production, industries have less water to share between them, resulting in fewer symbiotic relationships or smaller amounts of water being shared. Consequently, the amount of reused water decreases, necessitating the use of other water sources, such as freshwater. Desalination is not utilized by any industry in this scenario, due to its costs and environmental impacts.

Similarly, the costs decrease with lower wastewater production. Indeed, reducing wastewater reduces the need for treatment and of symbiotic connections which leads to decreased transportation costs due to shorter distances to be covered.

Environmental impacts follow a similar pattern as costs, decreasing with reduced wastewater generation. With a lower amount of wastewater to be treated, it is logical that the environmental impacts associated with water production and supply of treatment stations decreases. Consequently, the volume of freshwater supplied is higher, therefore increasing the respective associated impacts. As for transportation impacts, they decrease for the same reason as the costs.

Individually, it is reasonable for companies to aim for reduced wastewater generation, as it offers some environmental advantages and lowers their treatment costs before disposal. However, when considering the broader challenge of freshwater scarcity and the potential of industrial symbiosis, industries may alter their perspective. Rather than solely focusing on minimizing wastewater generation, they may prioritize the advantages that could be gained through IS as a solution.

Comparing the base scenario - To-Be (1) - with the scenario of a 30% reduction in wastewater generation for each unit of production, it is observed that this variation does not seem to significantly alter the network structure. In fact, although there are some changes in water intake, costs, and environmental impact across the four scenarios considered, these differences are not substantial. The primary objective of freshwater and seawater intake is the most affected by the changes, where the solutions vary almost proportionally with the parameter variation. On the other hand, costs and environmental impacts are less sensitive to the reduction in wastewater generation.

To gain a deeper understanding of the impacts of this parameter variation on the network structure, Table 20 was analysed.

Table 20 - Connections established for each scenario considering the variation of the bill of materials for wastewater generation

		Beverage	Paper	Refinery	Brewery	Agriculture
30% increase	Self-reuse	x	x	x	x	
	IS Sender	x	x	x		
	IS Receiver	x	x	x	x	x
	Public Network Receiver	x	x	x	x	x
	Desalination Receiver					
Base	Self-reuse	x	x	x	x	
	IS Sender	x	x	x		
	IS Receiver	x	x	x		x
	Public Network Receiver	x	x	x	x	x
	Desalination Receiver					
30% decrease	Self-reuse	x	x	x	x	
	IS Sender	x	x	x		
	IS Receiver	x	x	x		x
	Public Network Receiver	x	x	x	x	x
	Desalination Receiver					
50% decrease	Self-reuse		x	x	x	
	IS Sender	x	x	x		
	IS Receiver	x	x			x
	Public Network Receiver	x	x	x	x	x
	Desalination Receiver					

Table 20 illustrates the different connections established throughout the variation of the parameter. The agriculture and paper industry do not suffer any alterations between the scenarios. However, taking as example the paper industry, even though it is still involved in symbiotic relationships as both sender and receiver, the amounts of water exchanged are lower since there is less water available for reuse, as seen in Figure 14. The brewery industry only participates in symbiotic relationships in the scenario with a 30% increase, which is reasonable given the increased water availability for sharing. The beverage and refinery industries also experience slight changes, primarily in the scenario with a 50% decrease, where the beverage industry discontinues self-reutilization, and the refinery stops receiving water from symbiotic relationships due to reduced water availability caused by decreased wastewater production.

Both Figure 14 and Table 20 confirm that the changes in connections across the four scenarios are relatively minor. Although this parameter is critical for the problem, its variation does not appear to significantly impact the results. Therefore, while wastewater generation is indeed an important factor, the sensitivity analysis suggests that other factors, such as freshwater availability, play a more significant role in influencing the network configuration and its associated costs and environmental impacts.

Costs

Cost parameters often have inherent uncertainty associated. However, they are only critical to the problem if they have potential to impact the final solution. This way, all parameters associated with the cost structure were studied in this analysis.

Building costs of treatment and desalination stations exhibit minimal influence on the results, despite their uncertainty. This is due to the optimization process, which indirectly, places a higher priority on maximizing water reuse, leading to the use of all treatment stations, regardless of their specific costs. In contrast, when incorporating the second and third objectives, the model avoids opting for desalination unless there are no other viable alternatives available. This is primarily attributed to the considerable costs and environmental impacts associated with desalination. Even with a substantial reduction in the building cost of the desalination station, the model still favours the public network, as it does not incur in such high building costs, nor the high transportation costs and environmental impacts associated with desalination.

The treatment costs associated with desalted water also have a limited impact on the overall results. There is a consistent prioritization of the treatment of wastewater for reuse, regardless of the associated costs, as its primary objective is to indirectly maximize water reuse. Furthermore, when weighing the choice between freshwater and seawater, there is a consistent leaning towards freshwater, as it incurs no treatment costs. Therefore, even if the treatment cost for desalination were to experience a significant decrease, the public network would still be preferred, thereby maintaining the overall network structure unchanged.

The same rationale applies to the price of desalted water. Despite its association with uncertainty, it lacks sufficient influence on the cost structure to impact the established network. Even when the price of desalted water decreases significantly, the model still prioritizes treating water for reuse rather than resorting to desalination, as determined by the objective prioritization. Additionally, the model's preference for the public network over desalination remains constant, as indicated by its consistent choice of the former despite the higher price of freshwater.

From this analysis, it can be deduced that individual parameters related to desalination do not have a significant impact in the connections established. Although desalination incurs higher costs, it is the combination of all its cost components that results in this elevated value. As a result, altering these parameters separately does not appear to significantly affect the network structure. However, it is worth noting that conducting a sensitivity analysis that simultaneously varies all parameters related to desalination may lead to changes in the network structure, being a possible future work complementation.

The piping costs function in a similar manner, as they are essential for water transportation between entities and remain consistent regardless the origin and destination entities. Therefore, any variation in piping costs would proportionally affect the final costs, while maintaining all connections as the impact of the fluctuation remains constant across the network. Another potentially critical parameter is the price of treated water. Due to its association with significant uncertainty and variation based on the quality obtained, it could potentially influence the established exchanges between entities. However, this parameter did not cause any significant changes either to the solutions' value or the connections established.

Considering one of the objective functions is regarding cost minimization, it would be expected that the parameters related with the cost structure would indeed have a significant impact on the final results. However, the sensitivity analysis conducted showed that their individual variation does not substantially affect the network outcome. This finding highlights the robustness of the model and suggests that these parameters do not heavily influence the ultimate decisions made through the optimization process.

5.4 Scenario To-Be (2): Most probable future situation with a constraint on public water network capacity

In this study, the demand for final products is projected to increase by 5% every four years, leading to a corresponding rise in water demand by industries. According to Dsilva Winfred Rufuss et al. (2022), this growing water demand will have an impact on the availability of freshwater, including for industrial use. To address this issue, the study establishes the new capacity of the public network at 60% of the highest water demand value for each industry. This percentage is derived from the article and aligns with the reasoning of the sensitivity analysis, which highlighted the considerable impact of freshwater availability on the optimal network design. The decision to establish the limit based on the highest water demand value is justified by the author's description of capacity limitations for future years. This specifically concerns the later time periods of the modelled case study, during which the high demand peaks are expected. This approach ensures that there is a predetermined threshold for freshwater supply that accounts for the highest demands in later periods, effectively planning for potential limitations in freshwater availability.

This way, scenario To-Be (1) that included industrial symbiosis, public network and desalination is adapted to a second scenario: To-Be (2). This situation now incorporates a limitation to the availability of freshwater by restricting the public network capacity, in order to accommodate a more realistic future approach. In accordance with the sensitivity analysis performed in section 5.3.1 and with the experts' predictions, this capacity is then limited to 60% of the largest water demand for each industry.

5.4.1 Single objective

Following the lexicographic approach, the results achieved for each optimization are presented in Table 21.

Table 21 - Results for Scenario To-Be (2) with single objective optimization

	Fresh and Seawater intake (m^3)	Total Costs (€)	Environmental Impact (Pts)
Case A: Min Fresh and Seawater Intake	330 588 670	2 024 764 639	119 453 194
Case B: Min Total Cost	435 192 740	1 507 143 966	140 840 700
Case C: Min Environmental Impact	330 588 670	2 172 215 500	74 781 088

Table 21 reveals the similarities between the solutions for cases A and C, with the exception of the environmental impact value. Both cases demonstrate the same level of freshwater and seawater intake, which is justified by the similar trends of the respective objectives. In case C, where the priority is to minimize environmental impact, the reduction in water intake aligns with this objective. However, the optimal environmental impact is not achieved in case A due to the prioritization order of objectives. Indeed, in case A, the primary goal is to minimize water intake, followed by the objective of cost minimization. Since this objective does not necessarily follow the same trend as minimizing environmental impacts, it can lead to a suboptimal environmental impact. Consequently, the final solution for the environmental impact objective in case A is significantly higher than it would be if the order of objectives was adjusted.

In order to better understand the gains and losses associated with this scenario when compared to the other two previously studied, Figure 15 is presented.

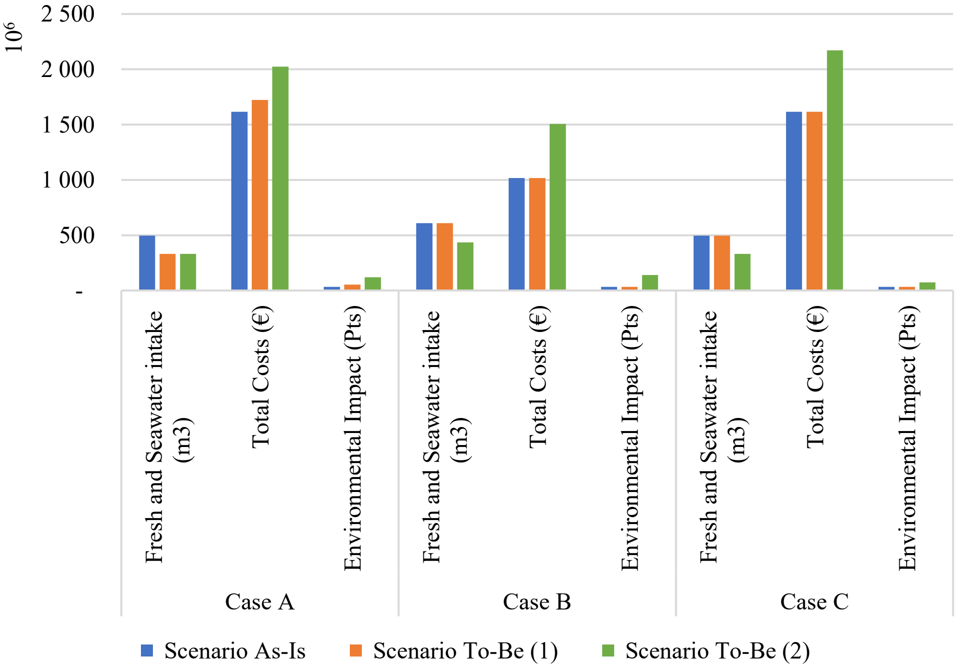


Figure 15 - Comparison of the results obtained for each case between each scenario

When comparing scenarios As-Is and To-Be (2), there is an evident decrease in water intake consistently across all cases. However, this 33% reduction is accompanied by an increase in the cost structure of 25% and by a substantial 252% increase in environmental impacts for case A. At the same time, when taking into account case A of scenario To-Be (1), it is possible to conclude the reduction had already been verified before. Indeed, in scenario To-Be (1), it was possible to obtain the same significant fresh and seawater reduction, but incurring in lower costs and environmental impacts. This was expected since scenario To-Be (2) represents a more pessimistic perspective. Certainly, by limiting the capacity of the public network, it forces the model to resort to desalination, which has significantly high environmental impacts.

Moreover, regarding cases B and C, there is an increase in costs and environmental impact of 48% and 120%, respectively, both when comparing with scenarios As-Is and To-Be (1). This increase is related with the capacity limitation established for the public network, forcing the model to opt for more costly and more environmental impactful alternatives. The variation is the same when comparing to scenarios As-Is and To-Be (1) since cases B and C present the same solutions for both scenarios.

The key takeaway from these findings is that if a choice between scenarios was to be made, scenario To-Be (1) would be the preferable option. It demonstrates a more reasonable balance between the decrease in freshwater intake and increase in costs and environmental impacts. However, it is important to acknowledge that scenario To-Be (2) is a much more realistic representation of the future context, where industries will be confronted with the challenge of selecting between these alternatives in an even more severe water scarcity context, possibly having to resort to costlier and more environmentally impactful options.

The water flows associated with cases A, B and C are given in Tables 22, 23 and 24, respectively. The reason behind analysing the flows of year 10 is due to capacity restrictions based on the highest water demand, that due to expected increases in final products' demand, occurs in the latest time periods.

Table 22 - Flows of water received by each industry from each possible source in year 10, for Scenario To-Be (2) with a constraint on the public network capacity for Case A

			From						Total Received
			Beverage	Paper	Refinery	Brewery	Public	Desalin.	
To	Beverage	Q5	-	-	-	-	6.02E+06	-	1.46E+07
		Q6	1.92E+06	6.64E+06	-	-	-	-	
	Paper	Q5	-	-	-	-	8.00E+06	-	2.00E+07
		Q6	-	6.04E+06	5.96E+06	-		-	
	Refinery	Q5	-	-	-	-	4.58E+06	-	9.16E+06
		Q6	-	4.12E+06	4.58E+05	-	-	-	
	Brewery	Q5	6.54E+05	-	-	1.07E+05	-	-	7.61E+05
		Q6	-	-	-	-	-	-	
	Agriculture	Q5	2.24E+06	-	-	-	-	1.67E+07	1.90E+07
	Total Sent		4.82E+06	1.68E+07	6.42E+06	1.07E+05	1.86E+07	1.67E+07	

In case A, the primary objective translates into maximizing water reuse, which leads to the installation of treatment stations by industries to make the most of their treated water, either through self-reuse or symbiotic relationships. However, the brewery industry does not produce enough wastewater to participate as a water symbiotic sender. As industries cannot solely rely on water reuse to meet their water demand, they must explore other alternatives. In this case, desalination is chosen exclusively for agriculture, one of the most water-intensive industries. Due to the higher costs and environmental impacts associated with desalination compared to the public network, it is the preferred option only for one industry, in this case agriculture. The paper industry, although supplying more water than desalination, remains slightly behind the public network. However, in total, the public network accounts for 28% of the circulating water, desalination for 26%, and self-reuse and industrial symbiosis for 46%. Comparing with scenario To-Be (1), the percentage of water reuse remains the same, but the previous 54% supplied by the public network is now divided between the public network and desalination. Thus, this case and scenario significantly alleviates freshwater consumption pressure while maximizing water reuse.

Table 23 - Flows of water received by each industry from each possible source in year 10, for Scenario To-Be (2) with a constraint on the public network capacity for Case B

			From						Total Received
			Beverage	Paper	Refinery	Brewery	Public	Desalin	
To	Beverage	Q5	-	-	-	-	7.51E+06	-	1.46E+07
		Q6	-	7.07E+06	-	-	-	-	
	Paper	Q5	-	-	-	-	1.12E+07	-	2.00E+07
		Q6	-	4.76E+06	-	-	-	4.07E+06	
	Refinery	Q5	-	-	-	-	4.58E+06	-	9.16E+06
		Q6	-	4.58E+06	-	-	-	-	
	Brewery	Q5	-	-	-	-	3.81E+05	-	7.61E+05
		Q6	-	3.80E+05	-	-	-	-	
	Agriculture	Q5	-	-	-	-	-	1.90E+07	1.90E+07
	Total Sent		0.00E+00	1.68E+07	0.00E+00	0.00E+00	2.36E+07	2.30E+07	

As it could be concluded from the analysis of previous scenarios, the public network is the less expensive option of all alternatives, therefore the preferred alternative when minimizing costs. However, due to its capacity limitations in this case, the model needs to resort to other alternatives to complement the water demand. The best combination the model could find was to resort to water reuse through the sole installation of a treatment station in the paper industry and rely on desalination to meet the substantial water requirements of the paper and agriculture industries. Although only these two industries receive water from this source, they are the primary consumers, making desalination a crucial component of the solution. Consequently, both the public network and desalination play significant roles, accounting for 37% and 35% of water circulation, respectively. The remaining 28% is attributed to water reuse facilitated solely by the paper treatment station. In comparison with case A, this case does not alleviate the freshwater consumption in such a significant way, being less ideal within a water scarcity context.

Table 24 - Flows of water received by each industry from each possible source in year 10, for Scenario To-Be (2) with a constraint on the public network capacity for Case C

			From						Total Received
			Beverage	Paper	Refinery	Brewery	Public	Desalin.	
To	Beverage	Q5	-	-	-	-	7.51E+06	-	1.46E+07
		Q6	-	7.07E+06	-	-	-	-	
	Paper	Q5	-		-	-	1.12E+07	2.21E+06	2.00E+07
		Q6	-	6.63E+06	-	-	-	-	
	Refinery	Q5	-		-	-	4.58E+06	-	9.16E+06
		Q6	-	2.82E+06	1.76E+06	-	-	-	
	Brewery	Q5	-	-	-	1.07E+05	3.81E+05		7.61E+05
		Q6	-	2.74E+05	-	-	-	-	
	Agriculture	Q5	4.82E+06	-	4.66E+06	-	9.48E+06	-	1.90E+07
	Total Sent		4.82E+06	1.68E+07	6.42E+06	1.07E+05	3.31E+07	2.21E+06	

When the primary objective is minimizing environmental impact, there is a prioritization towards maximizing water reuse. As a result, all industries opt to install treatment stations and utilize their own wastewater or exchange it with other industries. Considering the substantial environmental impacts associated with desalination, the model seeks to minimize its usage, resulting in the lowest proportion of water sourced from this option compared to cases A and B. However, to meet the water demand of the paper industry, which is one of the largest consumers, desalination becomes necessary as the industry's own wastewater reuse is insufficient due to variations in water quality requirements. Moreover, the wastewater production of other industries has already reached its maximum capacity, limiting further water reuse supply possibilities. In this case, reused water accounts for 46% of the total circulating water, aligning with the findings in case A. However, freshwater consumption rises significantly, representing 50% of the supplied water and indicating substantial pressure on this resource. The remaining 4% of water is sourced from desalination, since it is considered the last resort due to its high environmental impacts in this case.

Tables 22, 23 and 24 provide an overview of the network structure, including the connections between entities and the exchanged water quality. Nonetheless, since the main goal of this study is water intake minimization, the network structure for case A is presented in more detail in Figure 16.

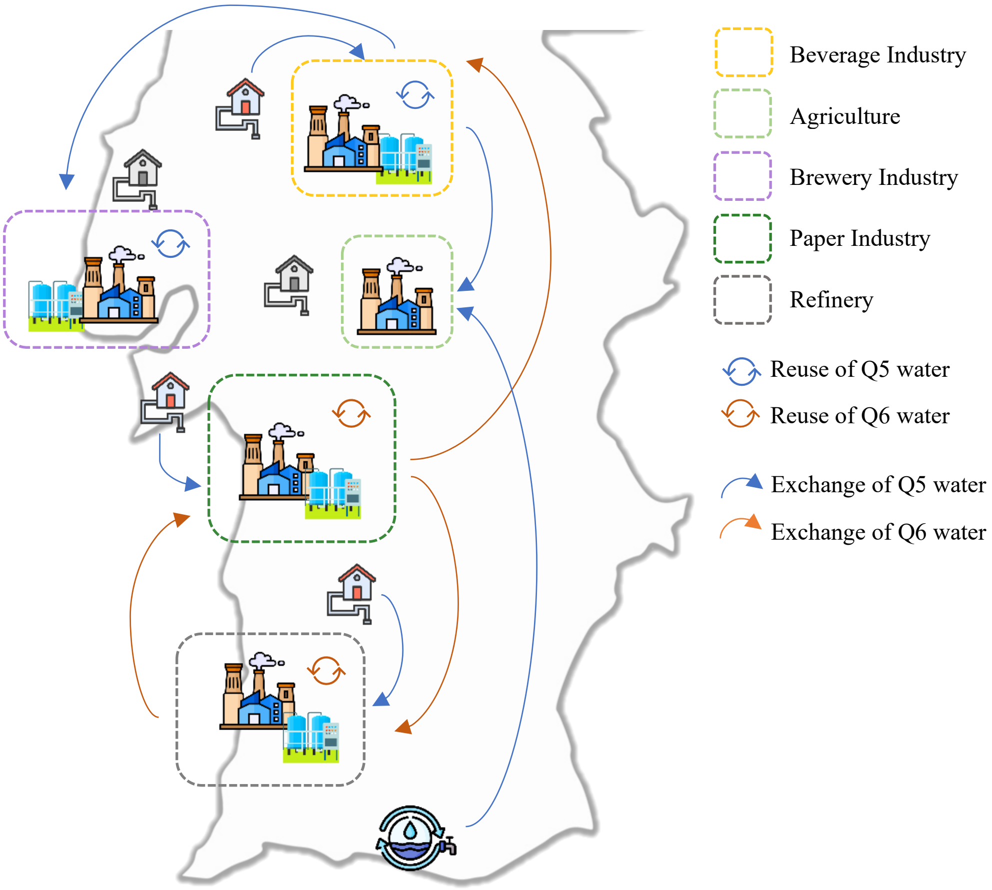


Figure 16 - To-Be (2) network with a constraint on public water capacity for case A

Figure 16 confirms the structure of the network deduced from the analysis of Table 22. The main goal is to minimize water intake by maximizing water reuse options like self-reuse and industrial symbiosis. However, these options have limited capacity, forcing industries to use the public network or desalination to meet their remaining water needs. Although desalination would be unpreferred because of its higher costs and environmental impacts, it is the chosen option due to the public network's limiting capacity.

In this network, the brewery and agriculture industries are not supplied by the public network. The brewery industry resorts to self-reuse and industrial symbiosis, while the agriculture industry relies on desalination and industrial symbiosis. Since these industries previously received water of quality Q5 from the public network, their alternatives for water supply now provide water of the same quality. For that reason, agriculture receives Q5 water from both the beverage industry and the desalination station. Similarly, the brewery receives Q5 water from the beverage industry, complemented by its own wastewater reuse. Considering the beverage industry's role in supplying Q5 water to two other industries, it follows that its self-reuse water is also of Q5 quality. The technology chosen for this purpose is again K1, the most cost-effective technology capable of providing Q5 quality water. Regarding the paper and refinery industry, the observed flows resemble those in scenario To-Be (1), involving the exchange of Q6 water between the two industries, self-reuse of water with the same quality, and reliance on the public network to fulfil their Q5 water requirements. Additionally, the paper industry maintains a connection with the beverage industry, supplying it with Q6 water. Both the refinery and paper industries continue to rely on the cost-effective technologies K4 and K5 for these water exchanges.

Regarding the cost structure, the distribution by cost type and by case is represented in Figure 17. It includes treatment costs regarding self-reuse, industrial symbiosis and desalination, and building costs associated with the installation of the treatment and desalination stations. It also considers transportation costs from each treatment station, public network location and desalination station to each receiving industry.

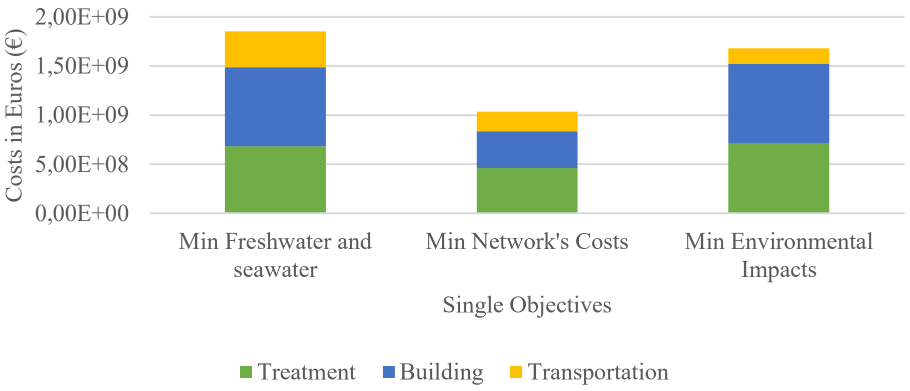


Figure 17 - Cost distribution of scenario To-Be (2)

Firstly, there is a clear difference between the cost structure from this scenario and the previous ones. One of the most relevant changes is the contribution of transportation costs across cases A, B and C. Indeed, these costs are considerably larger for the case of minimizing water intake than the ones obtained for both the cases of cost and environmental impacts minimization. In case B, this can be attributed to the fewer interindustry connections, and for case C, it is due to the shorter distance between the desalination station and the paper industry rather to agriculture in case A.

In addition, comparing case A across scenarios, it is possible to conclude there is an overall significant increase in costs. This increase is caused particularly by the transportation costs, which amount to 365M €

and represent 20% of total costs. This increase is due to the different connections from industrial symbiosis and to the supply of agriculture through desalination, leading to the construction of long pipelines. Building costs also experience a significant increase compared to scenarios As-Is and To-Be (1), reaching 860M € and accounting for 44% of the cost distribution. This increase is justified by the additional use of the desalination station and remaining need to install all treatment stations. Treatment costs also rise due to the large volume of water treated in the treatment and the desalination stations, amounting to 682M € and representing 37% of the overall costs.

In case B, the cost structure increases significantly since the model cannot solely rely on the public network as it did in the As-Is and To-Be (1) scenarios. This case now includes treatment and building costs, accounting for 45% and 36% of the overall cost structure, respectively. Transportation costs increase to 200M €, but their contribution to the overall costs decreases from 100% to 19%, due to the additional consideration of the two other cost components.

Comparing case C to its corresponding case in the As-Is and To-Be (1) scenarios, there is a significant increase in treatment costs, amounting to 710M € and representing 48% of the overall costs, compared to the previous 26%. This increase is solely due to the utilization of the desalination station, which treats a large volume of water, resulting in higher costs. Transportation costs follow the same pattern, increasing to 160M € and accounting for 10% of the overall cost structure, compared to the previous 2%. Building costs also increase to 860M € due to the installation of all treatment and desalination stations, but their contribution to the total cost decreases to 48%, primarily due to the significant increase in treatment and transportation costs.

Overall, this scenario exhibits the most homogeneous cost type distribution when compared to the previous scenarios, still predominantly dominated by building and treatment costs.

The environmental impacts studied in this scenario are the ones associated with the desalination station operation, as well as the impacts associated with transportation from the station to industries. This way, for cases A, B and C, figures 18, 19 and 20 are shown, respectively.

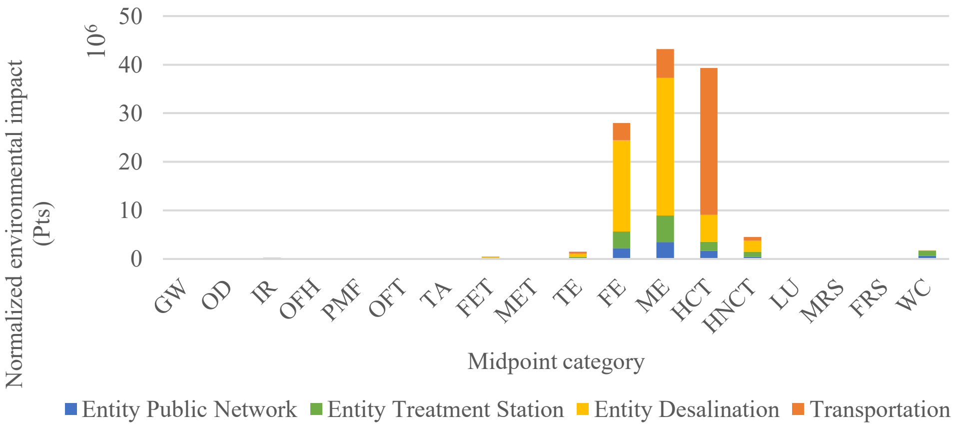


Figure 18 - Environmental impact distribution by midpoint categories in scenario To-Be (2) network for case A

Analysing Figure 18, it is possible to conclude that the categories of Marine Ecotoxicity (ME), Freshwater Ecotoxicity (FE), and Human Carcinogenic Toxicity (HCT) remain the most impactful in the network. However, there is another shift in the most contributing category comparing to scenario To-Be (1). In case A, the category of ME achieves higher impacts due to the inclusion of desalination as an alternative. This contribution is logical since desalination is associated with the production and discharge of brine, which can negatively impact the marine ecosystem. While transportation still plays a significant role in the overall environmental impact, the production of desalted water emerges as the highest contributor in case A.

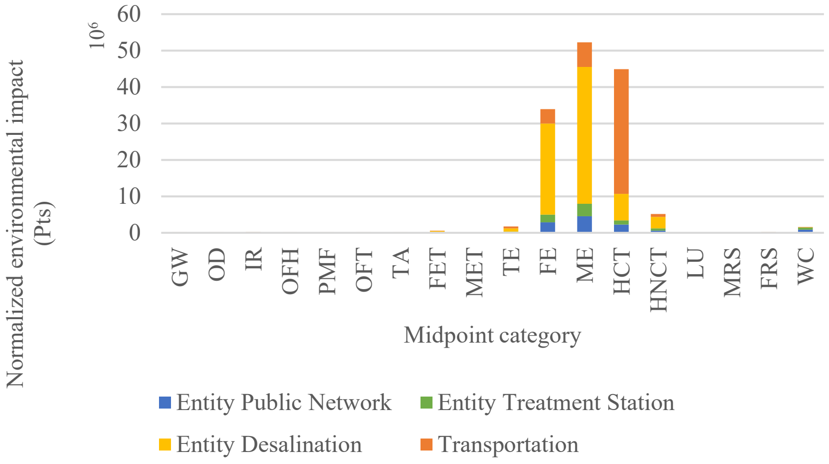


Figure 19 - Environmental impact distribution by midpoint categories in scenario To-Be (2) network for case B

For case B, the distribution of impacts across midpoint categories is similar to that observed in case A. Desalination continues to be the most significant contributor, followed by transportation. The categories of ME, HCT, and FE remain the most influential in terms of impact. However, the overall values are now higher due to the increased reliance on desalinated water, which involves transportation over longer distances, also increasing the transportation impact.

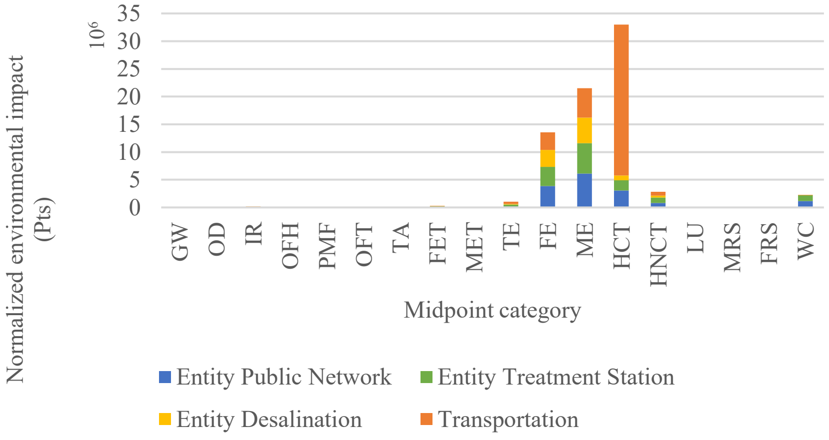


Figure 20 - Environmental impact distribution by midpoint categories in scenario To-Be (2) network for case C

In case C, the most impactful category reverts back to HCT, aligning with the impact distribution observed in case A of scenario To-Be (1). This is expected since case C involves the least utilization of desalination, similar to scenario To-Be (1) where desalination is not chosen. As a result, transportation emerges again as the most influential factor contributing to the final environmental impacts.

From the analysis of figures 18, 19, and 20, it can be concluded that Marine Ecotoxicity and Human Carcinogenic Toxicity are the most impactful categories in this scenario. The usage of desalination as an alternative water source significantly contributes to Marine Ecotoxicity due to the production and discharge of brine. On the other hand, Human Carcinogenic Toxicity is driven by the transportation infrastructure required for long distances, which involves materials and chemicals that can pose risks to human health.

Finally, it is relevant to understand the water consumption for each case, considering the three different alternatives. Table 25 presents those values.

Table 25 - Total water intake (in m3) distribution for the To-Be (2) solution considering each different objective function

	Min Freshwater and Seawater	Min Total Costs	Min Environmental Impact
Water Reused	2.78E+08	1.73E+08	2.78E+08
Freshwater	1.72E+08	2.25E+08	3.05E+08
Seawater	1.58E+08	2.10E+08	2.56E+07

In this scenario, desalination is employed for all cases due to the capacity restrictions. Cases A and C have the same amount of reused water, as they follow a similar trend in objectives. However, case B opts for a lower amount of reused water in order to reduce costs. Although cases A and C have the same amount of reused water, there is a difference in the quantities of freshwater and desalinated water. Case C aims to minimize environmental impacts, resulting in the lowest possible use of desalinated water due to its high environmental impact. On the other hand, case A prioritizes the minimization of both fresh and seawater, without specifically focusing on reducing seawater consumption. Consequently, case C relies on less seawater, but resorts to a higher amount of freshwater.

Figure 21 provides a clear representation of the evolution of water reuse, freshwater consumption, and seawater intake for case A across all studied scenarios. Case A is particularly important as it emphasizes the priority given to reducing the consumption of raw water in the context of water scarcity.

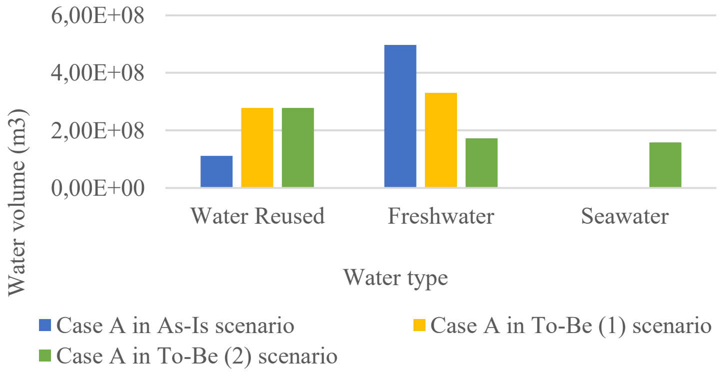


Figure 21 - Water intake from all sources for case A in each scenario

When comparing all scenarios, case A in scenario To-Be (2) reveals the lowest freshwater consumption. The main difference to scenario To-Be (1) is the usage of desalination in order to culminate the capacity limitation of the public network. By resorting to this other alternative, freshwater intake decreases 65% and 48% compared to the scenarios As-Is and To-Be (1), respectively.

It is worth noting that the findings of the sensitivity analysis in section 5.3.1 suggest the possibility of achieving a freshwater consumption volume of 0m^3, which would be the ideal scenario for mitigating the pressure on freshwater resources. However, reaching this null volume has significant implications in terms of costs and environmental impacts. Therefore, careful consideration of trade-offs is necessary when aiming to reduce freshwater consumption. This way, the solution found for case A of the To-Be (2) scenario allows industries adapt to a water scarcity context by relying less on freshwater, but at the same time balancing the costs and environmental impacts associated with this reduction.

5.4.2 Multi-objective: ε-constraint

Once the optimization of each objective function has been performed independently and their comparison has been analysed, it becomes relevant to explore their combination, which presents a multi-objective problem. This approach aims to identify feasible solutions that potentially improve at least one objective while keeping the other values optimal. In light of this, the ε-constraint method is applied, generating a set of non-dominated solutions that form the Pareto Front (Mavrotas, 2009). Each solution in the Pareto Front cannot be improved in terms of one objective without sacrificing performance in another criterion. In simpler terms, no solution on the Pareto Front is superior to another solution across all objectives.

Table 21 (in section 5.4.1), reveals that the optimal solutions can vary significantly depending on the prioritization of objectives. Some solutions of scenario To-Be (2) outperform the current network, while others perform worse. To gain deeper insights into the trade-offs between solutions and objectives, the interrelationships between each pair of objectives is studied by representing them bi-dimensionally. Firstly, the impact of decreasing fresh and seawater intake on the total costs is presented in Figure 22.

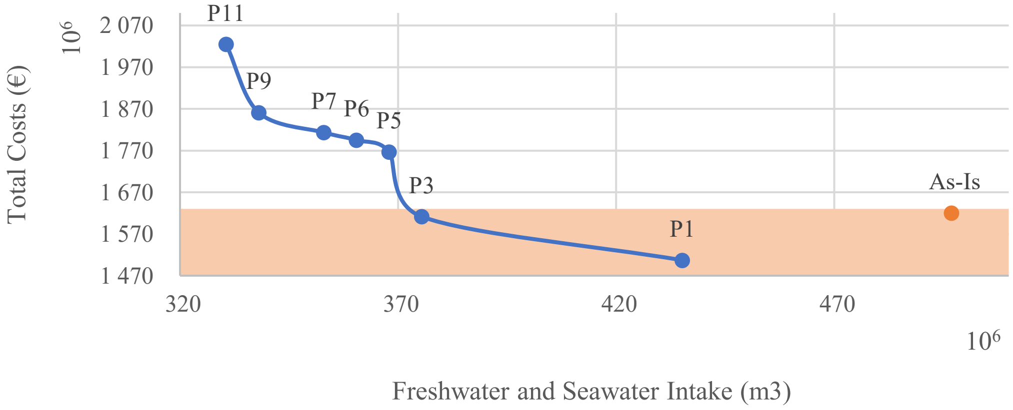


Figure 22 - Bi-dimensional representation of the Pareto front of Freshwater and Seawater Intake compared to Total Costs, including the As-Is solution

In Figure 22 only the non-dominated solutions are presented, which is the reason behind the omission of some points from this bi-dimensional representation. This exclusion is due to some cases where the cost variation within the considered range of increasing water intake was insufficient to warrant a change in the network configuration, resulting in solutions that presented the same costs for different levels of fresh and seawater intake. On the other hand, for the represented points, the increase of water intake caused a decrease in costs, allowing the model to consider other network structures. For instance, it might choose to replace a symbiotic relationship with the public network source, which has lower costs and higher freshwater intake.

The variation of water intake from its minimum value to its maximum in the efficient set corresponds to 32%. For this fluctuation, the impact on total costs is of approximately 26%. This way, it can be concluded that the amount of freshwater and seawater possible to intake, and consequently the water sources chosen, have significant impacts in the total network costs.

The solution of the current network scenario is also represented in Figure 22, as a way to compare it with the efficient solutions of the Pareto Front. The Front reveals two points that exhibit lower freshwater and seawater intake, along with reduced costs compared to the As-Is solution. These efficient solutions are enclosed within the orange rectangle, containing points 3 and 1. Furthermore, there is a considerable cost decrease observed between the P5 and P3 and between P3 and P1, indicating these two points may represent good trade-off solutions.

Comparing the improvements P3 and P1 offer over the As-Is solution, P3 achieves a 24% reduction in water intake and 1% reduction in total costs, while P1 achieves 12% and 7% reductions, respectively. Given the primary objective of minimizing water intake, P3 stands out as the superior option regarding the trade-off between water intake and total costs. It achieves values of 3.75E+8 m^3 for water intake and 1.61E+9 € for total costs.

Secondly, the focus turns to the effect that varying water intake has on environmental impacts. The bi-dimensional representation of the non-dominated solutions, along with the As-Is solution, are represented in Figure 23.

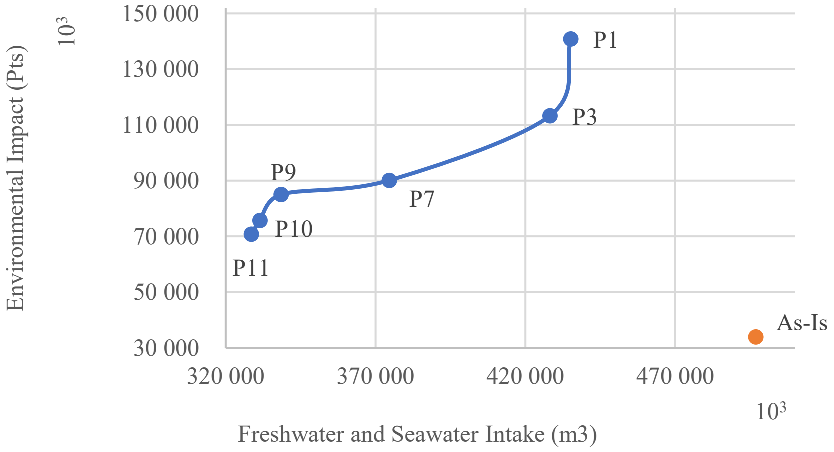


Figure 23 - Bi-dimensional representation of the Pareto front of Freshwater and Seawater Intake compared to Environmental Impacts, including the As-Is solution

Figure 23 shows a distinct pattern compared to the previous Pareto front chart, since an increase in water intake causes an increase in environmental impacts. This outcome is expected, as both objectives follow the same trend, meaning that directly or indirectly, they simultaneously minimize freshwater and seawater intake as well as environmental impacts. In this case, a 33% variation in water intake leads to approximately a 100% fluctuation in environmental impacts. This significant influence of water consumption on the network's environmental impacts can be attributed to desalination. For instance, when there is a lower amount of freshwater and seawater that can be consumed, the possibility of opting for desalination is also reduced, resulting in decreased environmental impacts.

Additionally, when comparing all points with the As-Is situation, another expected result arises: no solution from the To-Be (2) approach is ever better in terms of environmental impacts. At the same time, all points are situated to the left of the As-Is solution, meaning all points of the efficient set present lower volumes of water consumed. These results are easily explained by the context of scenario To-Be (2), which intends to represent the future situation of industries, where water scarcity requires them to adapt and resort to alternative water sources. While this adaptation helps alleviate water intake, it simultaneously results in higher environmental impacts, aggravating this component.

Although no solution offers superior results in terms of environmental impacts, the point that demonstrates the most significant reduction in both this objective and water intake is P11, with a 33% decrease in fresh and seawater intake and a 108% increase in environmental impacts.

Thirdly, the focus is given to the variation of total costs and the impact it can have on environmental impacts. The relationship between both and the resulting Pareto Front (non-dominated solutions) obtained are shown in Figure 24.

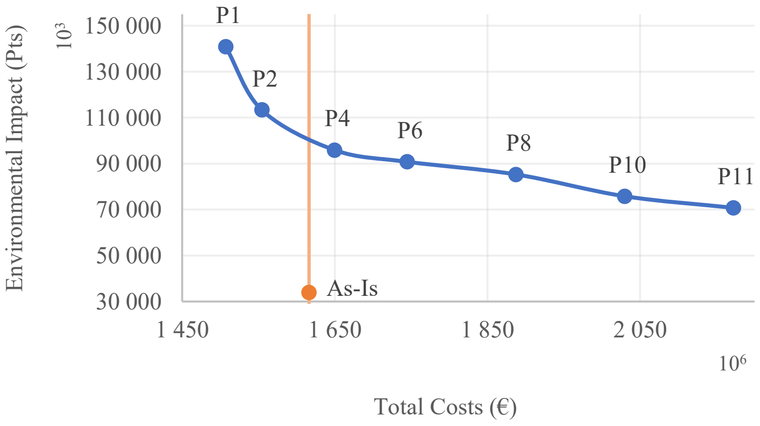


Figure 24 - Pareto Front of Total Cost and Environmental Impact with As-Is solution

Figure 24 presents the decreasing environmental impacts when increasing total costs. From this set of efficient solutions, it is possible to conclude that for a variation in total costs of 44%, the environmental impact can be reduced by 47%, meaning that each objective has a strong effect on the other one.

The figure also allows the comparison of the efficient solutions from the scenario To-Be (2) with the solution obtained in the As-Is situation. Two main conclusions can be drawn: Firstly, no solution in the To-Be (2) scenario achieves the low environmental impact observed in the As-Is solution. This is a consequence of the water scarcity context, being straightforward that the environmental impacts will be higher due to the need to resort to alternatives other than the public network. Secondly, there are two solutions in the Pareto Front that result in lower network costs compared to the As-Is solution, points P1 and P2. In terms of environmental impact, the solutions present an increase of 315% and 233%, respectively, when compared to the As-Is solution. However, in terms of costs, the improvement is of 4% and 7%, respectively. Despite the neglectable difference in costs improvement between the two solutions, the increase in environmental impacts is less accentuated for P2. Therefore, considering the trade-offs between cost reduction and environmental impact worsening, the P2 solution is the better candidate for the optimal network in terms of these two objectives.

Regardless, it is important to study the optimal solution considering the trade-off between the three objectives, not just in pairs. This way, in order to obtain the most complete and robust analysis possible, Figure 25 presents the Pareto Front of the combination of the three objectives. The order by which the objectives are considered remains consistent with the rest of the study: firstly, fresh and seawater intake; followed by total costs; and finally, environmental impacts.

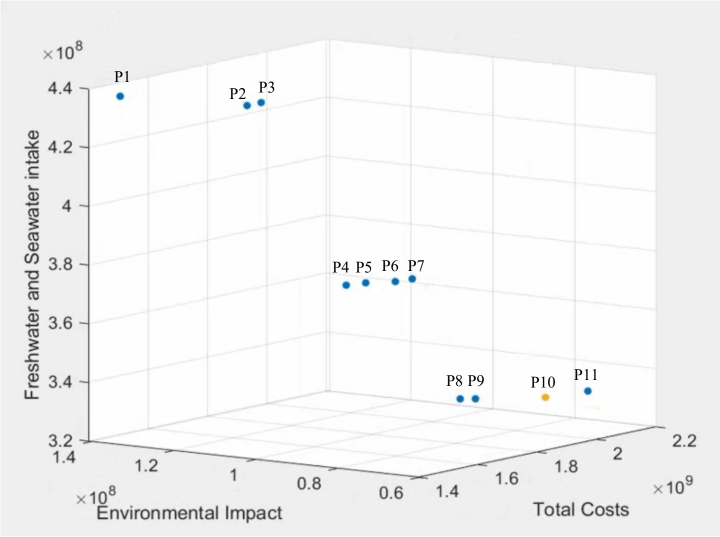


Figure 25 - Tri-dimensional representation of multi-objective optimization

Analysing Figure 25, it is possible to deduce the best solution is represented by P10. While it may not have shown the best trade-off in the two-dimensional objective representation, it offers the most favourable balance among all three objectives, suggesting it could lead to an optimal network structure. Table 26 illustrates the solution's values for each objective.

Table 26 - Results for the best solution considering the three objectives

	Fresh and Seawater intake (m^3)	Total Costs (€)	Environmental Impact (Pts)
Multi-objective solution: P10	331 457 445	2 029 700 171	74 816 116

Comparing the results obtained in Table 26 with the As-Is solution, it is possible to conclude there is a decrease in freshwater and seawater consumption, accompanied by an increase in both costs and environmental impact. Indeed, the decrease in freshwater and seawater intake is the same 33% verified when studying the single objective optimization. For this decrease in water intake, there is an increase of 26% and 120% on total costs and environmental impact, respectively.

Regardless, when comparing the solution with each of the single objective values from the To-Be (2) scenario, it is possible to conclude that the multi-objective solution provides the best trade-off between the three objectives. Indeed, the water intake and environmental impact values closely approximate the minimum values derived from the single objective optimizations. In terms of costs, the solution shows a minor increase in comparison to the optimal value achieved through the single objective approach.

Overall, by essentially achieving the minimum possible values for water intake and environmental impact, while only marginally penalising costs, the ε-constraint approach provides the best combination of all objectives. In the end, this solution presents the best results analysed to this point.

In order to compare the distribution of water consumption by water source for each situation analysed, Figure 26 is obtained.

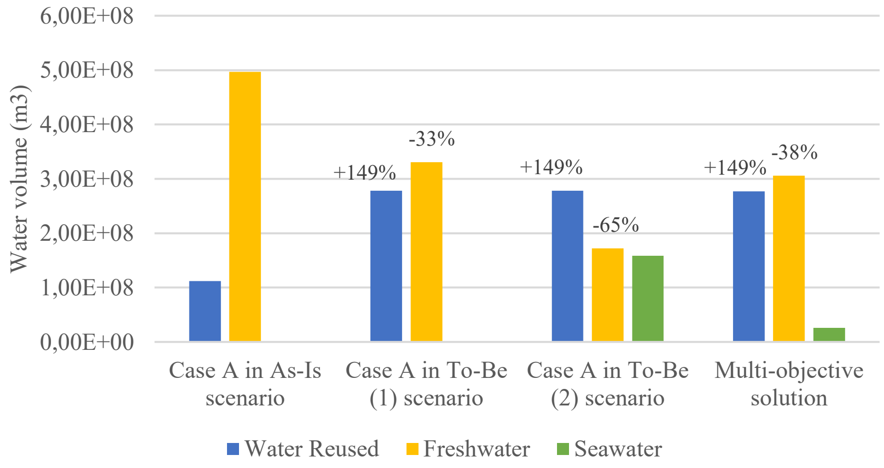


Figure 26 - Comparison of water intake between each scenario's single-objective case A solution and the multi-objective solution for scenario To-Be (2). The percentages represent the increase or decrease in m3 compared to the As-Is scenario.

From Figure 26, it is possible to deduce three relevant conclusions. Firstly, with the incorporation of industrial symbiosis and desalination options, a substantial reduction in freshwater consumption is evident, as depicted by the yellow columns representing the latter three scenarios. Secondly, regardless of the amount of freshwater and seawater sourced, the volume of reused water remains consistently at its maximum across the To-Be scenarios and the multi-objective solution. Thirdly, the scenario To-Be (2), which relies on the highest proportion of seawater, exhibits the lowest freshwater consumption among the scenarios. It is important to emphasize that although minimizing freshwater usage is vital in a water scarce context, it remains essential to consider economic and environmental aspects. Notably, while the freshwater consumption in scenario To-Be (2) may be 27% lower than that of the multi-objective solution, the associated environmental impacts are 60% higher. This underscores the necessity of a balanced approach, that can achieve low freshwater consumption volumes without compromising the other dimensions. Achieving this trade-off between objectives is what enables businesses' sustainable development.

The network configuration and flows between industries for this solution are presented in Table 27.

Table 27 - Flows of water between entities for the multi-objective solution

			From						Total Received
			Beverage	Paper	Refinery	Brewery	Public	Desal.	
To	Beverage	Q5	-	-	-	-	7.51E+06	-	1.46E+07
		Q6	-	7.07E+06	-	-	-	-	
	Paper	Q5	-	-	-	-	1.12E+07	2.31E+06	2.00E+07
		Q6	-	6.52E+06	-	-		-	
	Refinery	Q5	-	-	-	-	4.58E+06	-	9.16E+06
		Q6	-	2.82E+06	1.76E+06	-	-	-	
	Brewery	Q5	-	-	-	-	3.81E+05	-	7.61E+05
		Q6	-	3.80E+05	-	-	-	-	
	Agriculture	Q5	4.82E+06	-	4.66E+06	-	9.48E+06	-	1.90E+07
	Total Sent		4.82E+06	1.68E+07	6.42E+06	0.00E+00	3.31E+07	2.31E+06	

Table 27 provides insights into the changes in water sourcing for industries when comparing to case A in Table 22. For the multi-objective solution, all industries now resort to the public network, while reliance on desalination has significantly decreased. Indeed, the desalination station used to be the major supplier for agriculture, now supplying a lower amount to the paper industry. Although the paper industry's proximity to the desalination station might result in potential cost savings, it now serves as a water supplier to multiple industries, except for agriculture due to water quality requirements. As a consequence, its connections with more industries might counterbalance the cost decrease from changing the destination of desalted water. Moreover, both the beverage and brewery industries have ended their self-reuse of water. As a result, the brewery industry does not make use of its wastewater, while the beverage industry exclusively supplies water to agriculture.

The observed flow in Table 27 support the comparisons established in Figure 26 and the values obtained from Table 26. With reduced reliance on desalinated water, both the cost structure and environmental impacts have significantly decreased in comparison to case A of scenario To-Be (2).

Ultimately, this solution represents the best overall performance for all three objectives. However, it is crucial to acknowledge the significant amount of freshwater consumed. As this water resource will become increasingly constrained in the future, it is probable that the network will need to reduce its freshwater intake, which may lead to higher costs and environmental impacts.

5.5 Stochastic approach to take into account industries' demand uncertainty

To increase the study's applicability and closeness to real-world situations, it is relevant to consider the uncertainty associated with it. Although it was not the focus of the study, the demand for the final product plays a crucial role as it serves as the basis for all other flows within the industries, namely water demand

and wastewater generation, which affect the whole network established. Moreover, predicting demand accurately is essentially uncertain, mainly based on estimations.

Given the critical role of the final products' demand and its complex prediction, an uncertainty analysis is conducted to understand how the final solutions and network configuration are affected by different variations in the demand pattern. Considering a stochastic approach, a scenario analysis was performed, being possible to gain insights into how the network might adapt and perform under various conditions, providing a more robust and practical assessment for real-world applications. This way, the mathematical formulation was adapted by adding a new set 's', consequently adjusting the variables and constraints affected by the different scenarios. The main decision variable adjusted is $x_{m,i,j,q,t,s}$. The constraints affected by these alterations were also adjusted, and the stochastic objective functions substitute equations (22)-(24) in the water objective function, (25)-(38) in the economic objective function and (39)-(42) in the environmental objective function, now given by equations (43)-(45), (46)-(59) and (60)-(63), respectively.

<u>Freshwater and Seawater Intake Objective Function</u>

$$\min Freshwater\ and\ Seawater\ Intake\ = \sum_s prob_s * (WaterPublic_s + WaterDesal_s) \qquad (43)$$

$$\sum_{(m,i,j):(m,i,j)\in F^{pwINe}} \sum_{q:(q,i,j)\in A^{qOUTpINe}} \sum_{t\in T} x_{m,i,j,q,t,s} = WaterPublic_s \qquad \forall s \in S \qquad (44)$$

$$\sum_{(m,i,j):(m,i,j)\in F^{dwINe}} \sum_{q:(q,i,j)\in A^{qOUTdINe}} \sum_{t\in T} x_{m,i,j,q,t,s} = WaterDesal_s \qquad \forall s \in S \qquad (45)$$

<u>Total Costs Objective Function:</u>

$$\min TotalCostNetwork_s = \sum_s prob_s * (\sum_{i\in I_{ts}} CostSender_{i,s} + \sum_{j\in I_e} CostReceiver_{j,s})$$

$$+ \sum_{i\in I_{ts}} BldCost_i + \sum_{i\in I_d} BldCostDesal_i \qquad \forall s \in S \qquad (46)$$

$$CostSender_{i,s} = \sum_{(m,j):(m,i,j)\in F^{twINe}} (TreatCostIS_{i,j,s} + TranspCostIS_{i,j})/2\ -\ soldReuse_{i,s}$$

$$\forall\ i \in I_{ts}, s \in S \qquad (47)$$

$$TreatCostIS_{i,j,s} = \sum_{k:(q,k)\in S^{qOUTTech}} \sum_{m:(m,i,j)\in F^{twINe}} \sum_{t\in T} cTech_k * x_{m,i,j,q,t,s} \quad \forall\ (i,j) \in U^{te}, s \in S \quad (48)$$

$$TranspCostIS_{i,j} = \sum_{q:(q,i,j)\in A^{qOUTpINe}} cPipe * dist_{i,j} * y_{i,j,q}\ \forall\ (i,j) \in U^{te} \ (49)$$

$$soldReuse_{i,s} = \sum_{(m):(m,i,j)\in F^{pwINe}} \sum_{(q,j):(q,i,j)\in A^{qOUTpINe}} \sum_{t\in T} x_{m,i,j,q,t,s} * priceTreat_{q,t} \quad \forall\ i \in I_{ts}, s \in S \qquad (50)$$

$$CostReceiver_i = \sum_{(m,i):(m,i,j)\in F^{twINe}} (TreatCostIS_{i,j,s} + TranspCostIS_{i,j})/2$$
$$+ \sum_{(m,i):(m,i,j)\in F^{dwINe}} (TreatCostDesal_{i,j,s} + TranspCostDesal_{i,j})$$
$$+ \sum_{(m,i):(m,i,j)\in F^{pwINe}} TranspCostPublic_{i,j} + BuyReuse_{j,s} + BuyFresh_{j,s} + BuyDesal_{j,s}$$
$$\forall\ j \in I_e, s \in S \quad (51)$$

$$TreatCostDesal_{i,j,s} = \sum_{(m):(m,i,j)\in F^{dwINe}} \sum_{q:(q,i,j)\in A^{qOUTdINe}} \sum_{t\in T} cDesal_i * x_{m,i,j,q,t,s}$$

$$\forall\ (i,j) \in U^{de}, s \in S \qquad (52)$$

$$TranspCostDesal_{i,j} = \sum_{q:(q,i,j)\in A^{qOUTdINe}} cPipe * dist_{i,j} * y_{i,j,q} \ \forall\ (i,j) \in U^{de} \quad (53)$$

$$TranspCostPublic_{i,j} = \sum_{q:(q,i,j)\in A^{qOUTpINe}} cPipe * dist_{i,j} * y_{i,j,q} \ \forall\ (i,j) \in U^{pe} \quad (54)$$

$$BuyReuse_{j,s} = \sum_{(m):(m,i,j)\in F^{twINe}} \sum_{(q,i):(q,i,j)\in A^{qOUTtsINe}} \sum_{t\in T} x_{m,i,j,q,t,s} * priceTreat_{q,t} \quad \forall j \in I_e, s \in S \quad (55)$$

$$BuyDesal_{j,s} = \sum_{(m):(m,i,j)\in F^{dwINe}} \sum_{(q,i):(q,i,j)\in A^{qOUTdINe}} \sum_{t\in T} x_{m,i,j,q,t,s} * priceDesal_{q,t} \quad \forall j \in I_e, s \in S \quad (56)$$

$$BuyFresh_{j,s} = \sum_{(m):(m,i,j)\in F^{pwINe}} \sum_{(q,i):(q,i,j)\in A^{qOUTpINe}} \sum_{t\in T} x_{m,i,j,q,t,s} * priceFresh_{q,t} \quad \forall j \in I_e, s \in S \quad (57)$$

$$BldCost_i = cBldTreat_i * Open_i \quad \forall i \in I_{ts} \quad (58)$$

$$BldCostDesal_i = cBldDesal_i * Desal_i \quad \forall i \in I_d \quad (59)$$

Environmental Impact Objective Function

$$\min TotalEnvImp_s = \sum_s \sum_{g\in G} prob_s * NormFactor_g * EnvImpPerCateg_{g,s} \ \forall s \in S \quad (60)$$

$$EnvImpPerCateg_{g,s} = EnvImpTranspInf_g + \sum_{i\in I_p \cup I_{ts} \cup I_d} EnvImpWaterProdEnt_{g,i,s} \quad \forall g \in G, s \in S \quad (61)$$

$$EnvImpTranspInf_g = \sum_{(q,i,j):(q,i,j)\in A^{qOUTpINe} \cup A^{qOUTtsINe} \cup A^{qOUTdINe}} dist_{i,j} * y_{i,j,q} * envTransp_g \quad \forall g \in G \quad (62)$$

$$EnvImpWaterProdEnt_{g,i,s} = \sum_{(m,j):(m,i,j)\in F^{pwINe} \cup F^{twINe} \cup F^{dwINe}} \sum_{t\in T} \sum_{(q,i,j):(q,i,j)\in A^{qOUTpINe} \cup A^{qOUTtsINe} \cup A^{qOUTdINe}} x_{m,i,j,q,t,s} * envEntWaterProd_{g,i} \quad \forall g \in G, i \in I_p \cup I_{ts} \cup I_d, s \in S \quad (63)$$

Four scenarios were considered to account for uncertainties in the demand. The base scenario represents the originally expected demand, with a 5% increase every four years, based on historical patterns. However, acknowledging the unpredictability of future demands, scenarios s1, s2, and s3 were also analysed, each assuming different growth rates of 3%, 7%, and 10% every four years, respectively. In future approaches, it would be interesting to include different demand fluctuations for each industry specifically.

Considering the likelihood of these scenarios, the probabilities were assigned as follows: 45% for the base scenario, 15% for s1 and s3, and 25% for s2. The model was then optimized with a focus on minimizing freshwater and seawater intake, and the results were compared with the deterministic scenario To-Be (2), specifically case A. Table 28 presents the solutions for each objective, while Table 29 shows the amount of water used from each type of source, in each scenario.

Table 28 - Results for the deterministic and stochastic approach regarding each objective

	Freshwater and Seawater intake (m^3)	Total Costs (€)	Environmental Impact (Pts)
Deterministic	330 588 670	2 024 764 639	119 453 194
Stochastic	333 102 710	2 033 066 138	112 346 923

From Table 28, it is possible to conclude that the results for the deterministic and stochastic approach are quite similar between them. Indeed, the water intake and costs increase slightly, approximately 0.8% and 0.4%, respectively. The highest change is verified for the environmental impacts, decreasing 6%, which is positive but not considerably significant. These results indicate that the uncertainty in the final product's demand has a relatively minor impact on the overall outcomes. This suggests that the network structure, including the established connections between industries and associated investments, can remain unchanged.

Table 29 - Total water intake (in m3) for each scenario by each water source

	base	s1	s2	s3
Water Reused	2.78E+08	2.74E+08	2.82E+08	2.89E+08
Freshwater	1.72E+08	1.87E+08	2.79E+08	1.87E+08
Desalinated water	1.58E+08	1.38E+08	5.69E+07	1.57E+08

Table 29 shows that scenarios s1, s2, and s3, which represent variations in demand compared to the base scenario (case A of scenario To-Be (2)), demonstrate similar trends in the usage of water sources. The focus on maximizing water reuse remains consistent across all scenarios, leading to relatively stable levels of water reuse, whether from self-reuse or industrial symbiosis. However, there are notable differences in freshwater intake and desalination usage. Scenarios s1 and s3 exhibit an 8% increase in freshwater intake compared to the base scenario, while scenario s2 shows a more significant 62% increase. Conversely, desalination usage decreases by 13% in scenario s1, 64% in scenario s2, and only 1% in scenario s3.

The lower demand in scenario s1 results in reduced water necessity, which, in turn, leads to lower levels of reused and desalinated water and a higher reliance on freshwater. This can be attributed to the cost considerations involved in choosing between different water sources. The public network, being the least expensive option, is prioritized after maximizing water reuse to minimize costs. Nonetheless, the model still resorts to desalination, although less, to culminate the capacity restrictions of the public network.

In scenarios s2 and s3, the increased demand for final products results in higher water necessity and wastewater generation. Consequently, there is a slight increase in water reuse in both scenarios. However, when it comes to freshwater and seawater intake, scenario s2 shows considerably larger changes compared to s3, even though s3 has the highest water demand. The reason for this difference lies in the optimization strategy. The primary objective is to maximize water reuse, but the second priority is to minimize costs. As a result, the model prefers to use the public network whenever possible, as it is the least costly option. In scenario s2, the water demand is such that the optimal solution involves industries relying more on the public network rather than desalination. On the other hand, in scenario s3, the high-water demand makes it impractical to fully satisfy it solely through the public network. Indeed, due to capacity restrictions, there are instances where the public network alone cannot meet an industry's water demand, requiring the use of desalination as an alternative source. In such cases, it becomes more economic and environmentally favourable to rely solely on desalination instead of combining it with the public network. In this case, the optimal combination of alternatives leans more towards continued reliance on desalination, with a slight increase in the usage of the public network.

In conclusion, while there are slight differences in the amount sourced from each alternative due to demand uncertainty, the overall network configuration remains quite similar to the deterministic approach. Table 29 shows that the objectives' results are not significantly affected by the uncertainty in the demand for final products. Therefore, although considering uncertainty is still relevant, in this particular case, it does not have a significant impact on the outcomes.

5.6 Results overview: Recommendations

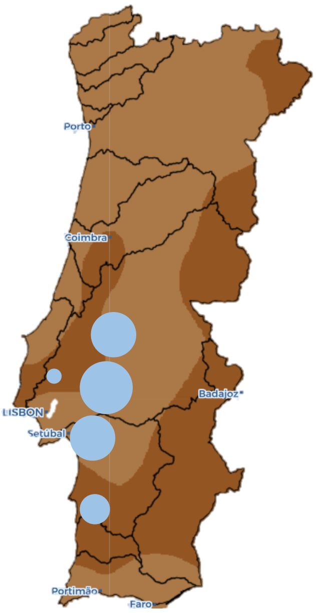
Throughout chapter 5, many scenarios and detailed analysis were undertaken, therefore this section aims to provide an overview of the most relevant points from a managerial perspective.

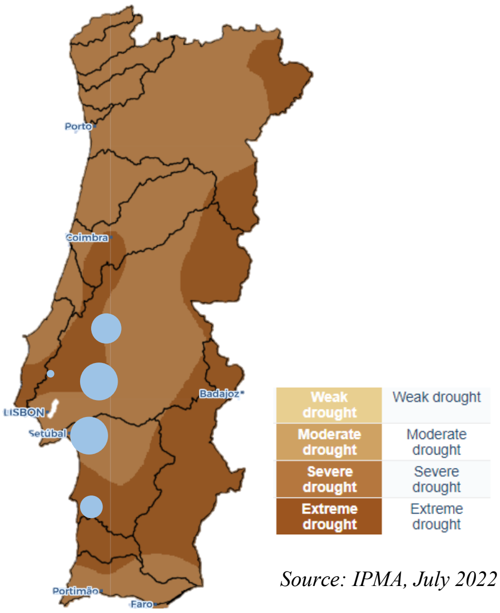
Firstly, it is important to highlight the relevance of the paper industry. By requiring high volumes of water, while at the same time generating large quantities of wastewater, it assumes a significant part as both a receiving and sender entity. Additionally, throughout the scenarios, it is possible to observe the decrease in freshwater intake, and therefore, in the reliance of public network. Consequently, there is an increasing dependency on self-reuse and IS. On the other hand, desalination is only opted for in scenario To-Be (2), when there is a restriction in the public network capacity and the reuse of water has reached its maximum. This option is avoided due to its high costs and environmental impacts.

After analysing the three scenarios, the most attractive solution would supposedly be scenario To-Be (1). Indeed, it presents the same reduction in water intake as scenario To-Be (2), while assuring more reasonable costs and environmental impacts. However, there are two important remarks to acknowledge when comparing these scenarios. First, even though the water volume intake is the same, the amount of freshwater consumed is not. In fact, by resorting to desalination, scenario To-Be (2) enables lower volumes of freshwater consumption, which is the main target when facing water scarcity. Second, the high costs and environmental impacts incurred by scenario To-Be (2) are simply due to the much more severe water shortage context it represents. Since this is the expected circumstance industries will face in the future, this is the most important outcome to study and seek to improve. Regardless, in both scenarios, no single solution achieved the low environmental impact observed in the As-Is solution. This underscores the relevance of industries to adapt to future freshwater restrictions by not only opting for alternatives to this resource, but also by improving the economic and environmental implications of these alternatives.

When considering all three objective functions simultaneously, the solution obtained is the most well-balanced outcome while still addressing the predicted restriction in freshwater availability. It allows for a 38% reduction in freshwater consumption, that even though is not the most substantial decrease observed, results in considerably more reasonable costs and environmental impacts. In the end, this is the recommended network solution, as it provides the best trade-off between objectives, while still achieving a considerable reduction in freshwater consumption.

Furthermore, an added advantage of opting for water industrial symbiosis and desalination is the potential to balance and distribute freshwater extraction points. In every country, certain regions face greater water scarcity, while others have more abundant natural supplies. Embracing these solutions allows water-scarce regions to decrease their freshwater withdrawals, for example by receiving treated wastewater from industries in areas with easier water access. This benefit extends to situations where there is a high concentration of industries in one area, which can put excessive strain on freshwater resources. The adoption of IS and desalination can alleviate this pressure. For a clearer understanding of this notion, figures 27 and 28 provide a visual comparison of freshwater extraction between the existing solution (As-Is) and the optimal outcome from multi-objective optimization. These illustrations use a map of Portugal, pinpointing the regions where the case-study industries are located with circles. Larger circles indicate higher freshwater extraction from nearby public network sources, while smaller ones imply lower pressure on this resource. The map's colour scheme adds another layer of information, where darker shades of brown denote regions facing extreme drought, whereas lighter ones indicate lower water stress.





Source: IPMA, July 2022

Figure 27 - Representation of freshwater consumption by each industry's region for the As-Is situation. The size of the circle is indicative of the amount of water extracted in that region.

Figure 28 - Freshwater consumption by each industry's region for the multi-objective solution. The size of the circle is indicative of the amount of water extracted in that region.

When comparing both figures, there is a clear pattern: the circles in Figure 28 are consistently smaller than those in Figure 27. This observation confirms there is indeed a reduction in freshwater extraction across all industries, resulting in lowered pressure on freshwater withdrawals within each respective region. In addition, this decrease leads to a more even distribution of freshwater consumption among different regions. This higher homogeneity benefits areas with higher water stress, as they can rely more on desalination and water exchange with industries situated in less water-stressed regions.

Therefore, an additional recommendation is to maximize the benefits of this positive effect by involving a larger number of industries. This would increase water exchange between them and thus further alleviate water stress in particularly affected areas.

6. Conclusions

This chapter presents the most relevant conclusions of the developed work in section 6.1. Section 6.2 outlines the limitations of the dissertation while section 6.3 indicates possible future work suggestions.

6.1 Main conclusions

In the context of water scarcity, seeking alternatives to reduce freshwater consumption, particularly in industrial and agricultural sectors, is crucial. Two potential solutions are water industrial symbiosis and seawater desalination. However, reviewing the existing literature revealed certain gaps regarding the application of these two alternatives. Most models developed are designed for smaller-scale purposes, neglecting uncertainty and the simultaneous consideration of economic and environmental aspects. Moreover, very few models optimize networks integrating all potential water sources: freshwater, treated wastewater exchange, and desalinated water. Hence, this study aims to contribute to the literature by developing an optimized industrial network that minimizes freshwater consumption, overall costs, and environmental impacts, simultaneously. For this purpose, a generic MILP model was developed, employing a simple stochastic programming approach to address uncertainty and consequently ensuring robustness. Furthermore, its versatility is enhanced by accounting for different water qualities, making it applicable to broader industrial and agricultural contexts.

The model developed was applied to a case study, providing valuable insights for the establishment of the optimal network solution. Firstly, through single-objective optimization, it was possible to deduce that the inclusion of water industrial symbiosis and desalination options led to a considerable 33% reduction in freshwater consumption by industries. Since desalination incurs in high costs and environmental impacts, this option is avoided, therefore this reduction is only due to the reliance on water industrial symbiosis. Regardless of this considerable improvement, a sensitivity analysis highlighted the significant impact of freshwater availability on network design and connections. Experts predict a future water demand surpassing the available freshwater supply, underscoring the need to examine the model's response to public network capacity restrictions. To address this, a scenario was simulated where the public network capacity was limited by 60%. Under this constraint, results demonstrated a substantial 64% reduction in freshwater consumption compared to the current situation (As-Is). This decrease proves advantageous in water-scarce conditions. Nonetheless, this positive outcome was associated with notable increases in costs and environmental impacts, mostly due to the option of desalination, commonly linked with these negative consequences. Therefore, while the substitutes of the public network source effectively decrease freshwater withdrawals, these alternatives still need to improve in order to ensure economic and environmental efficiency and viability.

When considering the multi-objective optimization, three Pareto sets are obtained by comparing each two objectives together. From this analysis, it is possible to conclude that no solution can provide better results for the environmental impacts of the As-Is solution. Although it is possible to make a compromise regarding costs and water intake, the environmental impacts are always significantly higher than the current network, mainly due to the transportation infrastructure, treated wastewater and desalted water production. When studying the Pareto Front considering the three objectives simultaneously, the best solution found provided a reduction of 38% in freshwater consumption. Even though this reduction was also associated with increases in costs and environmental impacts, the variation was far more reasonable than the single-objective optimization. This way, this solution provided the optimal trade-off between the three objectives, still achieving the significant freshwater reduction sought.

In conclusion, this study addresses the previously presented research questions by demonstrating the viability of water industrial symbiosis and seawater desalination as effective strategies for reducing industries' dependence on freshwater and consequently adapting to water-scarce conditions. However, this reduction is counterbalanced by the associated high costs and adverse environmental impacts, underscoring the necessity to either explore other alternatives or improve the existing ones by enhancing their economic and environmental feasibility. This way, a clear trade-off emerges, where the decision maker should choose the prioritization of the objectives based on the specific circumstances faced.

6.2 Limitations

Despite seeking for accuracy throughout the dissertation, there are still relevant limitations to the work developed. One of the primary limitations of this study is related to data collection. A significant portion of the parameters had to be estimated using various online sources. This not only introduced uncertainty into the values used but it also might have led to inconsistencies when comparing the same parameter across the different alternatives examined. For instance, the building costs of the treatment and desalination stations were derived from different sources, meaning that the difference between them could be significantly higher or lower, which could potentially affect the network establishment. Consequently, although a sensitivity analysis was conducted on the most uncertain parameters, drawing confident conclusions remains challenging due to the inherent variability and potential inaccuracies in the collected data.

Another limitation is the omission of pipeline transportation considerations. In reality, it is common to have aquifer storages to ensure timely access to water in case of pipeline maintenance or disruptions. Moreover, the lack of detail in mechanical and chemical factors can also be seen as a limitation. Indeed, the water pressure in transportation was not considered, ignoring the need for pumps or other devices. The overlook of this type of considerations leads to differences from an accurate real-world representation.

Regarding the consideration of the environmental impacts, it was rather difficult to find specific references in the SimaPro software that could accurately represent each process. For example, when considering the production of treated wastewater in the treatment stations, the only advanced technology available was ultrafiltration, which is not representative of all the technologies included in the case study.

Furthermore, a relevant limitation is the disregard for the process' efficiency. Throughout the water extraction, treatment and transportation, there is an inherent water loss that was neglected. However, these water losses should be included in the model, potentially leading to higher water consumptions. Also, the technologies and procedures used to treat wastewater, the quality obtained and then required, and the number of times the water can be treated and then reused were all significantly simplified.

6.3 Future work

Even though an important step was taken on the inclusion of different water alternatives that enable industries to adapt to water-scarce contexts, there are still many opportunities to be explored in future works in order to tackle the existing literature gaps.

Firstly, enhancing the robustness of this study would naturally involve a comprehensive examination of its limitations, such as exploring deeper into mechanical and chemical factors. This involves a detailed consideration of elements like water transportation and quality, water losses across every process, and other related components. Addressing these finer details is crucial for ensuring the practical applicability of the proposed work.

Secondly, it would consolidate the work if the optimization model accounted for the social component of the triple bottom-line, which is essential when discussing sustainable development. Furthermore, extending the model's applicability requires the incorporation of a wider range of industries and the exploration of transfers involving other by-products besides water. Indeed, extending the industrial symbiosis to other by-products would encourage symbiotic relationships among industries. While it may not be directly related to the freshwater intake issue, it would significantly contribute to waste reduction, further enhancing sustainable development.

Moreover, the possibility of choosing the location of the desalination station within the optimization model should also be considered, as this would potentially lead to a more optimized structure in terms of costs and environmental impacts. Additionally, integrating domestic wastewater from the municipal treatment stations in the network could boost the opportunity for lower freshwater consumption (Maryam & Büyükgüngör, 2019).

Beyond the direct water-related focus, there is the possibility of energy recovery in desalination processes, particularly Reverse Osmosis (Arenas Urrea et al., 2019). The inclusion of this energy benefits would add another level of complexity and sustainability to the model. Lastly, another important consideration that should be included is the water stress index of the regions where industries are located in. By ranking the locations based on this index, there would be an especial preference for IS and desalination in regions with higher water stress indexes. Additionally, it would be interesting to study the effect this decrease in freshwater consumption has on the water stress index, that is, understand how IS and desalination can delay the worsening of water scarcity in those regions.

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Appendix A

Demand data

Table 30 - Demand for all time periods

Time Periods	Beverage	Paper	Refinery	Brewery	Agriculture
1	134 400 000	1 445 600	61 867 500	2 205 420	41 947
2	130 500 000	1 295 000	61 867 500	2 226 000	41 947
3	104 300 000	1 460 000	61 867 500	823 071	41 947
4	117 000 000	1 518 000	61 867 500	2 100 420	41 947
5	141 131 157	1 518 000	64 966 011	2 315 874	44 047
6	137 035 833	1 359 857	64 966 011	2 337 485	44 047
7	109 523 658	1 533 121	64 966 011	864 292	44 047
8	122 859 712	1 594 026	64 966 011	2 205 615	44 047
9	148 199 430	1 594 026	68 219 704	2 431 860	46 254
10	143 899 000	1 427 963	68 219 704	2 454 553	46 254
Units	L	ton	boe	hL	ton

Normalization factor

Table 31 - Normalization factor by impact category

Impact category	Acronym	Normalization Factor
Global warming	GW	1,3E-04
Stratospheric ozone depletion	OD	1,7E+01
Ionizing radiation	IR	2,1E-03
Ozone formation, Human health	OFH	4,9E-02
Fine particulate matter formation	PMF	3,9E-02
Ozone formation, Terrestrial ecosystems	OFT	5,6E-02
Terrestrial acidification	TA	2,4E-02
Freshwater eutrophication	FET	1,5E+00
Marine eutrophication	MET	2,2E-01
Terrestrial ecotoxicity	TE	9,7E-04
Freshwater ecotoxicity	FE	8,2E-01
Marine ecotoxicity	ME	9,7E-01
Human carcinogenic toxicity	HCT	3,6E-01
Human non-carcinogenic toxicity	HNCT	6,7E-03
Land use	LU	1,6E-04
Mineral resource scarcity	MRS	8,3E-06
Fossil resource scarcity	FRS	1,0E-03
Water consumption	WC	3,8E-03

Appendix B

Sensitivity analysis results

Public Network Capacity

Table 32 - Detailed results of the sensitivity analysis to the public capacity network

Public Network Capacity	**10%**	**30%**	**60%**	**100%**
Freshwater and Seawater Intake (m3)	330 588 670	330 588 670	330 588 670	330 588 670
Water Reused	2.78E+08	2.78E+08	2.78E+08	2.78E+08
Freshwater	0.00E+00	9.33E+07	1.72E+08	3.31E+08
Seawater	3.31E+08	2.37E+08	1.58E+08	0.00E+00
Total Costs (€)	2 179 433 029	2 070 540 103	2 024 764 639	1 724 227 425
Treatment Costs	8.75E+08	7.70E+08	6.82E+08	5.04E+08
Building Costs	8.06E+08	8.06E+08	8.06E+08	5.80E+08
Transportation Costs	3.42E+08	2.28E+08	3.65E+08	9.60E+07
Environmental Impacts (Pts)	209 553 792	154 969 487	119 453 194	52 153 554
Entity Public Network	0.00E+00	4.73E+06	8.73E+06	1.68E+07
Entity Treatment Station	1.33E+07	1.33E+07	1.33E+07	1.33E+07
Entity Desalination Station	1.16E+08	8.45E+07	5.64E+07	0.00E+00
Transportation	7.86E+07	5.25E+07	4.10E+07	2.21E+07

Bill of materials for wastewater generation

Table 33 – Detailed results of the sensitivity analysis considering the variation of the bill of materials for wastewater generation

BOM Wastewater	30% increase	Base	30% decrease	50% decrease
Freshwater and Seawater Intake (m3)	254 068 104	330 588 670	414 007 377	469 616 150
Water Reused	3.55E+08	2.78E+08	1.95E+08	1.39E+08
Freshwater	2.54E+08	3.31E+08	4.14E+08	4.70E+08
Seawater	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Total Costs (€)	1 945 287 220	1 724 227 425	1 710 161 703	1 680 061 992
Treatment Costs	7.96E+08	5.04E+08	3.24E+08	2.52E+08
Building Costs	5.80E+08	5.80E+08	5.80E+08	5.80E+08
Transportation Costs	1.51E+08	9.60E+07	9.60E+07	7.52E+07
Environmental Impacts (Pts)	64 688 898	52 153 554	52 386 646	47 776 193
Entity Public Network	1.29E+07	1.68E+07	2.10E+07	2.38E+07
Entity Treatment Station	1.70E+07	1.33E+07	9.33E+06	6.66E+06
Entity Desalination Station	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Transportation	3.48E+07	2.21E+07	2.21E+07	1.73E+07

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