ALTERNATIVE NON-POTABLE WATER USE

DESIGN, COMPLEXITIES, AND OPPORTUNITIES

JESSICA MICHELLE WREYFORD

PROPOSITIONS

1. Alternative non-potable water sources and applications must be included in water management schemes. (this thesis)

2. Feasibility of alternative water use improves when management schemes focus on brine quality rather than the freshwater quality. (this thesis)

3. Data science creates a false sense of security for decision makers.

4. Exclusive reliance on geoengineering to mitigate climate change only offsets impending consequences.

5. Engineered solutions to environmental problems cannot be considered sustainable without the inclusion of all relevant disciplines and perspectives.

6. Money is the primary driver of any environmentally conscious initiative generated by a corporation.

Propositions belonging to the thesis, entitled
“Alternative Non-Potable Water Use: Design, Complexities, and Opportunities”

Jessica Wreyford, MSc
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Alternative Non-Potable Water Use

Design, complexities, and opportunities

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Dedicated to Chase, Knox, and Remington

TABLE OF CONTENTS

Summary 9

Chapter 1. Introduction 15

Chapter 2. Alternative Water Use 27
A critical review of reclaimed water sources, applications, criteria, standards, and overlooked opportunities

Chapter 3. Electrodialysis Modelling 57
Continuous mode electrodialysis modelling methods for brackish water desalination

Chapter 4. Treatment Train Analysis 87
Modelling framework for desalination treatment train comparison applied to brackish water sources

Chapter 5. Treatment vs. Transport 113
A framework for assessing the trade-offs between on-site desalination and off-site water sourcing for an industrial case study

Chapter 6. Discussion 143

References 171

Nomenclature 199

Supplementary Material 209

Acknowledgements 257

SUMMARY

Water scarcity is an undisputed global issue that is spurred by either a lack of availability or access to freshwater. The growing demand for available and accessible freshwater has resulted in increasing competition for water rights. Therefore, supplementing existing water supplies or meeting non-crucial needs with alternative non-potable water has been of growing interest. A common source of alternative non-potable water is reclaimed water. Reclaimed water sources have the potential benefit of long-term reliability and short-term flexibility, both of which are important factors in developing a sustainable and resilient water management scheme.

The objective of this research is to evaluate the complexities of alternative non-potable water use and explore which methods can support a more integrated and comprehensive water management scheme. This research will include the current state of alternative water use, identification of alternative water sources and applications, evaluation of treatment technology performance, and development of decision support methods for the purpose of identifying sustainable water management schemes. The output of this research will be an alternative water sourcing framework that accounts for impacts and factors beyond water quality so that the most appropriate and sustainable option can be identified.

Two types of reclaimed non-potable water are wastewater and brackish water, both of which are more typically overlooked or discharged due to their poor quality. These sources can be potentially reclaimed for non-potable applications or treated to achieve the necessary quality level. However, there are many limiting factors in the pursuit of reclaimed water use. These are loosely categorized into issues surrounding technical feasibility, economic viability, environmental impacts, and social considerations. In **Chapter 1**, it is concluded that, while these themes are generally understood, information is still missing that can intelligently connect reclaimed water sources with the appropriate applications.

A critical review on the state of alternative water use was completed in **Chapter 2**. This was done using a double literature review focusing on the state of reclaimed water use literature. The scope of the review included reclaimed water sources, potential applications,

relevant criteria, and available data and standards. In this chapter, the existing barriers and research gaps related to alternative water use schemes are identified. Through this review it was found that the most commonly investigated sources and applications were those sourced from or applied to human activities. For example, the primary focus of reclaimed water sources was on treated municipal wastewater. This was because of its close proximity to the relevant application and its reliable quantity. However, its quality is highly reliant on human behavior and can range widely based on activities and seasonal variations. Meanwhile, the primary focus of application research was on meeting human needs. However, these applications are prone to human exposure and risk. To improve the likelihood of reclaimed water implementation, it is recommended that the focus of future water application research should either shift to non-human centered applications or better identify the monitoring and collection criteria needs to better address and mitigate the relevant risks and concerns. This chapter concludes that future research must broaden its focus and improve the connection between alternative sources and applications.

One connection that is identified as needing more attention is the potential of technologies to assist non-potable sources in being relevant for application. In **Chapter 3**, a chosen treatment technology, continuous mode electrodialysis, was explored from a modelling perspective to help understand its potential in connecting sources and applications. It was found that continuous mode electrodialysis indeed has the capability to improve alternative water source quality, but there appears to be a lack of understanding of how to model this technology on a systems-level. A systems-level understanding would allow for this technology to be integrated and compared to other technologies to see how it performs in different configurations. An inventory of the existing continuous mode electrodialysis models was completed and two electrodialysis models were selected for implementation. These were then compared using common inputs from empirical data to make it possible to review their accuracy in capturing continuous mode electrodialysis performance. This performance was with regards to salt removal as well as energy demand. The output of this investigation found that semi-empirical methods were able to predicted performance accurately with the added benefit of being able to incorporate necessary modifications and phenomena to reflect changes in the operating conditions.

Given the systems-level modelling capabilities developed in the previous chapter, **Chapter 4** then explored combining different treatment methods into treatment trains. A unique

hybrid-modelling framework was developed for the purpose of evaluating and comparing treatment trains based on the same customizable inputs. This model incorporated the continuous mode electrodialysis model from the previous chapter as well as a slightly modified systems-level brackish water reverse osmosis model sourced from literature. Brackish water reverse osmosis was selected since it is a mature technology that has been widely implemented and the physics-based modelling of this technology was readily available in literature. It was found that the combination of these technologies could benefit from each technology's strengths while minimizing economic and environmental impacts. While the methodology was able to capture the trade-offs between different treatment train configurations, the results were found to be highly reliant on the accuracy of the evaluation methods for each technology. Further, the large number of outputs as well as the complexity of the indicator performance highlighted the need for a higher-level decision support method to help filter through and better comprehend the options generated.

In response to this discovery, a decision support framework using the Data Envelopment Analysis tool was developed in **Chapter 5**. This tool was developed to support decision makers in managing the integration of alternative sourcing options based on technical, economic, and environmental impacts. This framework was then applied to compare the options generated by the treatment train model with the outputs of a water transport networking model which optimizes water networking and transport. The framework assessed alternative water supply configurations of treatment and transport and then identified the most preferable configuration based on economic and environmental indicators. Through this decision framework it was found that these two alternative methods of water sourcing can be complementary measures depending on the scenario.

In the concluding chapter, **Chapter 6**, the state of alternative water use and potential improvements to the water use scheme are presented. The recommended modifications include a broadening of the water use scheme to account for non-potable sources and applications as well as expanding criteria and making standards available to promote alternative use while mitigating risks. In this reflection it is found that this and other research tend to focus exclusively on alternative water use schemes with a primary goal of meeting a product water target or requirement. The brine produced, however, can severely hinder or even limit these configurations. Reframing alternative water use schemes to focus on meeting a brine requirement is suggested to help resolve this issue and this approach was explored via a small exercise. The result of this exercise found that reframing the approach of water use schemes to focus on brine production can in fact improve the feasibility and reduce the adverse impacts. It is, therefore, recommended that future research further explore this idea in the pursuit of mitigating water scarcity issues while being conscious of environmental impacts.

I don't know why we ran out of water,

but apparently we drank it all.

– Fran Liebowitz, Pretend It's a City

CHAPTER 1

INTRODUCTION

1.1 Background

Water scarcity is an undisputed global issue caused by either a lack of availability or lack of access to fresh or potable water [1]. With 2.3 billion people living in water scarce countries, the effects of water scarcity on disease spread, poverty creation, and food insecurity has become increasingly clear through current events [2]–[4]. Poor access to clean water has resulted in annual deadly outbreaks of cholera in Nigeria [5]. The unsustainable use of water resources in Iran has led to the water system becoming bankrupt, sparking deadly protests and extreme political unrest [6], [7]. Drought in Madagascar has caused the country to be on the edge of a famine, with thousands of people currently malnourished [8]. These and other impacts of water scarcity are only becoming larger and more widespread as the climate continues to change and living conditions worsen.

The proven threat of water scarcity has resulted in increased competition for water rights and an urgent need for improved access to safe resources [4], [9]. Improvements to water security are commonly approached through either managing the demand (e.g. improving water use efficiency) or supplementing existing resources (e.g. harvesting rainwater) [10], [11]. The existing research for both approaches tend to focus on potable water (e.g. meeting potable demands with potable sources) [12]. However, alternative sourcing schemes which identify non-potable demands and include non-potable sources have the potential to indirectly help address water scarcity as well [13]. This is because, when properly treated and applied to applications, non-potable sources can potentially offset the demand for potable water [14], [15].

Though alternative sourcing is increasing in popularity, the implementation of reclaimed water accounts for less than 10% of the total water demand even in the most progressive water reclamation countries (e.g. Australia and the United States) [12]. When it is implemented, it is primarily in the form of internal reuse schemes (i.e. within a location or sector) where treatment technologies are used to convert non-potable water into usable water [16]–[19]. This is often seen as the most trustworthy and feasible application of non-potable water reclamation since the risks remain internal (e.g. health impacts and reliability) and the implementation can be managed on a smaller scale [20]. Note that the aforementioned risks are discussed further in Chapter 2. The industrial sector has been particularly proactive in pursuing these internal reuse and alternative water management schemes due to reliability issues of water sources and the resulting impact on production and finances [11].

Two commonly investigated non-potable sources are wastewater and brackish water [21]. The use of these alternative non-potable sources have the benefit of long-term reliability and short-term flexibility, both of which are important factors in developing a sustainable and resilient water management scheme [22]. Even with the increased interest and desire for alternative water sourcing, it was found that approximately 80% of global wastewater is still discharged without treatment or consideration for reuse [23]. This means that there is a potentially large amount of wastewater that could be reclaimed to meet water demands in water scarce areas. Further, brackish water sources are often overlooked when implementing alternative water schemes. Instead, desalination installations tend to focus on higher salinity seawater due to its proximity, quantity, and return on investment [24]. The reclamation of these typically discarded or overlooked sources can help alleviate the demand on potable sources while also minimizing their pollution and contamination [9]. To do so, however, requires knowledge on the available methods of treating and applying these sources so they can be safely implemented.

Desalination is one of the most popular methods for addressing water scarcity as it is relied on to produce over 95 million m^3 per day of potable water worldwide [25], [26]. Methods of desalination are typically classified into one of four technology types: membrane, thermal, electro/chemical, and emerging [27]–[29]. Of these, the most commonly implemented desalination technology is membrane-based reverse osmosis (RO). Globally, RO accounts for 69% of the installed desalination plants and has also been extensively researched in literature [25]. The reason for its popularity is its small physical foot print, modular design, and relatively low cost [27], [30], [31]. However, RO is also known to have a high energy consumption, fouling potential, and overly clean effluent [30], [31]. Since the optimization of this technology has been thoroughly exhausted, attention has shifted to other technologies that can minimize these impacts such as electro-based electrodialysis (ED). ED represents approximately 3% of the global desalination capacity and has received increased interest because of its decreased need for pre-treatment, energy savings (as compared to RO), and smaller operational footprint [32]–[34]. However, no single technology or technology type is best for all situations since technology selection depends on several factors [35], [36].

1.2 Problem definition

1.2.1 Omission of non-potable sources and applications

The primary focus when addressing water scarcity has been on supplementing freshwater sources and meeting potable water demand [12], [37]. As a result, the options considered for addressing water scarcity are often limited to potable sources and applications. Non-potable applications are often overlooked because they are considered to be of low importance (i.e. non-human related) or assumed to be met via natural hydrological cycles [38]. However, addressing non-potable demand can be equally important for addressing water scarcity. This is because non-potable applications may be relying on potable water sources even if this quality of water is not necessary [39]. Thus, the increase in availability and access to non-potable resources can significantly offset the demand on potable resources.

Non-potable applications can also play an important role in supporting and protecting human life and may experience their own water scarcity issues. For example, coastal estuaries provide ecosystem support and coastline protection and many have also experienced drought which has led to ecosystem losses and erosion of coastlines [40], [41]. The omission of these types of non-potable applications from regular water accounting may cause them to go further into water stress and exacerbate the impacts of water scarcity [42]. By not including these non-potable sources and applications, water management schemes will be limited in their considerations and a more resilient and sustainable scheme may be missed.

1.2.2 Limited impact assessments

Non-potable water reclamation is an effective way to meet growing demand in water scarce areas without the need to alter demand patterns or processes [43]. Desalination treatment is popular since it can provide potable water in water stressed locations, especially if those locations have access to saline water (e.g. coastal regions) [25]. However, desalination also has adverse impacts that are not always fully considered before implementation [44]. One such issue is the large quantity of brine produced which is increasingly difficult to dispose of [45]. Another issue is the elevated CO_2 output due to desalination energy costs, which is also not in line with current climate impact reduction policies [46]. Additionally, the energy demand required to operate desalination plants can increase the production of energy which, in turn, increases the amount of oil and gas consumed [47]. The increased demand for oil and gas then translates to an increased demand in water to extract these fossil fuels at the extraction locations. The result is meeting the immediate water scarcity issue in one location while possibly creating a water scarcity issue in another location [48]. Therefore, the true sustainability of these fit-for-purpose water treatment and reuse schemes may be questioned when a regionally wider and longer-term impact assessment is completed [49].

1.2.3 Internally focused water management schemes

Relying on internally generated or close proximity non-potable water reclamation is often seen as the holy grail of sustainability as it meets a direct need, reduces waste, and is internally managed [50]–[52]. While this internal focus may meet the definition of sustainability within the bounds of the location, it may have adverse impacts on health or the environment that could be avoided through other approaches [53]. Alternatives to internal water management schemes have been explored to include integrated and cross-sectoral water schemes which expand the boundary of reuse [12], [54]. In cross-sectoral water reuse, the effluents from one location or sector are used as influents for another location or sector. This is not to be confused with water stewardship which is defined as an approach that emphasizes water use equality through collective action [55]. In this case, cross-sectoral water reuse would be seen as one of many actions that could be taken within the context of water stewardship. Within the focus of cross-sectoral water reuse, the expansion of the investigation boundaries can potentially present more sustainable methodologies of water sourcing since the repurposing of water may have less adverse effects than fit-for-purpose water [21].

1.2.4 Lack of treatment technology performance clarity

A common and sometimes required method for exploring and applying non-potable water sources is the application of treatment technologies. Treatment technologies are used to achieve a desired water quality for application while also removing potentially harmful contaminants and minimizing risks to end users [20]. To date, the majority of treatment technology research has focused on the optimization and improved efficiency of specific treatment technologies with specific product water quality requirements [56]. However, the pursuit of single technology optimization appears to be reaching saturation [57].

Moreover, single technology approaches are sometimes unable to offer solutions for water reclamation and reuse.

Combining treatment technologies into treatment trains is, therefore, seen as the next step in advancing reclaimed water use possibilities [27]. Combining technologies, however, creates an exponential growth in potential options and configurations. Understanding which of these are the most sustainable and appropriate configurations is quite complex [20]. Therefore, to reduce this complexity, treatment trains are typically evaluated on a case specific bases for specific technologies pairing or combinations rather than viewing the true range of possibilities in a generic way [58], [59]. The true performance capabilities of treatment trains and the optimal configurations are, as a result, not well studied and insufficiently understood and accounted for.

1.3 Objective

The objective of this research is to evaluate the complexities of alternative non-potable water use and explore which methods can support a more integrated and comprehensive water management scheme at a regional scale. This research will cover the current state of alternative water use, investigate treatment technology modelling methods, evaluate the potentials of treatment trains, and develop a decision support method to support the pursuit of alternative water management schemes. The output of this research will be an alternative water sourcing framework that accounts for technical, economic, and environmental impacts so that the most appropriate and sustainable option can be identified. Though it is acknowledged that alternative non-potable sources may often include a variety of contaminants, for research clarity the scope of this investigation will be focused on salt removal. With this in mind, however, the research will be pursued in a way that the framework can be easily modified and expanded to address other contaminants in the future.

1.4 Overview of research

This research will explore all aspects of alternative water reuse from source to disposal. This will be founded on the conventional water use scheme presented in Figure 1.1. In this more linear scheme, water is usually taken from potable sources, undergoes a method of

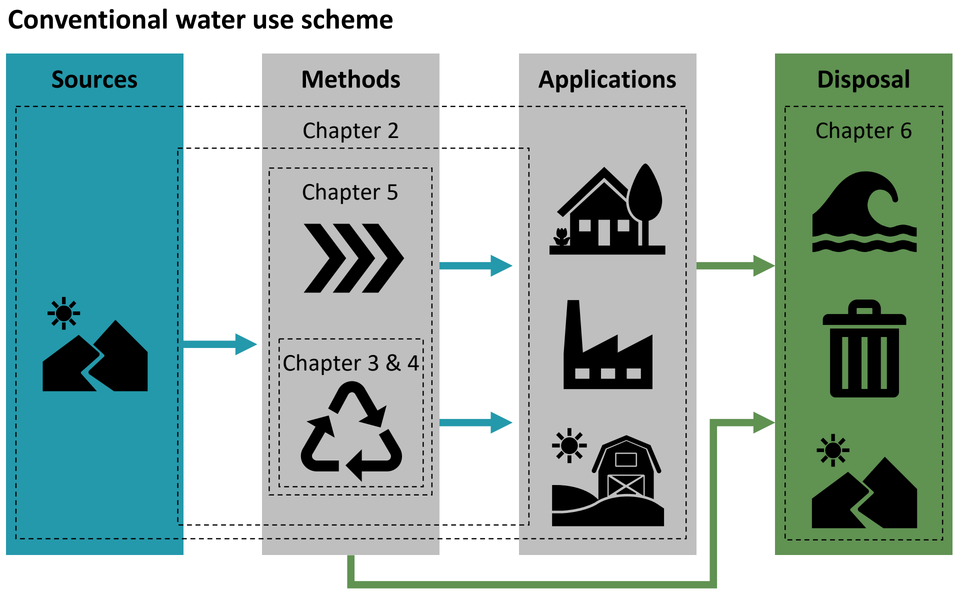

Figure 1.1 Overview of the focus of each chapter within the framework of a conventional water use scheme. Chapter 2 will cover alternative sources and applications, Chapter 3 will investigate treatment technology modelling, Chapter 4 will develop a treatment train model, Chapter 5 will develop a decision science approach to compare different alternative sourcing methods, and Chapter 6 will explore reframing brine management.

Sources: Environment. Methods: Direct use or recycling. Applications: Residential, industrial, or agriculture. Disposal: Surface water, disposal, or environment.

connection such as treatment or transport, is used for a particular application, and then discharged to the environment. This research will focus on each aspect of the conventional water use scheme and investigate how these can be expanded or improved to include alternative water sources, methods, and applications.

This research will begin with a critical review on the state of alternative water use presented in Chapter 2 with extra attention on the known non-potable water sources and their possible reuse. Because of the extent of this literature review, this introduction chapter will remain brief. In this chapter, the existing barriers and research gaps related to the alternative water use scheme will be identified. Because of the extensive elaboration of the state-of-art knowledge and existing knowledge gaps in current literature, as a basis for all the research described in this thesis, this introductory chapter is concise and only summarizes here the overall findings of that chapter. The scope of the review includes reviewing reclaimed water sources, potential applications, relevant criteria, and available data and standards. Through this review it was found that the most common sources and applications investigated were those sourced from or applied to human activities, in comparison to industrial and environmental applications. However, these are also the most prone to human exposure and risk as compared to industrial or environmental applications. This chapter concludes that future research must broaden its focus to include non-human centered applications and improve the connection between alternative sources and applications. One mode of connection that requires more investigation is treatment technologies. Specifically, more information is needed on what treatment technologies are capable of and how their operations can effect technical, economic, and environmental concerns.

To further understand the potential of treatment technologies within the alternative water use scheme, one treatment technology (i.e. ED) will be selected and explored (Chapter 3). ED is selected as it has been proven to effectively desalinate water but represents only a small share of the global desalination installed capacity. Further, there is a lack of consensus on the proper method of modelling this technology on a systems-level which can account for changes in the feed water and operating conditions as well as provide insight on potential impacts such as energy use. An additional goal of having a systems-level model of ED is that it can then be integrated and compared to other technologies based on the same inputs and can even be combined with other technologies to find novel and beneficial pairings. The exploration of the ED modelling begins with an inventory of the existing ED models in literature. From this, two ED models were selected for implementation. These were then compared using common inputs from empirical data and then compared to the empirical results to assess the accuracy of their predictive performance. This performance was reviewed with regards to the predicted salt removal and specific energy demand. The output of this investigation found that semi-empirical methods were able to predict performance somewhat accurately. However, it was also found that the inclusion of additional phenomena such as boundary layer resistance and water transport could potentially improve their accuracy. Once the systems-level modelling for ED is established, the next step would be to see how ED compares to other technologies which are modelled on the same level using the same inputs.

Chapter 4 explores comparing and combining different treatment methods into treatment trains. A unique hybrid-modelling framework is developed for the purpose of evaluating and comparing treatment trains based on the same customizable inputs. This model incorporated the ED model from the previous chapter as well as a slightly modified systems-level brackish water reverse osmosis model sourced from literature. It was found that the combination of these technologies could benefit from each technology's strength while minimizing economic and environmental impacts. While the methodology was able to capture the trade-offs between different treatment train configurations, the results were found to be highly reliant on the accuracy of the evaluation methods for each technology. Further, the large number of outputs as well as the complexity of the indicator performance highlighted the need for a higher-level decision support method to help filter through and better comprehend the options generated.

A decision support framework using the Data Envelopment Analysis tool is then be presented in Chapter 5. This tool was developed to support decision makers in managing the integration of alternative sourcing options based on technical, economic, and environmental impacts. This framework was then used to compare the options generated by the treatment train model with the outputs of a water transport networking model which optimizes water networking and transport. Through this decision framework it was found that these two alternative methods of water sourcing can be complementary measures depending on the scenario. This approach also identified that, while considering economic and environmental impacts are necessary, this method cannot always account for non-quantifiable impacts which should also be considered. Such non-quantifiable impacts include public perception, logistical feasibility, and byproduct production such as brine.

In the concluding chapter, Chapter 6, the state of alternative water use and potential improvements to the water use scheme are presented. The recommended modifications include a broadening of the water use scheme to account for non-potable sources and applications. In addition, it is also necessary to expand criteria and make standards available to promote alternative use while mitigating risks. In this reflection, it is found that this and other research tend to focus exclusively on alternative water use schemes with a primary goal of meeting a product water target or requirement. The brine produced from this approach, however, can severely hinder or even limit these configurations. Reframing alternative water use schemes to focus on meeting a brine requirement is suggested and explored via a small exercise. The result is that, indeed, reframing the approach of water use schemes to focus on brine production can potentially improve the feasibility and reduce economic and environmental impacts. It is, therefore, recommended that future research further explore this idea in the quest for mitigating water scarcity issues while being conscious of their secondary impacts.

I am one big myoma that thinks,

My planet supports only me,

I see my ancestors spend with careless abandon,

Assuming eternal supply

– Bad Religion, Modern Man

CHAPTER 2

ALTERNATIVE WATER USE

A critical review of reclaimed water sources, applications, criteria, standards, and overlooked opportunities

2

ABSTRACT

Reclaimed water use is increasing in popularity due to increased demands and worsening water scarcity. A comprehensive and critical review of the state of reclaimed water research was completed through a double literature review which covered alternative sources, potential applications, relevant criteria, available data, and application standards. It was found that research on this topic focused heavily on human-based sources and human centered applications. However, these are the most difficult sources and applications as they are affected by variable human behavior, can pose direct health risks, and implementation can be limited by public perception. To mitigate these issues, it is recommended to either: i) offset freshwater demand by addressing non-human centered applications or ii) improve source data availability to address the concerns and risks associated with the potential applications. The former approach requires increased research focus on environmental and industrial applications while the latter requires significant investment into monitoring and standardization of water quality criteria. It is recommended that both trajectories be pursued to facilitate reclaimed water use in the future.

A slightly modified version of this chapter is under review as:

Wreyford, J. M., Chen, W. S., Widyaningrum, D. S., & Rijnaarts, H. H. M. A critical review of reclaimed water reuse: sources, applications, criteria, standards, and overlooked opportunities.

2.1 Introduction

2.1.1 Background

Water scarcity is spurred by either a lack of availability or access and its presences is growing around the world [60]. The primary drivers of water scarcity include over exploitation (e.g. population growth and urbanization), climate change (e.g. droughts), and contamination (e.g. salt water intrusion and pollution) [61]. The issues surrounding freshwater availability have caused an increase in competition for water rights which has resulted in devastating impacts on both local and global levels [4].

Current water management strategies tend to focus on 'soft path' approaches such as application optimization through water use efficiency improvements or internal water recycling [62]. However, such soft path approaches are not enough to resolve water scarcity issues. 'Hard path' approaches, therefore, are becoming increasingly necessary [4]. The most common hard path approach is the implementation of alternative water sources. Alternative water sources such as reclaimed water can supplement the existing water supply, improving water security [4]. However, many factors such as technical feasibility and public perception must be addressed for reclaimed water sources to be deemed both viable and non-threatening for end users and the public.

Reclaimed wastewater specifically has been regarded for both its long-term reliability (i.e. constant quantities produced each day) and short-term flexibility (i.e. readily available and quality can be modified when needed). It can also be competitive in terms of energy efficiency and cost effectiveness [63], [64]. Reclaimed water has the additional benefit of reducing wastewater discharge, thus reducing contaminant discharge, alleviating pressure on overburdened infrastructure, and/or minimizing economic and environmental consequences [4], [65], [66]. While technically feasible, additional factors such as public perception, financing, and reliability can limit its implementation [64], [67]. When these additional factors are properly identified and addressed, reclaimed water can become an asset in the development of a sustainable and effective water management strategy [62], [67], [68].

A structured overview or roadmap to help direct and promote the use of reclaimed water is currently lacking. Existing research is often context specific and the available criteria and standards often vary. This makes it difficult to compare or exchange knowledge between sectors, cities, or regions [64]. This lack of clarity can result in hastily implemented water management strategies that do not fully vet the range of options or source risks [63], [67]. Further, these improperly implemented schemes can create negative impacts which can further tarnish the image and acceptance of reclaimed water use.

2.1.2 Aim

This critical review intends to facilitate future research on reclaimed water use by assessing the state of the existing literature. The aim of this critical review is to get both a comprehensive overview of the state of reclaimed water reuse and identify the existing barriers and research gaps. The scope of this investigation will be divided into two primary themes. The first will focus on reclaimed water sources and applications (2.4.1). This section will focus on the considered sources and applications and identify where the main focus of the existing research is and where there is room for improvement. The second focus will be on the reclaimed water criteria, data, and standards present in the existing literature (2.4.2). This section will focus on what criteria are relevant to reclaimed water use and extract the included data and standards to identify which aspects are key for reclaimed water use and how these can help promote this research further.

2.2 Material and methods

This research will be based on two systemic literature reviews. The first will be focused on identifying reclaimed water sources and applications. This will be done through a systematic literature review based on the methodology of Voskamp et al. [69]. This methodology uses three phases: i) search strategy; ii) relevance and quality assessment; and iii) data extraction and synthesis [69]. For the first literature the follow search terms were used for the search strategy:

[water] AND [reuse OR recycl* OR reclaim*] AND [application* OR end AND use*]*

It is important to state that the term 'wastewater' was not included as this research aims to focus on all types of reclaimed water. Wastewater, in this case, is only one specific type as reclaimed water can also encompass other overlooked resources such as brackish and non-potable surface water.

The second systematic literature review focused on reclaimed water criteria, data, and standards. This was completed using the same aforementioned approach but with an altered search strategy. The keyword search terms for this literature search were instead:

> *[criteria] AND [water reuse OR water reclamation OR reclaimed water OR recycled water]*

For both literature searches the article type was limited to articles or review papers from peer reviewed journals published after 2005 in the English language. The literature search was completed using two different databases, Scopus and Web of Science, to make sure all relevant publications were discovered.

2.3 Results

2.3.1 Systematic literature review results

2.3.1.1 Reclaimed water source and application literature review

The reclaimed water source and application systematic literature review resulted in a final set of 47 relevant publications. An overview of the filtering process is presented in Table 2.1. Within the final set of publications, six different research aims were identified. These included: i) presenting a treatment technology; ii) optimizing an existing reuse scenario; iii) assisting in decision support; iv) addressing public perception issues; v) providing an overall assessment; or vi) investigating technological feasibility. In addition, it was found that these publications could be further classified based on their scope, which was one of the following:

- *Specific application:* Publication assesses several different sources of reclaimed water to meet the needs of one specific application.
- *Specific source:* Publication assess the use of one single reclaimed water source for multiple applications.
- *Specific connection:* Publication assess the use of one single reclaimed water source for one specific application.
- *General overview:* Publication provides a general assessment including multiple reclaimed water sources and applications.

Classifying the publications based on both their aim and scope was done to help get a better overview of the trends in this field. These trends are discussed in the following sections which are grouped by the publication scope classification. Further information on the final set of publications and their classifications are presented in the supplementary material (S1).

Specific application

Publications with a specific application scope represented 19% of the final literature set. These publications included aims at optimization of reuse [70], decision support [71], public perception [60], [65], overall assessment [72], [73], and technological feasibility [4], [66], [74].

The public perception research aim was the most present in the specific application scope. This is because public acceptance is generally tied to the specific application. For example, Ntibrey et al. investigated reclaimed water used for a public high school while Pham et al. focused on greywater acceptance in residential reuse schemes [60], [65]. While these both tried to identify the perception of reclaimed water and what could be used to improve its acceptance, Alcaide Zaragoza et al. had a more technical approach by trying to use the optimization of reuse to better educate farmers on alternative water reuse for crops [70]. While this was initially intended to prevent over fertilization, this education approach could also be used to improve public perception and acceptance.

Specific source

Specific source publications also represented 19% of the final literature set but only covered three different aims. These were treatment technology investigations [75], [76], overall assessments [77], and technological feasibility [78]–[83].

A good portion of the specific source publications focused on technology implementation. This is somewhat expected since technologies would be applied to sources. In some cases these publications focused on a single technology [75] while others included and compared multiple technologies [76]. Notably missing from this scope was the research aim of investigating public perception. As previously stated, public perception is almost exclusively tied to the intended application. [60], [84], [85]. However, since public perception is also considered to be one of the most limiting factors of alternative source implementation, it is necessary to address this at the source as well [64], [67]. If public

Table 2.1 Systematic literature search results using the Voskamp et al. methodology for reclaimed water sources and applications [69].

	No. of Publications	
Search strategy		
Search terms for title, abstract, and keywords	141[a]	34[b]
[a] *Scopus;* [b] *Web of Science*		
Relevance and quality assessment		
Merge and removal of duplicates	160	
Title screening	64	
Abstract and keyword screening	49	
Document located	47	
Data extraction and synthesis		
Identification of relevant publications through review papers	57	
Text screening	47	
Final set	**47**	

perception issues are identified from the creation of the alternative source, it is possible that these could be better mitigated and the image of these sources could improve.

Specific connection

The most commonly pursued scope was the specific connection scope (39%). It is theorized that this is the most investigated scope as it has the most clearly defined boundary. This can help legitimize investigations and improve both accuracy and reliability of the results. An additional benefit to the clear scope boundaries is that the research aim could be a bit freer to explore different topics. As a result, the specific connection scope was the only scope that covered all six research aims: treatment technology [86], optimization of reuse [87], [88], decision support [63], [89], public perception [84], [85], overall assessment [9], [90], and technological feasibility [68], [91]–[98].

The most common scope-aim pairing of the entire literature set was the specific connection scope with a technological feasibility aim. This is arguably the most clearly defined pairing which is useful for demonstrating proof-of-concepts or reporting on a specific implementation scheme. Examples of these types of publications include the effects of wastewater for irrigating poplar trees [9] and the reuse of greywater for washing machines [68]. However, this narrow focus on a specific reclaimed water pairing limits its relevance for a larger scale hard path approach.

General overview

The publications with a general overview scope represented 24% of the final literature set and included research aimed at decision support [22], [99], [100], public perception [64], [67], overall assessment [42], [61], [62], [101], [102], and technological feasibility [103].

Those publications which had an overall assessment research aim did not actually connect any specific sources and applications. Rather, these publications provided information about the possibilities for water reclamation and reuse on a larger scale. This included identifying barriers [62], reviewing assessment methods [61], or presenting trends in the field of reclaimed water [42]. As such, these publications were typically not associated with any country or location and can be seen as the foundation for a hard path approach [64], [67].

2.3.1.2 Reclaimed water criteria, data, and standards literature review

The reclaimed water criteria, data, and standards literature review resulted in a final set of 45 relevant publications. An overview of the filtering process is presented in Table 2.2. Though this final set was used to identify the relevant criteria, the data and standards presented in both literature reviews were combined to try and accumulate as much relevant information on this topic as possible.

The research aims identified in the reclaimed water criteria, data, and standards literature were found to be the same as those identified in the reclaimed water source and application review (Section 2.3.1.1). The scope of the reclaimed water criteria, data, and standards literature, however, was found to be different. The scopes identified in this literature review were the following:

- *Identification:* Publication focuses on identifying criteria through investigations.
- *Presentation:* Publication presents criteria in the form of a model or assessment framework.
- *Application:* Publication applies criteria to a case study or other application.

Generally speaking, the final literature set was almost equally distributed between these three scopes. Criteria identification publications represented 29% of the final set while

Table 2.2 Systematic literature search results using the Voskamp et al. methodology for reclaimed water criteria, data, and standards [69].

	No. of Publications	
Search strategy		
Search terms for title, abstract, and keywords	349[a]	5,798[b]
[a] *Scopus;* [b] *Web of Science*		
Relevance and quality assessment		
Merge and removal of duplicates	109[a]	86[b]
Title screening	140	
Abstract and keyword screening	64	
Document located	64	
Data extraction and synthesis		
Identification of relevant publications through review papers	72	
Text screening	45	
Final set	**45**	

criteria presentation represented 33% and criteria application represented 38%. The publications are further discussed in the following sub-sections based on their scope. Further information on the final set of publications and their classifications are presented in the supplementary material (S2).

Identification

The publications which identified criteria included research aimed at presenting treatment technologies [104], decision support [105], [106], public perception [107]–[109], overall assessment [15], [99], [110]–[112], and technological feasibility [14], [113]. The wide range of research aims can be seen as reflective of the complicated nature of criteria identification. Reclaimed water use criteria can be both quantitative or qualitative and can be approached from multiple perspectives such as technical feasibility [108], economic viability [112], environmental impacts [109], [111], and public perception [106], [113]. Additionally, the range in criteria identification methods (e.g. surveys, interviews, and general assessments) makes this one of the more difficult to pursue research paths. However, without identification of relevant and accurate criteria, reclaimed water schemes would not be properly assessed.

Presentation

Publications that had the scope of presenting criteria spanned three specific aims. These were optimization of reuse [114], [115], decision support [50], [116]–[120], and overall assessment [12], [39], [121]–[125]. These publications were primarily focused on presenting these criteria through modelling and assessment frameworks to assist in assessing viability [39] or determining the optimal configuration of a reclaimed water scheme [114], [115]. This scope is necessary for research to expand on the topic of reclaimed water as presenting the impacts and criteria that are relevant can help further promote novel or applicable schemes.

Application

The publications that applied criteria covered only two different aims. These were decision support [126], [127] and overall assessment [49], [61], [128]–[132]. Criteria application publications typically used modelling or developed frameworks to assess or evaluate case studies or configurations However, the application of criteria is reliant on the identification scope to be accurate. Therefore, this is the most generally interesting research topic but is not always the most pivotal.

2.3.1.3 Study location

The frequency of the study location for both literature reviews were plotted in relation to the national water scarcity index (WSI) (Figure 2.1a) and the per capita gross domestic product (GDP) (Figure 2.1b). The implemented water reuse per capita was also plotted with regards to the reclaimed water source and application literature review (Figure 2.1c) as well as the presence of source data and application standards across both literature reviews (Figure 2.1d).

The literature reviews shown displayed no notable correlation between the publication frequency and the WSI (Figure 2.1a). However, locations with higher water stress appeared to be less present in the literature. For example, Greece and India are both facing considerable water stress, but neither were well represented in the literature [94], [96]. It was hypothesized that the low presence of literature reported for highly water stressed regions was due to an increased focus on application [101]. In other words, the need for implementing reclaimed water use is so urgent there is not enough time to also investigate this from a research publication point of view. In Figure 2.1b, a generally positive correlation was found, however, at a certain threshold the focus on publication drops off almost entirely. This communicates that research and implementation generally follow each other, until the need to implement becomes a higher priority. For example,

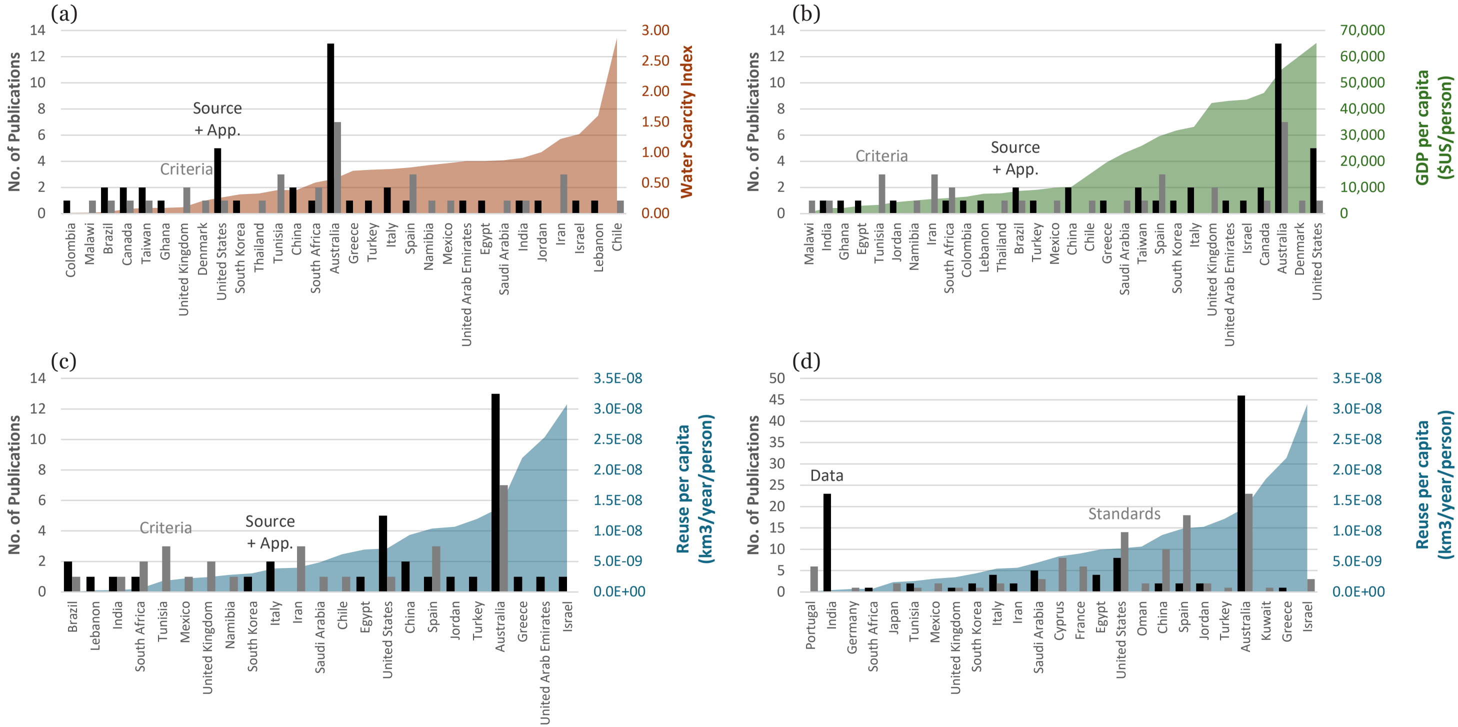

Figure 2.1 (a) The number of publications based on their study location as compared to the national WSI based on Water Resources Institute [133]; (b) The number of publications based on their study location as compared to the national GDP per capita based on The World Bank Group [134]; (c) The water reuse per capita based on Sato et al. as compared to the publication frequency for each literature review [135]*; (d) The water reuse per capita based on Sato et al. as compared to the presence of source data and application standards in the literature [135]*.

**Only shows countries with available water reuse per capita data.*

Israel has one for the highest implementation rates of wastewater reuse but is barely present in the literature [136]. While this shift in priorities could be a factor, it is also theorized that resource availability (i.e. financial support) could be a more limiting factor. Indeed, Figure 2.1b showed that the GDP per capita had the most consistent and positive correlation of the investigated factors on the literature review results.

While this highlights the importance of financial resources for research, it is also clear that all three factors (i.e. WSI, reuse per capita, and GDP per capita) play a role in the decision of where reclaimed water is investigated. Australia is an example of a location that scores relatively high in all three factors. It has an increasing dry climate, is experiencing increased urbanization allowing for reclaimed water schemes to be implemented, and has a relatively high GDP per capita [68]. In this case, all three factors have contributed to this study location showing up the most frequent in the literature review. However, this is not to say that other locations are not equally deserving. It is, therefore, recommended that future research try to incorporate and focus on locations that may be lacking in resources but are equally deserving of reclaimed water interventions to address their water scarcity issues.

With regards to source data and application standards, a total of 120 source datasets and 124 application standards were collected across the two literature reviews. The frequency of data and standards were then compared to the reuse per capita (Figure 2.1d) where a positive correlation was indeed found. However, there appears to be an implementation threshold, where data and standards disappear from the literature. It is believed that this threshold is where the need to implement outweighs the need to investigate, therefore the focus shifts solely to implementation. This should cause alarm, as hastily implemented reclamation schemes without clear standards and data can miss easier source-application connections and pose health risks if not properly vetted. This can potentially lead to negative consequences that can tarnish the perception of reclaimed water use.

2.4 Discussion

2.4.1 Reclaimed water sources and applications

While the literature review encompassed both reclaimed water sources and applications, this discussion will address each individually to highlight the state of each.

2.4.1.1 Sources

Sources of reclaimed water are primarily broken into four categories: environmental, residential, municipal, and industrial [103]. The representation of these categories and their sub-categories in the literature are presented in Figure 2.2, with additional information in the supplementary materials (S3).

Municipal

An overwhelming majority of the literature focused on municipal-based sources (65%). Further, municipal wastewater was the most commonly investigated source for all applications [68]. This coincides with the fact that municipal wastewater is also the largest alternative water source already in use [65]. The applicability of reclaimed municipal wastewater, however, is largely dependent on factors such as source application, infrastructure, legislation, guidelines, and social acceptance [80]. Further, the municipal sub-category (i.e. treated, untreated, or stormwater) poses different benefits and barriers.

Treated municipal wastewater (i.e. wastewater treatment plant effluents) is often regarded as reliable due to its stable flowrate, monitored quality, and scalability [80]. Because of this, treated municipal wastewater was shown to be the most common focus for both literature and implementation [86]. However, treatment plants require significant infrastructure with intensive treatment methods. This can result in cost implications, energy demand concerns, and brine disposal issues. Further, the scopes of these implications are completely reliant on the influent quality (i.e. untreated municipal wastewater) and effluent requirements [80].

While untreated (i.e. raw) municipal wastewater is considered less intensive, it can contain a fluctuating and wide range of contaminants. This is because municipal wastewater is comprised of urban effluents as well as residential, environmental, and, in some cases, industrial sources. While the combination of sources can result in a largely reliable quantity of water, it is less reliable with regards to its quality [80]. Further, the increased disposal restrictions placed on industries often leads to industrial wastewater being discharged to municipal wastewater streams. This increases both the range of contaminants and the likelihood of harmful chemicals ending up in municipal wastewater [80]. A preventative method for managing the diverse quality is to keep different quality streams separate. However, this requires significant infrastructure which can be cost-prohibitive or not technically feasible.

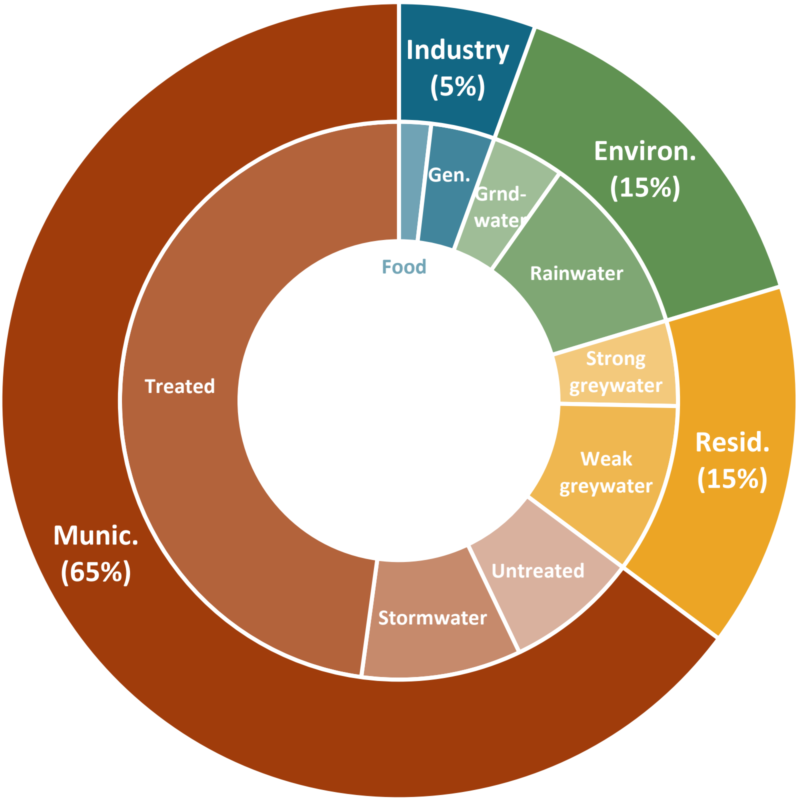

Figure 2.2 Overview of water reuse source categories and sub-categories arranged based on their presence in the literature.

Stormwater is one of the municipal streams that could benefit from these infrastructure improvements [82]. Stormwater is a seasonally dictated source that is typically comprised of runoff from paved roads and surfaces [81]. Though stormwater is originally of high quality (e.g. rainwater), the method of its collection can result in a heavily polluted stream containing heavy metals, hydrocarbons, or even pesticides [66], [81]. If infrastructure can allow for stormwater to be captured safely and kept separate from other municipal wastewater streams, it is possible that it could be a more popular alternative source [82].

In general, municipal sources can be considered a highly reliable source of water with considerable quantity that is conveniently located near to where it is needed. However, municipal sources can also contain a high range of contaminants with varying qualities. These contaminants need to either be removed via treatment methods or controlled via infrastructure improvements. Both, however, can be cost-prohibitive, energy-intensive, and complex. Ideally, it would be better to find ways to use this water with minimal need for mitigation efforts, however, the range in quality and contaminants can pose both human and environmental risks.

Residential

Reclaimed residential sources are primarily divided into low contaminated greywater and highly polluted blackwater. Investigations almost exclusively focus on greywater (see Figure 2.2) since blackwater (e.g. toilet effluent) is heavily polluted and can pose significant health risks if reused [102]. Because of this, blackwater is only considered under the most extreme circumstances [103].

Greywater, on the other hand, has a higher social acceptance rate, represents the majority of residential effluents, and can reach almost drinking water level qualities depending on its initial application [4], [60], [93]. To improve the scope of reclaimed greywater use, greywater is often further classified as either weak or strong [93].

Though not as polluted as blackwater, strong greywater (e.g. dishwashers and kitchen sinks) can have high contamination rates. This high level of contamination requires considerable treatment making it less attractive for reuse [103]. Weak greywater, on the other hand, is characterized as a low contaminant effluent sourced from sinks, bath, showers, and laundry machines [79]. Even though weak greywater is considered higher quality, it can still contain human sourced organic matter [79].

While the quality and quantity of residential greywater can be favorable, its application in a reclaimed water use scheme will always require some additional infrastructure or treatment. Infrastructure can be used to keep residential waste streams separated, which prevents contamination and improves reuse feasibility. Treatment is often needed to achieve the desired water quality but also to remove human-based organic matter that, if not treated, can pose health risks. Additionally, the quantity and quality of residential greywater depends on several factors including lifestyle, location, house size, and water stress which varies between countries, regions, and even houses [60]. As a result, investigations of reclaimed greywater often remain small scale, focus on non-potable applications, and are limited within the scope of a building or home [88], [93].

Environmental

Though environmental sources are typically seen as the original source of freshwater, there are alternative environmental sources with poor quality that are typically excluded from both water management schemes. These alternative sources include but are not limited to wetland effluents, poor-quality groundwater, and harvested rainwater [79], [86], [94]. Though these alternative environmental sources are often mentioned in literature, they are rarely investigated in depth (Figure 2.2).

Wetland effluent which can be used for polishing domestic or industrial wastewater, was found to be missing from the literature entirely. However, constructed wetlands have received increased interest as a nature-based method for removing contaminants from wastewater, providing a reclaimable effluent [137]. While constructed wetlands can improve wastewater quality, they are also highly reliant on the influent quality, require a large footprint, and need considerable time [138].

Poor-quality groundwater (i.e. brackish or contaminated groundwater) is a more generally accepted alternative water source, most commonly used in water scarce areas to address non-potable needs [66], [94]. Poor-quality groundwater is the result of salt water intrusion, over-withdrawal, poor irrigation management, or contamination via pollution [139].

Rainwater harvesting, in this manuscript, differs from stormwater as rainwater is collected and managed by private operators while stormwater is runoff from roads or land that is collected and managed by municipalities. Rainwater harvesting was represented quite well in the literature because of its higher quality, positive public perception, and decentralized distribution [88], [140]. However, it is also characterized as being unreliable, seasonally dictated, and requiring considerable infrastructure [4], [79], [88].

It was surprising that environmental sources were not well represented in the literature since they are, in general, of higher quality and can significantly supplement supplies and address non-potable applications. However, the lengthy replenishment times, seasonal variability, and decentralized nature can be seen as significant barriers to their implementation.

Industrial

Industrial sources are most notable for both their reliability and careful monitoring [66], [94]. However, industrial sources are also known for their large variance in quality and potential for dangerous contaminants which lead to a poor public perception. As a result, industrial sources were the least present in the literature (Figure 2.2). While this research aimed to identify the different industry sources within the literature, only one industry type was clearly differentiated: food processing. Therefore, all other references to industrial sources were grouped in a 'general' category.

The quality and risk associated with industrial wastewater reuse is highly reliant on the industry type. For example, a chemical plant may have a reduced risk for microbial pathogens but an increased risk of chemical hazards [103]. Meanwhile, a food processing plant may have less chemical risk but higher levels of BOD, COD, oil, and TSS [102]. Further, the wastewater composition within a given sector can vary between plants. This difficulty in scaling has directed research to focus on internal, soft path, efficiency improvements rather than on creating connections to other end users [66]

The negative public perception is not only connected with quality concerns but also how it is portrayed in media. Industrial wastewater is most often made noteworthy when it is improperly discharged and having negative impacts on human health or the environment [66], [94]. This can relate back to the application literature specific source scope which was found to be missing the public perception aim. If more focus was put on the public perception of this source, it could remove a barrier to what could be a controlled and reliable source. Further, the improved treatment and monitoring could result in reduced discharge to the environment and municipal streams thus preserving source and improving municipal sources [94]. It is also possible that more localized connections between industrial wastewater and applications are being overlooked.

2.4.1.2 Applications

This review found four primary categories for applications: environmental, agricultural, domestic, or industrial [4], [99]. The representation of the application categories and their sub-categories in the literature are presented in Figure 2.3, with additional information in the supplementary materials (S4). Further, the connections between the aforementioned applications and the previously discussed sources were investigated (Figure 2.4).

Applications were further categorized based on their potential contact with humans and animals (i.e. direct or indirect exposure) and required quality (i.e. potable or non-potable) [100]. In general, indirect non-potable applications were the most investigated because of their reduced risk and achievable water quality. Direct potable applications, on the other hand, were only considered in locations experiencing severe water stress. With that said, the ability to use reclaimed water for direct potable applications is slowly increasing due to improvements in technology capabilities and access [102]. Additionally, the need for potable quality water can change based on cultural customs, economic development, seasonality, and local water availability [4], [68].

Domestic

Sixty percent of the specific application publications were focused on domestic reuse. Of these, the overwhelming majority targeted the application of wastewater reuse for non-potable residential uses.

The domestic application category was the most diverse as well as the most investigated (45%) category. This coincided with domestic being the primary focus of water reuse (32%) (Figure 2.5), but contrasted with actual global water demand (12%) [4], [23], [67]. Based on the global demand, it was found that agriculture was in fact the most prominent application (69%). The discrepancy between where water is needed and what is investigated could be the result of disproportionate distribution of applications between countries. For example, agriculture is a major focus in underdeveloped countries (e.g. South America, South-East Asia, and North Africa), meanwhile, developed countries (e.g. Australia, US, and Europe) primarily concentrate on domestic uses to maintain a certain standard of living [102]. This leads to questioning if the need for domestic water reuse is truly the most relevant application or if this focus is more dictated by wealth distribution factors.

The largest focus of the domestic application investigations was on residential applications, both potable (e.g. bathing, sinks and dishwashing) and non-potable (e.g. gardening, laundry, and toilet flushing) [79], [140]. Laundry and toilet flushing, specifically, were found to be the most investigated due to their consistent demand, low-quality need, favorable public perception, and minimal human exposure [68], [79], [85]. However, these do not necessarily represent the largest demand and still require significant considerations such as costs, infrastructure requirements, and impacts to machinery [92], [141].

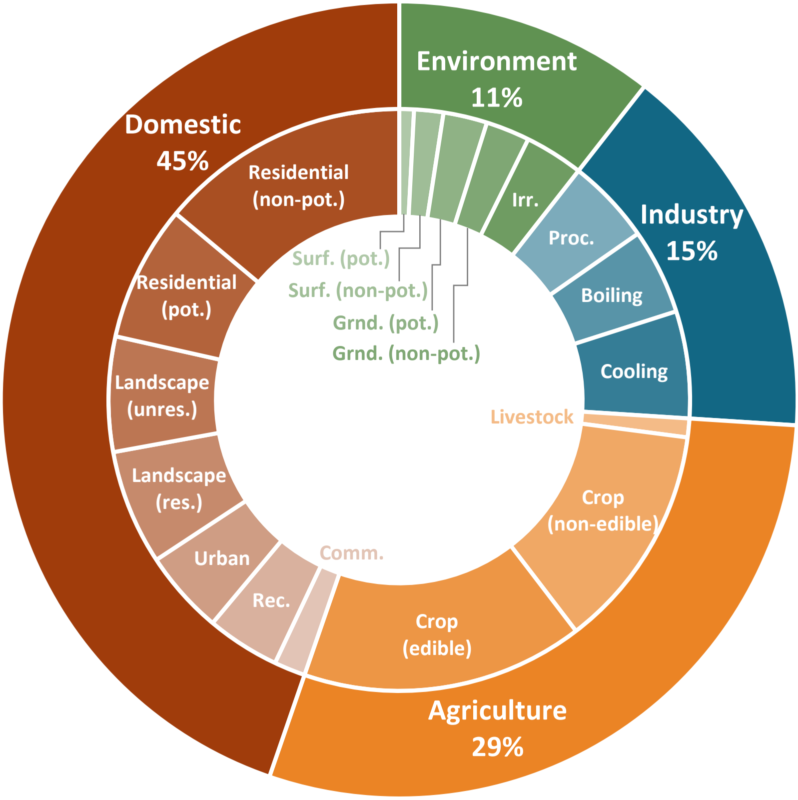

Figure 2.3 Overview of water applications categories and sub-categories based on their presence in the literature.

The next most investigated was landscape and recreation which represents a considerable demand during low-water availability seasons [80]. Its feasibility, however, depends on location specific properties (e.g. topography, plants, and soil) and human exposure. Therefore, landscape and recreation were divided into three categories: restricted landscape, unrestricted landscape, and recreational.

Restricted landscapes (e.g. cemeteries, greenbelts, and non-recreational (artificial) lakes) can allow for poorer quality water since the limited access can reduce concerns related to human health and exposure [67], [86]. Unrestricted landscapes (e.g. athletic fields, water features, parks, and playgrounds) require more stringent requirements as these are either located in or are for the purpose of having high human contact [102]. Recreational applications (e.g. swimming pools, lakes, and artificial snow) have both unrestricted access and a high probability of human contact or exposure [142]. In addition to having high quality standards, recreation also requires high aesthetic standards (e.g. color and smell). Therefore, considerable treatment and reliable monitoring methods are required for recreational applications, resulting in it being one of the least investigated sub-categories [22].

The more general category of urban applications include construction, fire protection, sewer flushing, and other cleaning process use within the urban setting. Urban applications can often use poor-quality water and have a low risk of human exposure. However, the implementation of reclaimed water for urban applications is often limited by the required infrastructure which are frequently complex, technically infeasible, or cost-prohibitive [67].

Commercial applications (e.g. car washes, laundry services, and office buildings) are one of the most commonly implemented applications for reclaimed water use schemes [102]. Car washes and laundry services, specifically, are highly pursued due to their visible water-based practices and non-potable water needs. Additionally, rain and greywater reclamation are often well matched with commercial buildings due to their low demand but high (re)capture potential (i.e. roof space) [4]. However, commercial applications represent only a small portion of total demand and were minimally present in the literature [141]. Therefore, the role of public perception, scalability, and fit appear to have more influence on the direction of implementation rather than general need.

Though, in general, this application category has a reputation for requiring high quality potable water, it was discovered that up to 85% of domestic applications could use non-potable sources [62]. For residential applications, specifically, it was found that only 4% of residential demand requires drinking water quality [100], [140]. However, residential infrastructure typically only allows for one service water type, therefore, the service water quality must meet the highest water quality need [4], [80]. As such, domestic infrastructure is both a major limiting factor and an important point of investigation that could help open up a large market for reclaimed water use [63], [68].

This is exemplified by the strong investigation connection between rainwater sources and domestic applications [63], [91], [93]. Because of the impacts of treatment on costs, energy, and infrastructure, it is beneficial and often preferred to match water sources

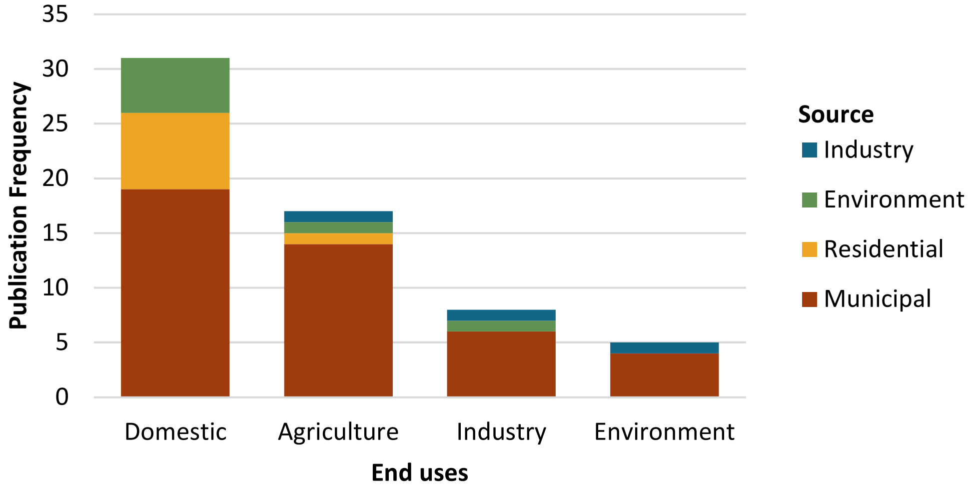

Figure 2.4 Overview of source and application connections in the application literature review.

with similar in quality applications [62]. While this is interesting to investigate due to scalability and fit-for-purpose, its low implementation rate is related to cost-prohibitive infrastructure and low pay-off [67].

Industrial sources, on the other hand, were a potentially reliable source that were entirely missing from the domestic application category (Figure 2.4). This is in part due to its poor public perception and the potential for harmful contaminants [67]. It is, therefore, seen as a missed opportunity that could be implemented if proper treatment, education, and monitoring were completed.

Agricultural

Agricultural applications represent the largest global demand (69%) but were the second most investigated in the literature (29%) [80]. Agriculture is heavily affected by water scarcity and climate change since decreasing precipitation and increasing temperatures can result in lower crop yields [70], [75], [94], [98]. This has impacts beyond the local environment since agriculture is often one of the more prominent parts of a country's global economy and has a direct human impact [70].

The stability and reliability of reclaimed water as well as the ability for some crops to tolerate poor-quality water makes the use of reclaimed water for agricultural applications both feasible and well matched [95], [98]. Further, reclaimed water use can be competitive from both an energy and cost perspective when compared to existing agricultural irrigation practices (e.g. groundwater pumping) [67]. Further, reclaimed water often contains nutrients which can offset the need for fertilizers, having a beneficial impact on both crop yields and production costs [70], [80], [98].

The use of reclaimed water for agricultural applications also includes many points of concern, since reclaimed water can also contain heavy metals, salts, organic micropollutants (e.g. pharmaceutical, hormonic, and pesticides) and pathogens. This can pose significant short- and long-term risks [9], [89], [98]. In the short-term, polluted soil can adversely affect yields and compromise edibility [98]. Long-term damage to soil and groundwater may take years to become apparent and can develop into long-term or even permanent soil quality damage [9]. Therefore, an appropriate level of monitoring and treatment is required to minimize risks while also retaining the beneficial components.

Reclaimed water use for agriculture also relies on several factors such as soil composition, climate, crop type, and topography [94]. The application type of reclaimed water for agriculture is primarily divided into crop irrigation, frost protection, or livestock applications.

Crop irrigation for both edible (e.g. grains, soy beans, fruits, and vegetables) and non-edible (e.g. decorative plants, trees, and textile related) crops were the primary focus of agricultural applications [95], [98]. While both must consider impacts to crop yields and soil quality, they differ on their risk for human exposure. While non-edible crops have limited human exposure risks, edible crops must be dealt with more cautiously since these could eventually be consumed by humans [97]. Therefore, more attention to the water quality, consumption type (i.e. raw or processed), and potential health risks need to be extensively investigated [95], [98]. Additionally, edible crops are also more sensitive to public perception, specifically farmer and consumer health. Therefore, any application of reclaimed water to edible crops should also include a reliable health risk assessment [80], [89], [98].

Frost protection is a tangential application to crop irrigation, however, it differs in that it may directly touch the surface of crops [98]. This definition is important since some reclaimed water is only approved for agricultural applications contingent upon the fact that it does not wet or come into contact with edible parts of the plants [98]. This risk and institutional barrier may explain why it was almost completely omitted from the application literature.

Livestock applications (e.g. dairy farming, fisheries, and pastures) represent a significant water demand that could be a great opportunity for water reclamation [80]. However, this application is minimally investigated as it also comes into direct contact with both humans and animals. The potential for illness to both animals and farmers has resulted in a common distrust and reluctance to implement [22]. It is, therefore, necessary that the health risks be heavily investigated for this application to be considered.

It is also interesting to note that agricultural applications were almost exclusively met with treated municipal wastewater. This is a result of both the low-quality requirement of agriculture and the reliability and quality of treated municipal wastewater effluents [94], [95], [98]. However, the consistently high exposure potential to both humans and animals make any source with pathogen or contaminant issues difficult to implement without reliable treatment and monitoring.

Industrial

The use of reclaimed water for industrial applications is already quite common in developed countries (e.g. Japan, Germany, and the US) [9]. This is because some industrial process are reliant on large quantities and access to water (e.g. hydrogen production) [143]. However, if any water availability issues occur, industrial applications are generally the first to be cut off [67]. This can result in the halting of production which can cause significant economic impacts [87]. The need for secure and reliable sources of water have led the sector to (pro)actively pursue and incorporate alternative water sources into their processes [99]. However, this activism is not well reflected in the included literature. This is primarily due to scoping and scalability issues, as each sector and plant is unique in their needs and operations. Since this is most typically tackled on a case by case basis, it is difficult to draw conclusions and disseminate knowledge between sectors and plants. Therefore, the research that is available tends to focus on three common industrial applications: cooling water, boiler feed water, and process water [80].

Cooling water is responsible for controlling and maintaining efficient industrial process temperatures. It also represents the largest demand of industrial water use (up to 50%)

and is also regarded as one of the most feasible applications of reclaimed water [80]. Boiler feed water is used in either regular or high pressure operations [77]. While regular boiler feed water has a more relaxed water quality requirement, high pressure boiler feed water must be of high quality since contaminants can lead to equipment or process damage [61]. Process water is the least uniform industrial application as it can be used for a range of applications (e.g. dilution, cleaning, construction, or lubrication). While these vary between and within different industrial sectors, almost all applications require a high if not extremely high quality of water (e.g. ultrapure) [102], [144]. While the specific quality of water needed for each of these sub-categories may vary, all require a certain level of treatment and monitoring. This is needed to reduce the risk of equipment damage or process impacts such as corrosion, biological growth, scaling, and fouling [80]. With that said, the quality in some cases is much more attainable than those of applications that come into contact with humans. Additionally, limiting factors such as public perception are heavily reduced, making this a more favorable application of reclaimed water.

Environmental

Environmental applications were the least investigated in the literature (Figure 2.3) and have often been overlooked in global demand accounting (Figure 2.5) [4], [23], [67]. This is presumably because environmental demand is assumed to be met via natural hydrological cycles which is not necessarily true. Further, even when an environmental need is identified, it is often ignored over opportunities to service human and agricultural needs [9], [96], [97].

This is short-sighted in two ways. First, the prioritization of human needs does not acknowledge that environmental applications are also necessary to ensure a healthy living environment. The use of reclaimed water for environmental applications, for example, can restore environmental habitats while also minimizing unmonitored discharge and pollution [87], [145]. Second, by addressing non-human centered activities the risk to humans is minimized as is the demand on freshwater sources. Therefore, if lessons are to be learned about the ecological health of the world, environmental applications must be both accounted for and included [9]. As with all applications, however, several factors must be considered including exposure to animals, water quality, and microbial growth [80]. Environmental applications are primarily divided into three themes: groundwater, irrigation, and surface water.

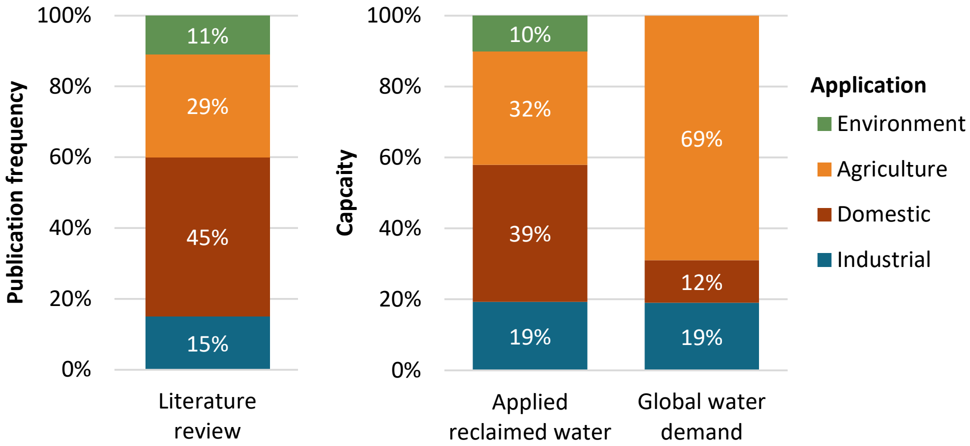

Figure 2.5 Overview of application presence in the literature review as compared to applied water reuse applications and global water demand. The applied water reuse and global water demand data is derived from the outputs of the UNESCO World Water Assessment Programme (WWAP) [23].

Groundwater injections can be either potable or non-potable. Potable groundwater injection can be used to supplement existing supplies and prevent the consequences of over-extraction and salt water intrusion [76]. However, this requires a very high quality of water to prevent adverse effects or contamination of groundwater sources. Non-potable groundwater injection, on the other hand, has a lower water quality standard and can be used to either protect or indirectly supplement potable groundwater [76], [146]. While this has already been applied in the field, more research is needed to verify both proper application and long-term effects.

Irrigation applications (e.g. forestry, subsidence control, or environmental enhancement and augmentation) have a long history of using reclaimed water [102]. Ensuring these environmental applications are properly irrigated can contribute to flooding prevention, aquifer recharge assistance, and wildlife habitat recovery [60].

Some surface waters can be safely supplemented with reclaimed water to offset the demand on freshwater sources, however, this is often not pursued due to public perception and perceived risk [74]. Therefore, this should be done only when the quality and reliability of the source has been fully vetted.

2.4.2 Reclaimed water criteria, data, and standards

Reclaimed water assessments are used to assess technical feasibility, prevent economic loses, minimize environmental risks, and address social concerns [61]. Therefore, the associated criteria typically fall into one of these primary criteria categories (i.e. technical, economic, environmental, or social) [100]. The associated sub-categories and criteria for these categories are presented in the supplementary materials (S5). It is commonly acknowledged that assessments should include all four categories to be comprehensive and objective [22]. This was supported through the criteria literature review which found 53% of the publications included criteria from all four categories (Figure 2.6a).

The presence of comprehensive criteria in the form of standards is also crucial for implementation. The lack of application standards is often cited as a major limiting factor in reclaimed water implementation [91]. It is even argued that strict standards can improve the rate of reclaimed water implementation since it can improve public perception that the water is indeed safe to use [87]. The following sections will explore the four main criteria categories and discuss the crucial criteria relevant for comprehensive assessments.

2.4.2.1 Technical

Technical criteria were included in 84% of the criteria literature and were mostly quantitatively based (Figure 2.6a). While most technical criteria contribute to a pass/fail feasibility test, some quantitative criteria are more pivotal in the success of other categories. For example, characteristic criteria (e.g. odor and color) do not necessarily dictate feasibility but are directly related to public perception [81]. This emphasizes that a clear and exhaustive list of criteria is needed for a comprehensive assessment [9].

Source data and application standards focused almost exclusively on technical criteria (6.3.2S6). This is because technical criteria are typically used to determine initial feasibility while economic, environmental, and social criteria are used to determine limitations. While some technical criteria were considered equally important from a source and application perspective (e.g. total suspended solids and pH), the importance or presence of other criteria differed (see the supplementary material S6). Specifically, source data focused primarily on measurable criteria (e.g. electroconductivity) while application standards focused on risk-based criteria (e.g. presence of pathogens) [66]. It is imperative, however, that the priorities and needs from both perspectives be aligned for

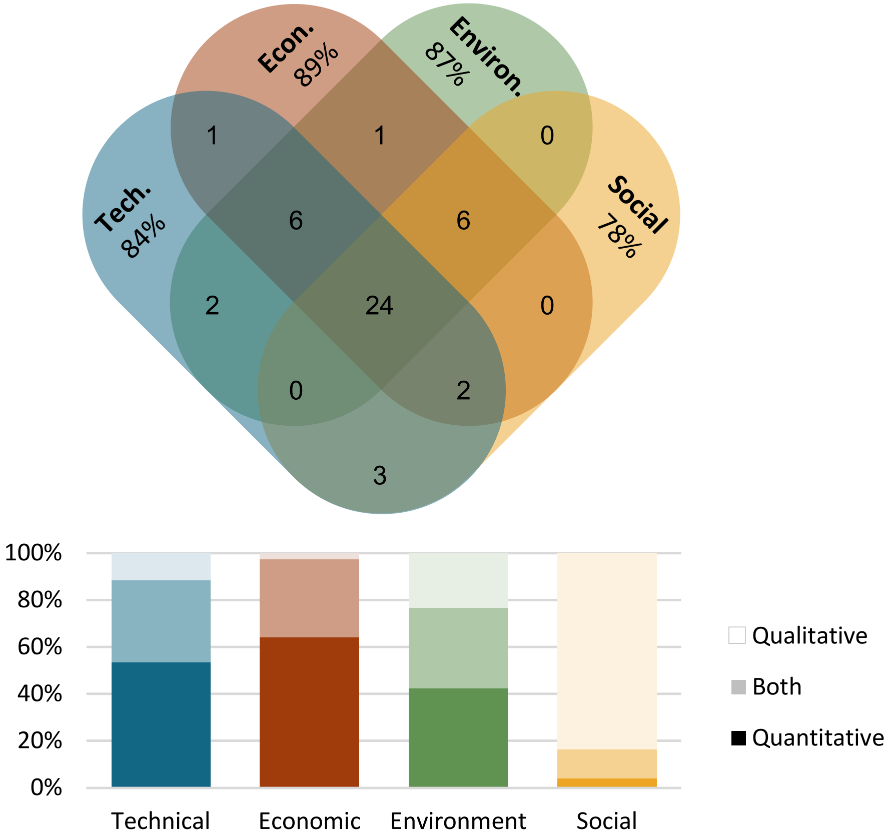

Figure 2.6 Overview of the criteria base on (a) its presence in the literature and (b) the type of criteria presented per category.

source-application connections to be made. If end users are concerned about pathogens, then source data must reliably include these criteria so that end users know both the feasibility and safety of the source [91].

Additionally, neither the source data nor application standards included any quantifiable information regarding micropollutants or pharmaceuticals. While identified in the literature as important topics, the lack of understanding or ability to accurately measure has limited their inclusion in these datasets.

2.4.2.2 Economic

Economic criteria were found to be largely quantitatively based (Figure 2.6b). However, these criteria were also found to be heavily influenced by other categories and criteria.

For example, the unit product cost is affected by social (e.g. price of water and subsidies), technical (e.g. infrastructure), and environmental (e.g. discharge costs) factors. Further, if the resulting price of the effluent is too expensive it may not be affordable for consumers [66]. Conversely, if it is too cheap consumers may distrust the quality and stakeholders may not be able to afford production costs and could return to discharging methods [9]. This can also negatively affect the rate of return which is a key indicator for financing [66], [87]. This is all to say that economic assessment criteria, though primarily quantitative, must account for qualitative factors and changes in other criteria must be accurately connected and reflected.

2.4.2.3 Environmental

Environmental criteria are often associated with risks and impacts to the environment including pollution, risks to species, over-extraction, and other potentially long-term impacts [145]. However, these criteria can also highlight the need for interventions or present the positive impacts of reclaimed water use schemes. Existing condition criteria, for example, can communicate the need for an intervention leading to improved public willingness or assisting in political agenda communication. Additionally, effects to freshwater supplementation are seen as one of the most important factors as it can address the potential for pollution but also the increased availability of usable water [4], [100].

The scope of these criteria are also important. For example, accounting for greenhouse gas emissions may highlight that water treatment can lead to increased emissions, having a negative effect on the environment. However, if this scope also includes the offset of treatment-based emissions through plant and tree irrigation, net negative emissions may be seen. Therefore, a full environmental assessment should be included in any reclaimed water proposal to fully evaluate how reclaimed water can both positively and negatively affect the surrounding environment and concerns.

2.4.2.4 Social

The social criteria category is regarded as the most important barrier to reclaimed water use and is also notorious for being difficult to assess. This is in part because the social category is almost entirely based on qualitative criteria (Figure 2.6b) but is also viewed as essential for a reclaimed water project to proceed [60], [68], [77], [91].

Social acceptance, specifically, is reliant on several factors such as culture, application, safety, water availability, and the all-important yet impossible to define 'yuck' factor [60], [65]. The 'yuck' factor is an example of the vagueness of some social criteria as it is an instinctive disgust for reclaimed water influenced by factors such as water stress, potential exposure, and level of education [60], [64]. Therefore, this type of criteria is contextually based and ranges in severity since it includes multiple perspectives and concerns that are impacted by a variety of difficult to define factors [103]. The proper identification of social criteria is, therefore, crucial for understanding the social based needs, potential benefits, and promotional levers.

When better understood, social criteria can be used to both inform or even leverage the use of reclaimed water. As an example, identifying the local water stress (i.e. need) and the potential for water security through the pursuit of alternative sources (i.e. benefit) can be used as the foundation for promoting reclaimed water use (i.e. lever). With these items clearly identified, the stakeholders can better select locations for reclaimed water use by either focusing on high water stressed locations or assist local governments in developing policies and guidelines, both shown to improve social acceptance, financial feasibility, and better business practices [66], [67], [77], [84], [100]. Therefore, the inclusion of clear and accurate information is a crucial factor for addressing social criteria [60], [64].

However, while straight forward connections can be identified, the social category remains complex as some opinions may be based purely on perception or intuition. While some studies recommend improved education, others state a 'paradigm shift' is needed to help reframe reclaimed water [62]. It is, therefore, research should better address these criteria to give more insight on what and how to review the socially based obstacles [100].

2.5 Conclusions

Reclaimed water use has been shown to be a reliable, flexible, and an efficient alternative water source which can alleviate the demands on limited freshwater sources. However, in order to effectively implement, it is important to address factors such as public perception, financing, and risks. This research used a double literature review to investigate the state of reclaimed water use with regards to sources, applications, criteria, standards, and data. The following conclusions were made through this investigation:

Existing sources and applications

- Most of the publications focused on municipal sources (e.g. treated municipal effluents) due to its relatively good quality, quantity, scalability, and reliability.
- Though domestic applications are the most investigated, they actually represent the smallest global demand. This mismatch between research focus and real-world need is shown to be connected to wealth distribution and quality of life standards.
- Infrastructure connecting sources and applications requires more investigation since this is both a common issue and major barrier.

Criteria, standards, and data

- To better assure feasibility, acceptance, and safety, comprehensive and clearly defined criteria are needed that address end users concerns.
- Source data and application standards criteria need to be better aligned to promote reclaimed water use. Currently, source data primarily focuses on measurable criteria while application standards focus on health risk criteria.
- Source data transparency and the presence of application standards are both necessary to make informed decisions when implementing reclaimed water. Intelligent implementation is necessary to prevent negative impacts and repair the image of reclaimed water use.

Missed source-application connections

- Risk to humans is among the most limiting factors in reclaimed water use. Therefore, either addressing these risks (e.g. improving criteria and monitoring) or focusing on non-human centered applications (e.g. environment) is needed.

- Focusing on environmental applications can help offset freshwater demand and improve ecosystem health but is barely present in research. Showing the feasibility of reclaimed water as a nature resource can also help improve its image and likelihood of implementation elsewhere.
- Industrial sources are the least present in the literature due to the potential of harmful contaminants but also have notable potential for appropriate applications due to its reliability and heavy monitoring.

If you can't explain it simply,

you don't understand it well enough

– Albert Einstein

CHAPTER 3

ELECTRODIALYSIS MODELLING

Continuous mode electrodialysis modelling methods for brackish water desalination

3

ABSTRACT

Electrodialysis is a membrane-based desalination technology with emerging scientific and commercial interest. Modelling can help predict the potentials of electrodialysis, however, there is no consensus on which model is preferred. This is because existing electrodialysis models range in their approach, scope, and assumptions. The aim of this study is to both review existing models and compare select models using the same experimental inputs to assess their accuracy. Existing continuous electrodialysis models were first identified through a literature review and then the most relevant models were selected for replication. The two models selected (the Campione et al. model and Nakayama et al. model) were chosen based on their validated feed salinity range and their ability to provide in-channel performance outputs. While both the Campione et al. model and the Nakayama et al. model were somewhat accurate under specific conditions, the limits of the resistance calculations in the Nakayama et al. models resulted in a poorer performance prediction of the specific energy use. Further, the Campione et al. model was more flexible and able to incorporate additional phenomena such as the boundary layer resistance and water transport, both of which were able to improve the accuracy of the model.

A slightly modified version of this chapter is under review as:

Wreyford, J. M., Prajsnar, S., Bruning, H., Dykstra, J. E. & Rijnaarts, H. H. M. Continuous mode electrodialysis modelling methods for brackish water desalination.

3.1 Introduction

Electrodialysis (ED) represents approximately 3% of the world's desalination capacity and has received increased interest as a desalination method [32]–[34]. This is largely because of its decreased need for pre-treatment and smaller operational footprint as compared to other available treatment technologies [32].

ED is an electrically-driven desalination process that consists of several stacked cell-pairs sandwiched between two electrodes [147]. Each cell-pair consists of two semi-permeable membranes: an anion exchange membrane (AEM) and a cation exchange membrane (CEM). These membranes are alternated across the stack, forming channels between them. As the feed water flows along the membranes in the channels, ions are transported through the membranes via various mass transport phenomena [148]. Figure 3.1 depicts a simplified ED design consisting of a single cell-pair stack.

The three primary mass transport phenomena occurring in ED are diffusion, migration, and advection [148]. Diffusion is caused by the ion concentration gradient of the solution

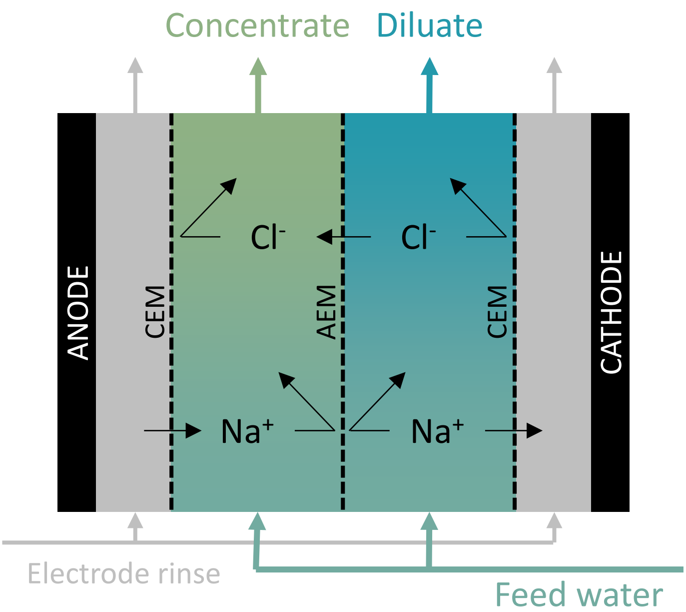

Figure 3.1 Overview of a simplified ED design consisting of a single cell-pair stack sandwiched between two electrodes.

in the channels [148]. Migration, also referred to as conduction, occurs when the applied external voltage creates an electrical potential gradient across the cell-pairs, driving the ions through the membranes [148]. Advection of water occurs in the form of osmosis and electroosmosis, and due to ion water friction is coupled with the ion transport [148], [149]. The result of these transport phenomena are that ions move from one channel to the next creating a diluate channel (i.e. desalinated water) and a concentrate channel (i.e. brine).

ED can be operated in either batch dynamic or continuous mode [33]. Batch dynamic mode (Figure 3.2a) recirculates the diluate and the concentrate through the ED stack until the required quality of water is achieved. However, batch dynamic mode is limited in the quality of water it can produce and is typically only used in small-scale operations [150]. Continuous mode (Figure 3.2b) is when the feed water passes through once but is typically part of a multistage operation. The result is that it is able to produce a higher quality of water while also being less energy-intensive, more efficient, and more widely applicable [150]. As such, continuous mode ED is typically used in industry-scale applications [33], [151].

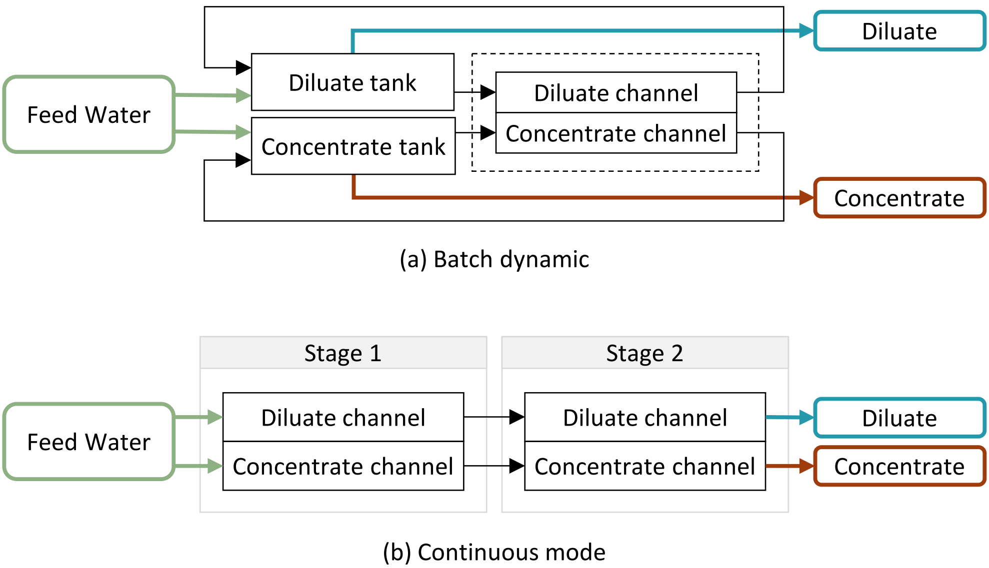

Figure 3.2 Diagrams of the basic operating process for (a) batch dynamic and (b) continuous ED designs [33], [151].

ED has been applied to both brackish water and seawater, with application to brackish water gaining increased attention due to its widespread availability [17], [32], [152], [153]. Brackish water ranges from slightly brackish (1,000 – 5,000 mg/L) to heavily brackish (15,000 - 35,000 mg/L) and is found in ground, surface, and wastewater [152], [154], [155]. It has also been shown that brackish water desalination can be economically competitive and environmentally beneficial [156]. Further, when brackish water is sourced internally it can reflect positively on a company's image [32], [152]. However, the wide salinity range and varied conditions of brackish water makes it difficult to predict how desalination technologies such as ED will perform [157]–[159].

Modelling is a potential method for testing ED operations under different conditions while also incorporating systems-level impacts (e.g. energy use) [160]. This is necessary for continuous mode evaluations which require multiple inputs and have multiple transport mechanisms to consider. Existing continuous models have currently only been presented independent of each other and applied to a variety of scenarios. To date, there are no reviews of existing continuous mode models nor is there a consensus on which modelling method performs best when applied to the same source [33], [151], [160]. In order to better understand the capabilities of the continuous mode process for brackish water application it is necessary to first identify which models exist, review their scope and assumptions, and test their performance and accuracy.

3.1.1 Research objective

The aim of this research is to identify existing continuous mode ED models, filter them based on relevance to a systems-level modelling scope, and then evaluate their output performance. Models will be selected based on their ability to fit within the general overview presented in Figure 3.3. This overview is based on the intent to have an ED model which can be integrated into a larger comparative model. This comparative model will use common inputs for different technologies and then compare these technologies based on their salt removal efficiency and energy demand. Therefore, the objective in this research is to identify models which can be reflective of changes to the feed quantity and quality while also accurately depicting the associated energy demand. The scope of this research is limited to continuous mode ED models which use physics-based evaluation methods that can accurately capture both the removal rate of a two ion (Na^+ and Cl^-) solution and the resulting energy demand for brackish feed water desalination.

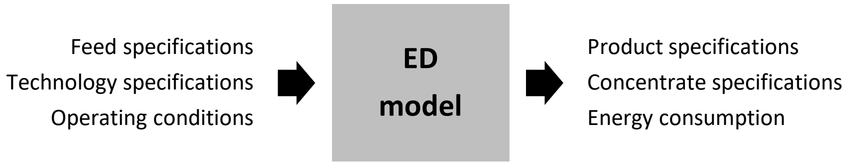

Figure 3.3 General overview of the inputs that will be provided and the outputs that are expected of a systems-level ED model.

In Section 3.2, the methodology of this research will be outlined. The continuous ED models identified in the systematic literature review will then be assessed and categorized in Section 3.3. The theory of the selected models will be outlined in Section 3.4 and the experimental data will be explained in Section 3.5. The results will be presented in Section 3.6 and a summary of the paper will be given in Section 3.7.

3.2 Methodology

This research will be conducted in three steps: systematic literature review, implementation of select models, and performance review.

3.2.1 Systematic literature review

The systematic literature review will follow the framework presented by Voskamp et al. [69]. This method uses three phases: i) search strategy; ii) relevance and quality assessment; and iii) data extraction and synthesis. This search will be conducted using Scopus to ensure replicability. The search strategy will include all peer reviewed articles written after 1995 that meet the following keyword search term:

Electrodialysis AND Desalination AND Model

The year, 1995, was selected to reduce the chance of pursuing outdated models. It is also expected that theories and methods which predate 1995 will be captured or included in the review papers present in this timeframe.

Once the initial set of papers is collected, the relevance and quality assessment will then be completed using the model scope criteria presented in Table 3.1. These criteria were developed with the goal of identifying a model which can be integrated into a larger comparative model of different desalination technologies. The aim of the larger comparative model is to both compare different treatment technologies using the same inputs and also optimize the configuration based on systems-level metrics such as energy usage. Therefore, the pursued models should include physics-based methodologies that can accurately reflect both changes in the input and operating conditions. The inputs, however, must be limited as evaluations methods and technology performance are known to vary significantly based on the salinity range of the input water. Therefore, the scope of this research will focus on brackish water salinity ranges as this field of research still requires some attention.

The evaluation methods should also account for transport phenomena within the channel. While some models may exclude the spacer, the effects of the spacer may be significant. Therefore, it was deemed important that realistic aspects such as the spacer material should be present in the model. Further, only models operating under the limit current will be considered since operating above the limiting current does not necessarily contribute to improved ion transport. It is also expected that the selected models should already be validated empirically so that an initial quality control has been completed before application to other empirically based studies.

With regards to implementation scope, the selected models should not rely on any secondary or specialty software and should have a reasonable (less than 10 second) run time. This is because when the models are incorporated into the larger iterative model, the model will need to be run thousands of times. Therefore, access to alternative software or long execution times should be avoided.

Data extraction and synthesis will be comprised of categorizing the remaining papers and then reviewing their modelling methods in depth. The models which meet the modelling criteria scope will then be selected for implementation.

3.2.2 Implementation of select models

The select models will be recreated and implemented in Python. The recreated models will then be applied using the same feed water conditions and operating conditions as the empirically based data. This will allow for the model performance to be more justly compared.

Table 3.1 Scope of model criteria used for the relevance assessment in the systematic literature review.

Item	Scope
Channel properties	Accounts for channel spacer
Computational power	Can be run repetitively with a reasonable run time
ED Operation	Continuous ED system
Feed water range	Brackish water (1,500 to 15,000 mg/L)
Implementation	Does not require specialty or licensed software
Limiting current	Operating below the limiting current
Modelling level	Systems-level
Scope	Focuses on simulation of ED channel performance and properties
Validation	Empirically validated

3.2.3 Performance review

The outputs of the implemented models will be compared to the empirical results. The comparison will primarily focus on salt removal and energy demand to determine which models were the most accurate in their predictions. At this point, relevant phenomena will also be reviewed and a discussion into the performance of the models will be completed.

3.3 Review of existing continuous ED models

The initial search strategy returned 108 publications. The relevance and quality assessment reduced this to 30 relevant publications as presented in the supplementary materials (S7). The omitted papers were often excluded because their model focus was not on the simulation of ED channel performance but rather on topics such as the incorporation of renewable energy, operating over the limiting current, or predicting environmental impacts. The number of relevant papers were further reduced during the data extraction and synthesis stage, where the scope and aim of each paper was more closely scrutinized. As a result, 12 final papers were selected for an in-depth literature review.

The final 12 papers were categorized based on the fundamental methods used, presented in Figure 3.4. This is similar to the framework presented in Campione et al. [33]. The models broke down into two primary types: simplified and advanced [33]. Within these categories, sub-categories were formed to further classify the core methodology used.

3.3.1 Simplified models

Simplified models are computationally less intensive and can be used to quickly predict general performance. However, simplified models typically consist of empirically based constants which require calibration to fit specific scenarios [33]. Because of this, simplified models are based on several assumptions which can limit their applicability and reliability to scenarios which differ from the conditions they are developed for. This type of model tends to include a limited number of design equations making them suitable for general performance prediction but not optimization or performance outside of the operating limits [33].

3.3.1.1 Lumped models

Lumped methods use average compartment concentrations to estimate all process variables [33]. Lumped models are best suited to estimate pivotal aspects of initial ED design such as the approximate membrane area and energy use. Lee et al. presents a lumped modelling approach based on a set of fixed and variable parameters [161]. These parameters include the feed and product concentrations and velocities, stack configuration, membrane properties, current density, and recovery ratios. The model includes simple algebraic equations whose variables are based on empirical data.

A major drawback to the Lee model is that it is less accurate at salinities higher than 5,000 mg/L. This is partially due to the simplifications and neglect of important transport phenomena such as back-diffusion and water transport. The Lee model is therefore not able to accurately reflect different scenarios and is not fit for performance optimization.

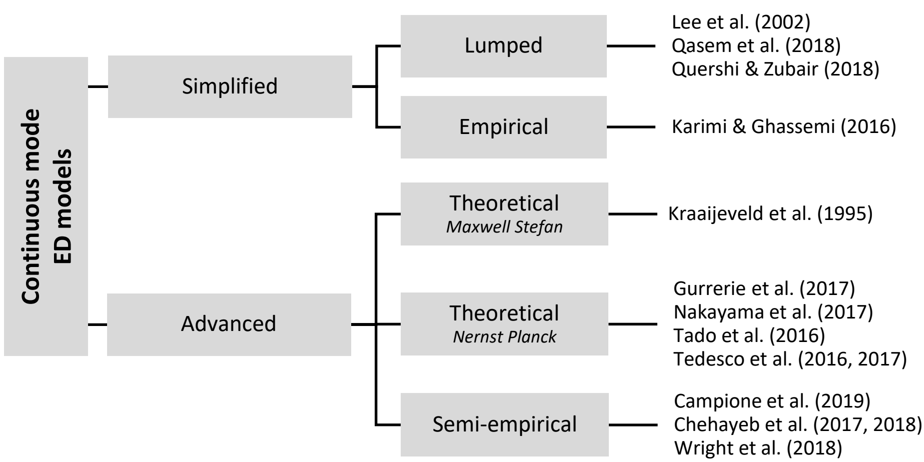

Figure 3.4 Categorization of existing ED models included in the final set of publications based on their fundamental basis.

As a result, other researchers have attempted to improve upon this method to improve its accuracy and reliability [33], [162], [163].

One expansion of the Lee model was completed by Qasem et al. who modified the method to include the Donnan potential. This improved the general accuracy of the model for low and moderate salinities, but not for higher feed salinities [162]. Qureshi & Zubair also attempted to improve upon the Lee model by replacing the constant conductivity equivalent assumption with an empirically based solution. This modification increased the models complexity but only slightly increased the accuracy of the model for feed salinities above 8,000 mg/L [163].

3.3.1.2 Empirical

Empirical models are based on dimensionless numbers and simulate only the most important ED processes for a static design [164]. Karimi & Ghassemi developed an empirical model for use with a wide range of operating conditions [164]. This model used the dominant dimensionless numbers from experimental data to predict the removal of both monovalent and divalent ions. While the Karimi & Ghassemi model was validated, it was only proven accurate within a narrow salinity range (1,000 – 2,000 mg/L). Moreover, the model can only produce an overall performance rather than detailing the internal processes within the channel.

3.3.2 Advanced models

Advanced models are widely used in modelling ED because they are able to capture non-ideal phenomena and compute the variable distribution (i.e. current density, flowrate, etc. over the length of the channel). While they are potentially more precise and accurate than simplified models, they are also much more complex [33]. Advanced models are sub-categorized into theoretical or semi-empirical models. The main difference between these sub-categories is the basis of their assumptions and the source of their coefficients.

3.3.2.1 Theoretical

There are two main foundations for theoretical models: Maxwell-Stefan and Nernst-Planck. In both, the microscopic properties of the membranes are used to determine the internal mass transport phenomena while simple geometry is used to describe in-channel characteristics.

Maxwell-Stefan

Maxwell-Stefan is most suitable for non-ideal, concentrated solutions as it accounts for interactions between ions using multiple transport coefficients [33]. These interactions include the friction with the water, pore walls, and other ions [165]. The Kraaijeveld et al. model (i.e. the Kraaijeveld model) is a Maxwell-Stefan based approach appropriate for capturing the complex interactions between ions, membranes, and solutions [33]. The Kraaijeveld model does obtain some model parameters from existing correlations (e.g. the Sherwood number and activity coefficients) [166].

This model includes multiple aspects of ED such as water transport and the boundary layer. The boundary layer is a thin stagnant layer between the bulk solution and the solution-membrane interface which can strongly influence the concentration profile [167]. Inclusion of the boundary layer typically results in a non-linear concentration profile, the shape of which is dictated by the transport phenomena [33], [167]. Water transport across the membrane occurs due to hydrostatic pressure differences, osmosis, and electroosmosis as well as in the form of a hydration shells around migrating ions [165]. Though the importance of including water transport is debated, some research has shown it is acceptable to neglect this within certain salinity ranges [149].

The base Maxwell-Stefan equation is represented as

$$-\frac{c_\mathrm{i}}{R_g T}\nabla\mu_\mathrm{i} - \frac{z_\mathrm{i} c_\mathrm{i} F}{R_g T}\nabla\phi = \sum_{\mathrm{j}=1}^{N_i} \frac{c_\mathrm{i} c_\mathrm{j}}{c_{total}\, D_\mathrm{ij}}(u_\mathrm{i} - u_\mathrm{j}) \qquad \text{Equation 3.1}$$

where i and j are given ion species, c is the concentration, R_g is the universal gas constant, T is the temperature, μ is the chemical potential, z is the ion charge number, F is the Faraday constant, $\nabla\phi$ is the potential drop, N is the total number of ions in the concentration, u is the average species velocity, and D is the Maxwell-Stefan diffusivity between two species [166]. It should be noted that when the friction between ions and between ions and the pore walls are neglected, Maxwell-Stefan becomes formally equivalent to the Nernst-Planck approach [165].

Nernst-Planck

The Nernst-Planck approach is suited for less concentrated solutions since it simplifies the interactions between ions and between the ions and the pore walls [33]. This approach determines the ionic flux through both short and long range interactions. Short range interactions include the effect of diffusivity while long range interactions include the effect of the externally applied electric field and electro-neutrality [168]. Nernst-Planck based approaches are typically focused on modelling the membranes but can also contribute to the overall understanding of ED performance [33].

The extended Nernst-Planck equation is based on diffusion, conduction, and advection and assumes an ideal dilute solution. It is expressed as

$$\vec{J}_i = -D_i \vec{\nabla} c_i - \frac{z_i F D_i c_i \vec{\nabla} \phi}{R_g T} + c_i \vec{u} \qquad \text{Equation 3.2}$$

where J is the ionic flux, D the diffusion coefficient in the solution, and u is the fluid velocity [169].

The ion mass balance for inert species is given by

$$\frac{\partial c_i}{\partial t} + \nabla J_i = 0 \qquad \text{Equation 3.3}$$

where t is time.

Existing Nernst-Planck models are either one- or two-dimensional [33]. One-dimensional models include more assumptions and are simplified to the direction of the flow, thus simpler to solve [147], [170]. Though classified as theoretical, one-dimensional models typically use experimental data inputs to describe two-dimensional features (i.e. spacer porosity, mechanical dispersion, and membrane resistance).

Both Tado et al. and Nakayama et al. developed one-dimensional models [147], [170]. The Tado model depicts ion transport based on diffusion, migration, and advection. It also accounts for the osmotic pressure [147]. The Nakayama et al. model builds upon the Tado model, presenting a boundary layer analysis describing the most crucial features of the ED process. This model then presents varied approaches for short and long channel applications [170].

Gurreri et al. and Tedesco et al. present two-dimensional models that included the changes in concentration in both the horizontal and vertical directions [165], [169], [171], [172]. The Gurreri model was developed to test different membrane/channel configurations using simplified geometry [171]. This model is able to capture important processes with high accuracy including the effect of membrane features, concentration profiles, residence time, and voltage drops. However, the Gurreri model requires a specific solver to solve the Navier-Stokes and Nernst-Planck equations.

The Tedesco et al. model is presented over a series of three papers which present the base model and the inclusion of additional aspects such as water transport [165], [169], [172]. The Tedesco et al. model uses simplified channel geometry which assumes a parabolic flow, therefore requiring a relatively low computational power. The Tedesco et al. model was validated using a Nelder-Mead method where the model parameters were fitted to the experimental data in both batch and reverse ED operations [165]. The model was also used to deliver a theoretical solution to desalinate seawater in continuous mode, though this was not empirically validated.

3.3.2.2 Semi-empirical

Semi-empirical models are multi-level evaluation approaches including both local and operational calculations. The local level includes transport phenomena (e.g. electromigration, back-diffusion, and water transport) while the operational level includes multistage operations [33], [151]. In semi-empirical models, differential mass balance equations are used to determine the concentration, flowrate, and current efficiency profiles over the channel length. These are achieved through use of empirically based membrane properties and correlations, such as Islam's correlation for conductivity and computational fluid dynamics (CFD) [33], [173]. All semi-empirical models identified assumed a single 1-1 electrolyte (e.g. NaCl) which allowed for the equations describing conductivity, diffusion, and transport to be simplified. Further, the use of empirically based data and equations allows the neglect of some theoretically based equations and has also shown to result in more realistic performance predictions for different channel geometries [33].

Campione et al. developed a semi-empirical model applicable for a wide salinity range and was tested with a feed salinities ranging from 3,880 to 30,340 mg/L [151]. This model was found to be highly accurate and was validated through experimental data. In literature, the Campione et al. model is regarded as a fully predictive tool that is relatively fast and potentially very accurate [174].

Chehayeb et al. carried out a semi-empirical simulation for desalination optimization based on entropy generation [167], [175]. The Chehayeb model demonstrated that energy consumption can be significantly lowered through multistage operations. La Cerva et al. confirmed the accuracy of the Chehayeb model for a hybrid system consisting of ED and reverse osmosis (RO) [176].

Wright et al. presented a semi-empirical model for a batch system including only electromigration and back-diffusion [149]. While the study was able to demonstrate that water transport can be neglected under certain salinity levels, the model was also only shown to be valid when the feed salinity was below 5,886 mg/L [149].

3.3.3 Model selection

Since brackish water salinity can vary widely and the feed salinity can significantly affect membrane performance, it was deemed important to select models that were both designed and validated for a wide range of feed salinities [149]. This showed to be the greatest challenge for the simplified models. While the Lee et al. model had the largest feed salinity range of the simplified models, it was not large enough to meet the range specified for this research [161]–[163]. Karimi & Ghassemi were also excluded based on their narrow feed salinity validation range as well as for the lack of in-channel performance descriptions.

While the Maxwell-Stefan approach was found suitable for highly concentrated solutions, it was concluded that this method would require much more complexity and implementation effort than that for a lower or more uniform salinity solution. It was, therefore, determined that the assumptions used in the Nernst-Planck method would be more valid for this research.

For the one-dimensional Nernst-Planck models, the Nakayama et al. model and the Tado et al. model were found to be very similar. This is because the Nakayama et al. model builds off the Tado et al. model. Therefore, the Nakayama et al. model was selected for further investigation as it was the most recent version of this approach.

The two-dimensional Nernst-Planck models were found to operate outside of the computational and implementational scope for this research. However, the Tedesco et al. model was unique as it had been experimentally validated, though not for continuous operation. Therefore, the modelled outputs of Tedesco et al. were selected to be used for comparison in the results section rather than being pursued as a modelling method.

Of the semi-empirical methods, the Campione et al. model was found to be the most accurate for the largest range of feed salinities. Therefore, the Campione et al. model was selected for implementation. An overview of the final papers and the reasoning for being included or rejected in this study is presented in the supplementary materials (S7).

3.4 Theory of selected models

3.4.1 Campione et al. model

The Campione et al. model is based on a set of local mass balance calculations for an ED cell-pair [151]. A cell-pair is defined as one CEM, the diluate channel, one AEM, and the concentrate channel. Included in this model are several assumptions including: i) only sodium and chloride ions are present; ii) concentration changes perpendicular to the flow direction are neglected; iii) permselectivity values are constant; and iv) a uniform flowrate is assumed along the cell-pairs [177].

The Campione et al. model was verified through comparison to single pass, continuous mode experiments. In these experiments, a variety of currents and velocities were applied to a wide range of feed salinity levels (1,000 to 30,000 mg/L). The conductivity of the diluate and concentrate were then measured at the outlet of the ED stack and compared to the model results.

3.4.1.1 Mass balance and transport phenomena

The foundation of the Campione et al. model is a set of four mass balance equations which depict the bulk concentration distribution (Equation 3.4 and 3.5) and flowrate (Equation 3.6 and 3.7) along the length of the ED channel. These are written as

$$\frac{dQ_{dil}(x)c_{dil}(x)}{dx} = -W * J_{total}(x) \quad \text{Equation 3.4}$$

$$\frac{dQ_{conc}(x)c_{conc}(x)}{dx} = W * J_{total}(x) \quad \text{Equation 3.5}$$

$$\frac{dQ_{dil}(x)}{dx} = -W * q_{total}(x) \quad \text{Equation 3.6}$$

$$\frac{dQ_{conc}(x)}{dx} = W * q_{total}(x) \quad \text{Equation 3.7}$$

where Q is the local volumetric flowrate, c is the salt concentration in the channel, W is the channel thickness, J_{total} is the total ionic flux, and q_{total} is the total water transport. Note dil and $conc$ denote the diluate and concentrate channels. This system of ordinary differential equations are then solved using a solver which then determines the concentration profile in the channel.

The Campione et al. model includes two primary ion transport phenomena: migration and diffusion. The total flux over the cell-pair is therefore defined as the sum of the conductive and diffusive fluxes, written as

$$J_{total}(x) = J_{cond}(x) + J_{diff}^{AEM}(x) + J_{diff}^{CEM}(x) \qquad \text{Equation 3.8}$$

where J_{cond} is the conductive flux, J_{diff}^{AEM} and J_{diff}^{CEM} are the back-diffusive fluxes across each ion exchange membrane (IEM), and x is the given location along the length of the channel [151]. Further explanation of the ion transport phenomena can be found in the supplementary materials (S8).

The Campione et al. model includes two water transport phenomena: osmosis and electroosmosis. The total water transport is expressed as

$$q_{total}(x) = q_{osm}^{AEM}(x) + q_{osm}^{CEM}(x) + q_{eosm}(x) \qquad \text{Equation 3.9}$$

where q_{osm}^{AEM} and q_{osm}^{CEM} are the water flux based on osmosis for each membrane and q_{eosm} is the water transport caused by electroosmosis [151]. Further explanation of the water transport phenomena can be found in the supplementary materials (S8).

3.4.1.2 Resistance

The resistance is directly related to the external applied cell-pair voltage through Ohm's law, written as

$$V_{cp,drop} = \eta(x) + R_{cp,total}(x)i(x) \qquad \text{Equation 3.10}$$

where $V_{cp,drop}$ is the voltage drop over a cell-pair, η is the non-ohmic voltage drop (i.e. the Donnan potential), $R_{cp,total}$ is the total ohmic resistance of a cell-pair, and i is the current density at the given location [151]. $R_{cp,total}$ can be calculated as the sum of four components, expressed as

$$R_{cp,total} = R_{AEM}(x) + R_{CEM}(x) + R_{dil}(x) + R_{conc}(x) \qquad \text{Equation 3.11}$$

where R_{AEM} and R_{CEM} are the resistance across the membranes, R_{dil} is the resistance across the diluate channel, and R_{conc} is the resistance across the concentrate channel [151]. Further explanation of the resistances can be found in the supplementary materials (S8.3).

3.4.1.3 Current efficiency

One of the most important indicators of ED performance is the current efficiency. The current efficiency represents the amount of current actually converted into salt flux and is defined as the ratio between the calculated current density based on salt removal and the current density obtained through Ohm's law (Equation 3.10). The current efficiency (ⓔ) can therefore be expressed as

$$ⓔ = \frac{\left(c_{dil}^{\text{in}} Q_{dil,total}^{\text{in}} - c_{dil}^{\text{out}} Q_{dil,total}^{\text{out}}\right) F}{I_{total}\, N_{cp}} \quad \text{Equation 3.12}$$

where c^{in} and c^{out} are the concentrations at the inlet and outlet, Q^{in} and Q^{out} are the volumetric flowrates at the inlet and outlet, I_{total} is the total current, and N_{cp} is the number of cell-pairs [151]. The total current is calculated as the integral of the current density over the active area, written as

$$I_{total} = \sum_{n=1}^{N_{sub}} i_n \frac{L * W}{n} \quad \text{Equation 3.13}$$

where N_{sub} is the number of subcells and L is the channel length.

3.4.1.4 Energy

The energy consumed in this process is calculated using a simpler approach that remains tied to the operating conditions. In order to calculate the specific energy consumption for the ED process, the total voltage drop (V_{total}) must first be calculated. This is expressed as

$$V_{total} = \frac{I_{total} R_{exp}}{A_{mem}} + \sum_{n=1}^{N_{cp}} V_{cp,n} \quad \text{Equation 3.14}$$

where R_{exp} is the resistance of the electrodes obtained from an experiment, A_{mem} is the area of a single membrane, and $V_{cp,n}$ is the voltage for each cell-pair [151]. For this research

R_{exp} is assumed to be 0.57 Ω [178]. Next, the total power consumption (E_{total}) needs to be determined, which is defined as

$$E_{total} = V_{total}\, I_{total} + \Delta p_{dil,total} Q_{dil,ave} + \Delta p_{conc,total} Q_{conc,ave} \quad \text{Equation 3.15}$$

where Δp_{total} is the overall pressure drop in the channels and Q_{ave} is the average volumetric flowrate over the length of the channel (see S8.4).

The specific energy consumption per unit volume of product (E_{spec}) is calculated as the total energy divided by the volume of produced water (Equation 3.16).

3

$$E_{spec} = \frac{E_{total}}{Q_{dil,total}^{\mathrm{out}}} \quad \text{Equation 3.16}$$

3.4.2 Nakayama et al. model

The Nakayama et al. model uses a novel boundary layer analysis and an analytical approach to estimating the limiting current density and stack voltage drop [170]. This is achieved through the application of the Nernst-Planck equation with local electro-neutrality in combination with an effective harmonic diffusivity and average volume theory [170]. This method defines the effective harmonic diffusivity (D_e) as

$$D_e = \frac{1 - \frac{z_\mathrm{i}}{z_\mathrm{j}}}{\frac{1}{D_\mathrm{i}} - \frac{z_\mathrm{i}}{D_\mathrm{j} z_\mathrm{j}}} \quad \text{Equation 3.17}$$

where the subscripts i and j refer to the two ionic species being evaluated (i.e. Na^+ and Cl^-).

3.4.2.1 Boundary layer thickness

The basis of the Nakayama et al. model is the Nernst-Planck equation (Equation 3.2) for a given ion species (Equation 3.3) and is represented as

$$\frac{\partial c_\mathrm{i}}{\partial t} + u_\mathrm{j} \frac{\partial c_\mathrm{i}}{\partial x_\mathrm{j}} = \frac{\partial}{\partial x_\mathrm{j}} \left(D_\mathrm{i} \frac{\partial c_\mathrm{i}}{\partial x_\mathrm{j}} + \frac{z_\mathrm{i} F D_\mathrm{i} c_\mathrm{i}}{R_g T} \frac{\partial \varphi}{\partial x_\mathrm{j}} \right) \quad \text{Equation 3.18}$$

where φ is the total voltage drop [170].

Applying Equation 3.18 to two different ionic species, summing these terms, and applying the effective harmonic diffusivity, the term for the channel velocity is simplified to

$$u_{dil}\frac{\partial c_{dil}}{\partial x}=\frac{\partial y}{\partial y}\left(D_e\frac{\partial c_{dil}}{\partial y}\right)$$ Equation 3.19

where it is assumed steady state and that $c_i=c_j=c_{dil}$. This equation is then used for determining the boundary layer thickness (ω_{bound}) expressed as the following equation.

$$\omega_{bound}(x)=\sqrt{D_e x/\bar{u}_{dil}}$$ Equation 3.20

The boundary layer in an ED channel with a spacer is thinner than in an ED channel without a spacer. This is because the spacer creates turbulent flow which causes the boundary layer to become thinner [179]. As mentioned earlier, the Nakayama et al. model uses a volume averaging theory to deliver solution for ED including and excluding spacers, however, only the methods including spacers will be included in this research.

3

3.4.2.2 Short and long channel definition

The Nakayama et al. model presents two methods for calculating ED channel performance: short channel and long channel. The short channel approach assumes a thin boundary layer that grows from the channel entrance. This is often more appropriate for practical processes. The long channel approach assumes a thick boundary layer that can potentially cover the entire thickness of the channel. This approach is more applicable for narrow channels with low velocity flows. Determining which approach to use is done based on the thickness of the channel as presented in the following equations.

Short channel: $$W\gg\sqrt{D_e L/\bar{u}_{dil}}$$ Equation 3.21

Long channel: $$W\ll\sqrt{D_e L/\bar{u}_{dil}}$$ Equation 3.22

It should be noted that for some cases both long and short channel regions may be present within the same channel. In these cases, the appropriate approach should be applied during the relevant region. This is determined through Equation 3.23 and 3.24 for the given location along the channel length (x).

Short channel region: $$x\ll\bar{u}_{dil}W^2/D_e$$ Equation 3.23

Long channel region: $$x\gg\bar{u}_{dil}W^2/D_e$$ Equation 3.24

3.4.2.3 Analytical solution: Short channel

The short channel flow profile is represented through the Navier-Stokes equation which assumes a parabolic flow through the channel. This is expressed as

$$u_{dil}(x,y) = 1.5\bar{u}_{dil}\left(1-\left(\frac{y}{0.5\,W}\right)^2\right) \qquad \text{Equation 3.25}$$

where y is the location across the thickness of the channel.

Assuming that the concentration profile is symmetrical, the concentration distribution across the diluate channel can be derived from Equation 3.19 and 3.25 to be written as

3

$$c_{dil}(x,y) - c_{md}(x) = \frac{iW}{8F\varepsilon D_e\left(1+\frac{\xi W\bar{u}_{dil}}{D_e}\right)}\left(1-\left(\frac{y}{0.5\,W}\right)^2\right) \qquad \text{Equation 3.26}$$

where c_{md} is the concentration at the membrane interface, ε is the porosity, and ξ is the empirical coefficient for mechanical dispersion. The concentration on the membrane for a short channel with spacer is then defined as Equation 3.27.

$$c_{md}(x) = \bar{c}_{dil}(0) - \left(\frac{ix}{0.886F\varepsilon D_e}\right)\frac{1}{2\left(1+\frac{\xi W\bar{u}_{dil}}{D_e}\right)\sqrt{\bar{u}_{dil}\,x\Big/\varepsilon D_e * \left(1+\frac{\xi W\bar{u}_{dil}}{D_e}\right)}} \qquad \text{Equation 3.27}$$

From Equation 3.27, the limiting current (i_{lim}) is then found to be expressed as Equation 3.28.

$$i_{lim} = 1.772F\bar{c}_{dil}(0) \times \sqrt{\frac{\bar{u}_{dil}\varepsilon D_e}{L} \times \left(1+\frac{\xi W\bar{u}_{dil}}{D_e}\right)} \qquad \text{Equation 3.28}$$

3.4.2.4 Analytical solution: Long channel

The analytical approach for a long channel is based off the Darcy flow accounting for the porosity of the spacer and the assumption that the flow is symmetrical. With these assumptions the concentration on the membrane for a long channel with spacer is defined as Equation 3.29.

$$c_{md}(x) = \bar{c}_{dil}(0) - \frac{iW}{12F\varepsilon D_e\left(1+\frac{\xi W\bar{u}_{dil}}{D_e}\right)} - \frac{i}{FW\bar{u}_{dil}}x \qquad \text{Equation 3.29}$$

Assumption that $c_{md}\,L$ =0, the limiting current is then defined as Equation 3.30.

$$i_{lim} \cong \frac{FW\bar{u}_{dil}\bar{c}_{dil}(0)}{L} \times \left(1 - \frac{\bar{u}_{dil}W^2}{12\varepsilon L D_e\left(1+\frac{\xi W\bar{u}_{dil}}{D_e}\right)}\right) \qquad \text{Equation 3.30}$$

3.4.2.5 Voltage drop

The total voltage drop in the ED unit cell (φ_{cell}) is calculated as the summation of the drop in the channels and in the membranes. This is expressed as

$$\Delta\varphi_{cell} = \Delta\varphi_{dil} + \Delta\varphi_{conc} + iR_{AEM} + iR_{CEM} \qquad \text{Equation 3.31}$$

where φ_{dil} is the voltage drop over the diluate channel and φ_{conc} is the voltage drop over the concentrate channel. The resistance over the membranes are found via experiments. Assuming the resistance for both membranes are the same (R_{AEM} =R_{CEM}=R_{IEM}), the voltage drops are then written for the diluate channel (Equation 3.32) and the concentrate channel (Equation 3.33).

$$\Delta\varphi_{dil} = \frac{R_{IEM}T}{F(D_\mathrm{i}+D_\mathrm{j})}\left[\frac{\xi iW}{F\bar{c}_{dil}(0)} - \frac{4D_e\left(\bar{c}_{dil}(0)-c_{md}(x)\right)}{\bar{c}_{dil}(0)} + 2\left(2D_e + D_\mathrm{j} - D_\mathrm{i}\right)\ln\frac{\bar{c}_{dil}(0)}{c_{md}(x)}\right] \qquad \text{Equation 3.32}$$

$$\Delta\varphi_{conc} = \frac{R_{IEM}T}{F(D_\mathrm{i}+D_\mathrm{j})}\left[\frac{\xi iW}{F\bar{c}_{conc}(0)} - \frac{4D_e\left(c_{mc}(x)-\bar{c}_{conc}(0)\right)}{\bar{c}_{conc}(0)} + 2\left(2D_e + D_\mathrm{j} - D_\mathrm{i}\right)\ln\frac{c_{mc}(x)}{\bar{c}_{conc}(0)}\right] \qquad \text{Equation 3.33}$$

3.5 Empirical data

3.5.1 Doornbusch et al. study

Doornbusch et al. performed desalination for both a single and multistage configuration [180]. The multistage system consisted of four ED stacks under two different operating conditions. The first operating condition applied a uniform current distribution while the second operating condition used a non-uniform current distribution. For the purpose of this exercise, the uniform current distribution will be used for comparing the selected models (see Table 3.2). While it is noted that a non-uniform current distribution is more realistic, using a uniform current distribution will make it simpler to witness the effects of the models performance.

Each ED stack consisted of ten cell-pairs (10 cm x 10 cm) containing 0.155 mm thick woven spacers with a 79% porosity. While this is not industrial scale, it is an appropriate size for assessing the accuracy of the model performance. The properties of the membranes

Table 3.2 Operating conditions for the Doornbusch et al. experiments with uniform current distribution [180].

Stage	Cell-pair voltage [V]	Current density [A/m^2]
1	0.08	75
2	0.097	75
3	0.114	75
4	0.180	75

applied in the Doornbusch et al. experiments are presented in Table 3.3. Additional details regarding the operating conditions applied to the selected models for the Doornbusch et al. comparison are presented in the supplementary materials (S9).

3.5.2 Tedesco et al. study

Tedesco et al. investigated the effect of water transport on the concentration profiles and current efficiency profiles [165], [169]. This research used a single stage configuration with 25 cell-pairs (10cm x 10cm). A cell-pair voltage of 0.3 was applied with membrane specifications matching those in Table 3.4. While the Tedesco et al. model is applied to continuous ED, Tedesco et al. limited its validation of the model to the case of reverse ED. While this validation proved the accuracy of the model, the validation for continuous ED was not included. However, the result of the model for continuous ED were still presented and assumed accurate. As such, the selected models will be compared to the Tedesco et al. model outputs for continuous ED, even though these outputs were not validated. Additional data used for the implementation of the selected models is present in the supplementary materials (S10).

3.6 Results

3.6.1 Comparison to Doornbusch et al.

The three models, Campione et al., Nakayama et al. (short channel), and Nakayama et al. (long channel) were first evaluated using the Doornbusch et al. inputs (Section 3.6.1). If a needed modelling input was not available in the Doornbusch et al. study, the original modelling values were used. Though the Campione et al. model is originally designed with the voltage as the input parameter, the calculations were revised so that the current became the input parameter, therefore, the models could be more easily compared. The

Table 3.3 Properties of the membranes used in the Doornbusch et al. experiments [180].

Membrane	Thickness [μm]	Perm-selectivity [%]	Water permeability [m^3/Pa s m^2]	Resistance [Ω/cm^2]
Fujifilm AEM type 10	146	96	2.22E-14	1.29
Fujifilm CEM type 10	155	97.6	2.22E-14	2.02

Table 3.4 Properties of the membranes used in the Tedesco et al. simulation [169].

Membrane	Thickness [μm]	Perm-selectivity [%]	Water permeability [m^3/Pa s m^2]	Resistance [Ω/cm^2]
Fumasep FAS (AEM)	80	85	2.78E-13	0.8
Fumasep FKS (CEM)	80	94	2.78E-13	1.2

outputs of all three models were then compared to the Doornbusch et al. experimental data for the outlet concentration and specific energy for each stage (Figure 3.5). In addition, the calculated cell-pair voltage was also graphed to provide context to the performance outputs.

With regards to the outlet concentration, the Campione et al. and Nakayama et al. (long channel) models produced very similar results that came within range of the Doornbusch et al. results (Figure 3.5a). The Nakayama et al. (short channel) prediction, on the other hand, was shown to be more conservative in estimating the salt removal for each stage. This is interesting since the Doornbusch et al. case is actually defined as a short channel case per the Nakayama et al. condition equations (Equation 3.23 and Equation 3.24).

The specific energy prediction of all three models were found to considerably underestimate the performance when compared to the experimental values (Figure 3.5b). This is not entirely unexpected since the models only consider the energy used within the ED channels. Empirical measurements such as Doornbusch et al. may also include other aspects of the ED system (i.e. pump and associated pressure losses) which would increase the total energy used in the process. Therefore, a slight underestimation was expected, however, this drastic difference should be accounted for or modified in order to present a more realistic expectation of the energy demand of the ED operations. Regardless of this underestimation, Campione et al. presented a similar rate of increase in the specific

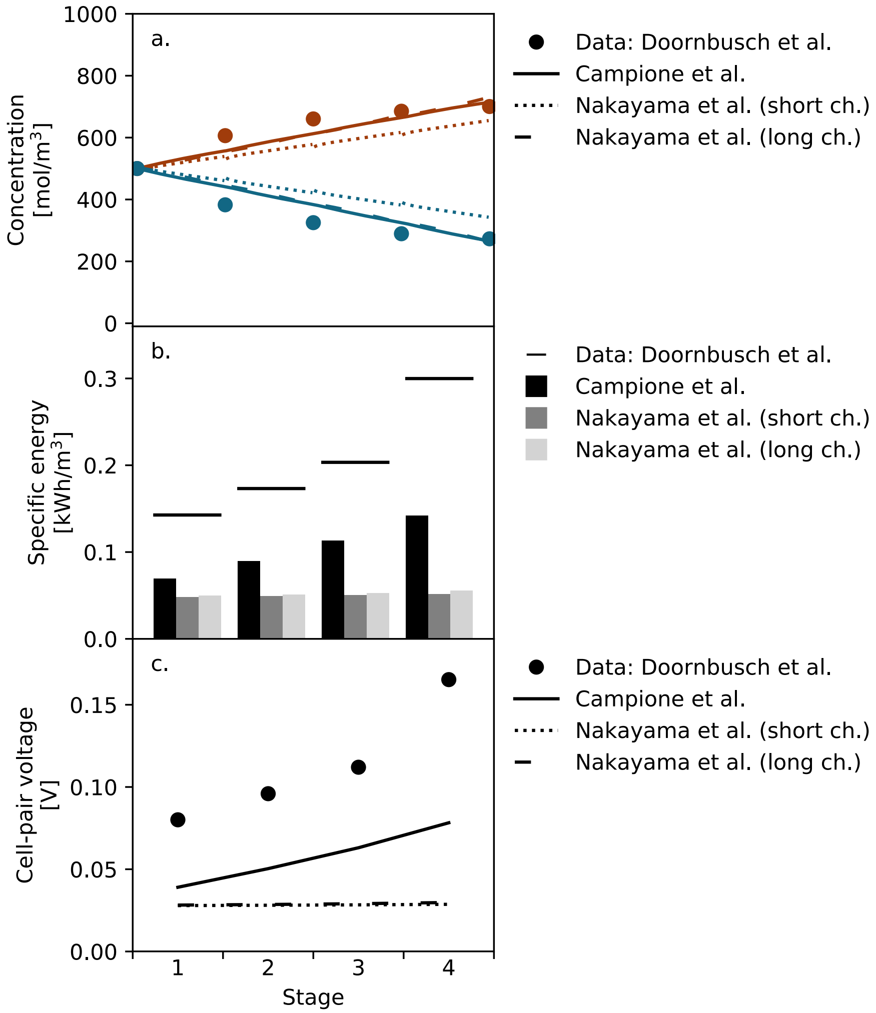

Figure 3.5 Concentration, specific energy, and cell-pair voltage results for each model compared to the Doornbusch et al. experimental outputs.

energy use as compared to Doornbusch et al. The Nakayama et al. models, on the other hand, showed only a slight increase in the per stage specific energy usage. To explore both the underestimation of all models and the small rate of change in the Nakayama et al. models, the calculated cell-pair voltage must be reviewed.

When reviewing the cell-pair voltage calculation for each model (Figure 3.5c), the Campione et al. model shows a similar increase as Doornbusch et al.. However, the cell-pair voltage is also significantly underestimated. To test what is the cause of this, the

Campione et al. model was rerun using its original voltage-based calculation method, the results of which are presented in the supplementary materials (S11). When reverted to a voltage-based calculation, Campione et al. was found to over predict the salt removal, specific energy use, and current calculation. This indicates that there is an issue in the calculation of the resistances which connect the voltage and current calculations. This also holds true for the Nakayama et al. models which show an almost stagnant cell-pair voltage across all stages regardless of the concentration accuracy. To explore this, the total resistance for each stage and for each model was plotted in Figure 3.6.

The Campione et al. resistance (Figure 3.6a) shows that the resistance calculated within the channels is significant and varies with the channel concentration. Therefore, the concentration within the channels directly effects the cell-pair voltage and specific energy calculations. Nakayama et al., on the other hand, calculates an almost fixed and practically negligible amount of resistance across the channels. This results in the cell-pair voltage and specific energy being calculated independent of the channel concentrations as they are primarily reliant on the input current and membrane resistances. While Campione et al. also shows that the membrane resistances are larger than the in-channel resistance, the small estimation of the channel resistances in the Nakayama et al. models' appears to be the primary source of the inaccuracy.

While the purpose of this exercise is to see how the models perform when compared to each other and to empirical results, it was found interesting to explore the effects of including additional phenomena such as the effect of the boundary layer resistance and

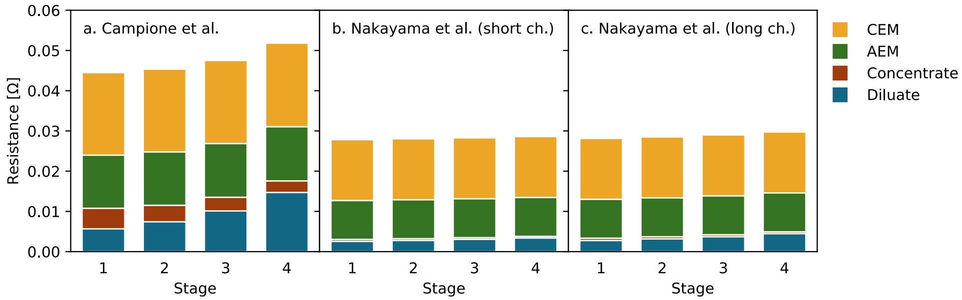

Figure 3.6 Calculated resistance per stage for each model: a) Campione et al., b) Nakayama et al. (short channel), and c) Nakayama et al. (long channel).

the effect of the spacer in the channel. While not explicitly studied in this research, these were briefly included in the models to see if any impacts to the results could be seen.

Inclusion of the boundary layer was possible for the Campione model, as this method included a boundary layer resistance calculation. This is presented in the supplementary materials (S8.3). Inclusion of the boundary layer resistance was found to greatly improve the resistance and, therefore, the cell-pair voltage accuracy. This, in turn, resulted in a more accurate specific energy calculation for each model. Though this improved the accuracy for the Campione et al. model, it was not possible to incorporate this into the Nakayama et al. models. Regardless, it was found that future research should include the boundary layer resistance to improve the accuracy of the models.

Inclusion of the spacer in the channel was also briefly explored. It was observed that the modelling approach of the spacer had a significant impact on the results due to the spacers effect on the boundary layer, however, this can become complicated and is dictated by the composition and geometry of the spacer. Therefore, it is recommended that investigation of the spacer effects should be considered in future research.

3.6.2 Comparison to Tedesco et al.

The Campione et al. and Nakayama et al. models were again applied, this time using the Tedesco et al. data (Section 3.5.2). To investigate the impact of the boundary layer resistance on the Campione et al. model, Figure 3.7 includes the Campione et al. model both with and without the boundary layer resistance. The boundary layer was included in this simulation as the Tedesco et al. model included a 30 second residence time. The slow flow of water through the channels allows the boundary layer to develop, therefore viewing the impacts of the boundary layer may become more significant. While Tedesco et al. validated their model for both reverse ED and batch dynamic ED, their model was not validated for continuous mode ED. Therefore, the comparison in this section cannot state which is more accurate, but rather review how the outputs of the different models compare.

Interestingly, the Campione et al. model excluding the boundary layer resistance matched well with Tedesco et al. One slight difference is that the salt concentration of the concentrate calculated by Campione et al. grows higher at first but then decreases.

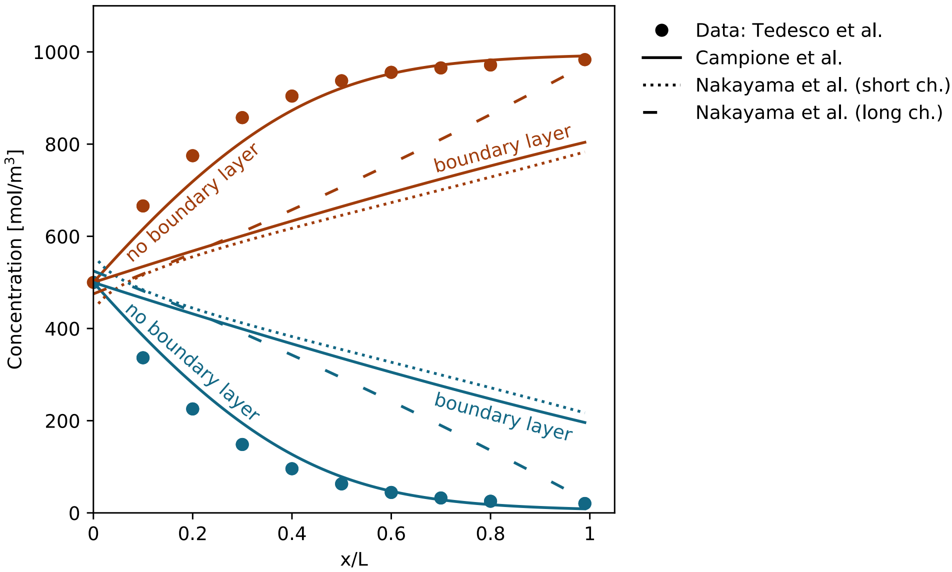

Figure 3.7 Concentration profiles produced by the Tedesco et al., Campione et al., and Nakayama et al. models using the same inputs as the Tedesco et al. model.

Meanwhile, the concentration calculated by Tedesco et al. increases steadily over the length of the channel. This communicates that Campione et al. predicts a lower water transport rate which results in a higher concentration at first but then decreases due to the increased water transport towards the end of the channel. This also communicates that Tedesco et al. uses a more direct correlation between salt and water transport, keeping the concentration levels steadier.

Meanwhile, the Campione et al. model including the boundary layer was found to be similar to the Nakayama et al. (short channel) model. The Nakayama et al. (long channel) model, on the other hand, predicted a similar outlet concentrations as Tedesco et al., though it did not predict a similar concentration profile over the length of the channel. The linear profile is again related to the restrictive resistance calculations mentioned in the Doornbusch et al. case.

Though not included in this evaluation, the Tedesco et al. model also presented results including water transport. When including water transport within the Campione et al. model (excluding the boundary layer resistance), it was found to predict the same concentration profile as Tedesco et al.. The water transport was included via the calculations presented in the supplementary materials (S8.2). When further compared to Figure 3.7, it was found that Tedesco et al. including water transport came to a similar output concentration for the concentrate channel as the Nakayama et al. (short channel). Since the inclusion of the boundary layer and water transport show a closer relation to the Nakayama et al. (short channel) results, it is concluded that the inclusion of these additional phenomena may increase the accuracy of the model performance and there is the possibility that the end result will be more in line with the Nakayama et al. (short channel) results seen in Figure 3.7. However, since this cannot be confirmed through this research it is recommended that these phenomena be further explored in future research.

3. Conclusion

This research identified and compared existing models for continuous ED for a specific systems-level scope. It was concluded that for an intended systems-level analyses, semi-empirical models are the best suited due to their relatively lower computational needs, high accuracy, and wide salinity application range. A systematic literature review of all models led to the selection and application of two existing models: Campione et al. and Nakayama et al.. The Campione et al. and Nakayama et al. model performances were then implemented and compared to the results of one experiment (Doornbusch et al.) and one validated model (Tedesco et al.).

While both Campione et al. and Nakayama et al. were somewhat accurate under specific conditions, the limits of the resistance calculations in the Nakayama et al. models resulted in a poorer performance prediction of the specific energy use. Further, the criteria defined the Doornbusch et al. case as a short channel design, when in fact the long channel modelling approach was more accurate. For these reasons, it is proposed that the Campione et al. model be included in the intended systems-level comparative model.

While exploring these models, the effects of key phenomena were also identified. These include the boundary layer resistance, spacer geometry, and water transport across the membrane. When briefly explored it was found that all three impacted the performance of the models and in some cases actually improved the accuracy of their outputs. It is, therefore, recommended that future research explore how to include these phenomena in the existing models to better predict ED performance.

Water is important to people who do not have it,

and the same is true of control.

– Joan Didion

CHAPTER 4

TREATMENT TRAIN ANALYSIS

Modelling framework for desalination treatment train comparison applied to brackish water sources

ABSTRACT

Desalination is known to have considerable energy, economic, and environmental impacts. Treatment trains are receiving increased interest for their potential to meet produced water standards while both minimizing impacts and increasing the range of eligible input salinities. However, determining which technologies to combine and predicting their performance is both difficult and case specific. This research will present a unique hybrid-modelling framework (the DESALT model) for evaluating and comparing desalination treatment trains based on the same customizable inputs. This comprehensive discrete-based approach generates treatment trains and then systematically evaluates them using physics-based evaluation methods that are reflective of changes in their operating conditions. The DESALT model also accounts for technology limitations, product water requirements, and user preferences. The modelling outputs are filtered using a combination of a Pareto front analysis and data envelopment analysis decision support. The result is a list of eligible and preferred treatment trains with their corresponding operating conditions. The framework's performance was tested by applying two different technologies, electrodialysis and brackish water reverse osmosis, to a brackish water case study. While the methodology was able to capture the trade-offs between treatment trains and individual technologies, the results are highly reliant on the accuracy of the evaluation methods used.

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4.1 Introduction

Water scarcity is an increasing concern across the world due to a geographic mismatch of freshwater demand and availability [181], [182]. Business-as-usual scenarios predict that by 2030 the demand for freshwater will exceed supply by 40% [183]. The finite amount of accessible and available freshwater is further impacted by over-withdrawal, changes to the hydrological cycle, and contamination [3], [182]. The most common form of contamination is salinization which is primarily caused by either salt water intrusion or wastewater discharge [23]. Salinization ranges from brackish (1,000 – 35,000 mg/L) to seawater (35,000+ mg/L) [154].

Desalination is the process of removing salts from saline water and is one of the most popular methods for addressing water scarcity [25]. Desalination produces around 95 million m3 per day of freshwater and its installed capacity is rapidly increasing [25], [26]. There are four main desalination technology types: membrane, thermal, electro/chemical, and emerging [27]–[29]. The most common form of desalination is reverse osmosis (RO) which accounts for 69% of all desalination plants globally [25]. However, no single technology or technology type is best for all situations since technology selection depends on several factors [35], [36]. These factors include feed water quality, product water requirements, operating conditions, technology parameters, and local information.

To date, desalination optimization research has primarily focused on reducing the impacts of individual technologies [27], [57]. This includes reducing energy demand, lowering costs through optimal configurations, and other technological advancements [27], [57]. As many of these optimization paths have been exhausted, research has now turned towards improving performance through combining technologies (i.e. treatment trains) [184], [185]. Treatment trains are defined as a sequence of treatment technologies used to desalinate a saline water source [186].

Treatment trains have the potential to both achieve produced water quality standards while also reducing the associated impacts [187]. However, research and application of desalination has been primarily focused on high-salinity sources [167]. Fortunately, technological improvements coupled with treatment train benefits make it possible to widen the input salinity eligibility [188]. By increasing the range of eligible feed salinities, the number of viable sources also increases thus creating more options to meet freshwater demand.

Determining which treatment trains are worth pursuing is complicated due to the variety of available technologies, the range in their operations, the variance in their performance under different operating conditions, and the needs of the user [189]. Modelling is a potential method to analyze and compare the expected performance of different treatment trains. A treatment train model, however, must include multiple aspects and take into account a myriad of considerations in order to accurately predict treatment train performance and reflect the operating conditions.

4.1.1 Research objective

The objective of this research is to design a comprehensive systems-level decision support tool that can evaluate and compare desalination treatment train performance. This paper will present a unique modelling framework based on this objective, hereafter referred to as the Desalination Evaluation, Screening, And Learning for Treatment Trains (DESALT) model. The DESALT model will present how to integrate physics-based technology-specific evaluations into a larger treatment train assessment through a hybrid-modelling structure. This approach allows for the effects of varied operating conditions for specific technologies to be reflected in the treatment train performance, while still being based on the same input criteria (i.e. feed water specifications) and case specific constraints. The decision support aspect of the DESALT model will expand outside of technical and economic considerations to include both energy and environmental indicators.

The DESALT model will be designed to support either water systems planning or research and development. For water systems planning, the DESALT model can be used as a screening tool which presents the potential capabilities and impacts of treatment trains to convert available water (i.e. brackish water) into desired water (i.e. freshwater). The model can be used by planners or engineers in the initial investigation of waste or brackish water (re)use. For research and development, this model will provide a tool in which the performance of emerging technologies can be reviewed, compared, or matched with existing mature technologies. In this capacity, the DESALT model can be used to identify which treatment trains should be further investigated prior to investing in lab-scale testing.

This paper begins by determining the guidelines of treatment train modelling through a review of the existing treatment train models (Section 4.2). The DESALT modelling framework design is then presented in Section 4.3 and the model results are illustrated in Section 4.4. To conclude, a summarization of the paper and crucial findings are presented in Section 4.5. Supplementary information regarding additional calculations are presented in the appendices.

4.2 Model guidelines

4.2.1 Existing hybrid treatment train models

Existing treatment train models tend to fall into one of three categories: detailed, general, or hybrid [190]. Detailed evaluation models focus primarily on mimicking the exact performance of a specific treatment train and are not meant to assess how different combinations perform [27], [31], [191]–[193]. General assessment models are more commonly focused on estimating performance, costs, or environmental impacts [114], [194]. However, general assessment models typically do not include technological limitations and neglect crucial interactions between operating conditions and performance.

Hybrid-modelling has the potential to integrate detailed evaluation and general assessment models in order to provide a comprehensive systems-level analysis [20], [35], [189]–[191], [195]–[198]. An example of this is the mixed integer nonlinear programming method (MINLP) developed by Skiborowski [191]. This method uses a hybrid-modelling approach for evaluating treatment trains that breaks down the components of each individual technology and optimizes based on the specific technology. The evaluation then uses a step-wise optimization strategy for achieving a set economical objective [191]. This approach results in both an accurate evaluation and a manageable optimization process, however, does not include a comprehensive decision support tool [191].

In incorporating a decision support tool it is important to focus on impacts outside of technical performance such as economic and environmental decision criteria [191]. Al-Nory and Graves present one of the most comprehensive and thorough approaches to desalination decision support including both environmental and economic impacts as well as long-term performance [35], [195]. Additionally, Al-Nory and Graves address the complexities of decision support by providing an interactive visualization of the modelling outputs. The user can select two decision parameters which are then plotted on a Pareto Optimal graph depicting the trade-offs [35]. Though very thorough, the approach presented in Al-Nory and Graves does not account for the impact of the operating conditions on treatment train performance.

Operating conditions are important for assessing treatment train performance as they can directly link to the technical, economical, and environmental decision criteria. Technology-specific evaluations, therefore, are crucial to accurately assessing treatment train performance and impact. Some models address this by using secondary technology-specific software that is operated separately from the model [189], [196]. However, requiring multiple models makes the evaluation process much more complex and can sometimes result in accessibility issues [189], [196], [199]. Gassemi and Danesh addressed this by developing their own technology-specific evaluations within their model making the model reflective of the operating conditions and simpler to use [198]. However, Gassemi and Danesh did not incorporate customization as a feature in their model, instead focusing on pre-set scenarios.

Customization capabilities for both the input criteria and technology evaluation methods are necessary since the former allows for the model to be case specific and the latter allows for the model to remain up to date. The input criteria should include multiple data points including feed water quality, local conditions, and user preferences as exemplified by the evaluation tool of environmental and economic performance for drinking water (the EVALEAU model) developed by Mery et al. [189]. The EVALEAU model monitors 168 water quality criteria for producing high quality drinking water. The customization capabilities of these input criteria allow for the model to be reflective of the given scenario. However, EVALEAU does not include customization of the technology evaluation or internal generation of treatment train combinations. Instead, EVALEAU uses an existing database of pre-determined treatment trains. Limiting the treatment train length [35], [191] and/or combination possibilities [189], [196] limits the discovery of unconventional combinations that could be effective. Additionally, relying on a database for treatment train evaluations can limit the applicability to a given situation, especially if a specific technology needs to be considered. Therefore, it is recommended that in addition to the input criteria being customizable, the technology evaluations and treatment train composition should be customizable as well.

4.2.2 Desalination treatment train modelling guidelines

While each model reviewed can reach its own target, no single model was able to meet the full objective for the DESALT model. From the literature review, five desalination treatment train modelling guidelines were compiled (Table 4.1). These guidelines were referred to during the development of the DESALT model to assure that this research both builds upon existing knowledge and expands the accuracy and potential of treatment train modelling.

4.3 Model design

The evaluation uses a step-wise approach followed by a filtering process which makes sure all modelling outputs meet specific qualifications and requirements. The remaining treatment train options are then assessed using a multi-criteria analysis which highlights those options which perform best based on the decision criteria. This modelling framework is considered unique as it is the first to apply hybrid-modelling to treatment trains while also including the effect of operating conditions and multi-objective optimization.

4.3.1 Treatment train evaluation process

The treatment train evaluation in the DESALT model follows four major steps (Figure 4.1). First, the input criteria are applied which include the feed water quality, treatment train combination, operating condition combination, and technology-specific parameters. This information is used to set up the treatment train steps and apply the appropriate evaluation method and operating conditions.

Second, the treatment train evaluation begins by applying the feed water to the first technology (e.g. Tech A). The evaluation output from Tech A is determined using the technology-specific evaluation method, parameters, and operating conditions. The product water from Tech A is then passed to Tech B and so on until the treatment train is complete.

Third, the modelling output is broken into three aspects: product, brine, and impacts. The product is the desalinated water coming out of the final technology in the treatment train. The associated brine water and impacts, on the other hand, are accumulated over the course of the total treatment train evaluation.

Table 4.1 Desalination treatment train modelling guidelines as gathered from existing literature and their explanations.

Guideline	Explanation
Hybrid-modelling design	• Include and integrate multiple levels of evaluation, including detailed technology evaluations and general treatment train performance assessment. • Use common input criteria and technology parameters for all treatment train evaluations so that they are operating under the same conditions. • Use a modular modelling structure to allow for individual components to operate independently and include their own necessarily level of detail. • Treatment trains should be generated within the model without pre-set combinations and the model should be able to evaluate any combination of the included technologies.
Decision support	• Use a multi-objective optimization decision support tool. • Include technical, economic, energy, and environmental indicators as decision metrics. • Reduce the number of options to a manageable number for user review. • Provide a visualization of the modelling outputs that can assist in understanding the trade-offs between treatment trains.
Technology-specific evaluations	• Develop evaluation methods that are specific to a technology or technology type. • Base evaluation methods on physical processes that include the impacts of operating conditions on the determined indicators. • Operating conditions should include feed water characteristics, site-specific data, and technology parameters. • Include the limitations of the technology to prevent technologies from operating out of their normal scope. • Technology evaluations should not rely on external modelling software.
Customization capabilities	• Both the input criteria and technology evaluation methods should be customizable. • Input criteria should include multiple data points including feed water quality, local conditions, and user preferences that can be easily edited separate from the model. • A modular modelling structure should be used to allow individual aspects to be updated as needed (i.e. technology evaluation, decision support method, etc.). • Model should make it possible for new technologies to be added to the database.

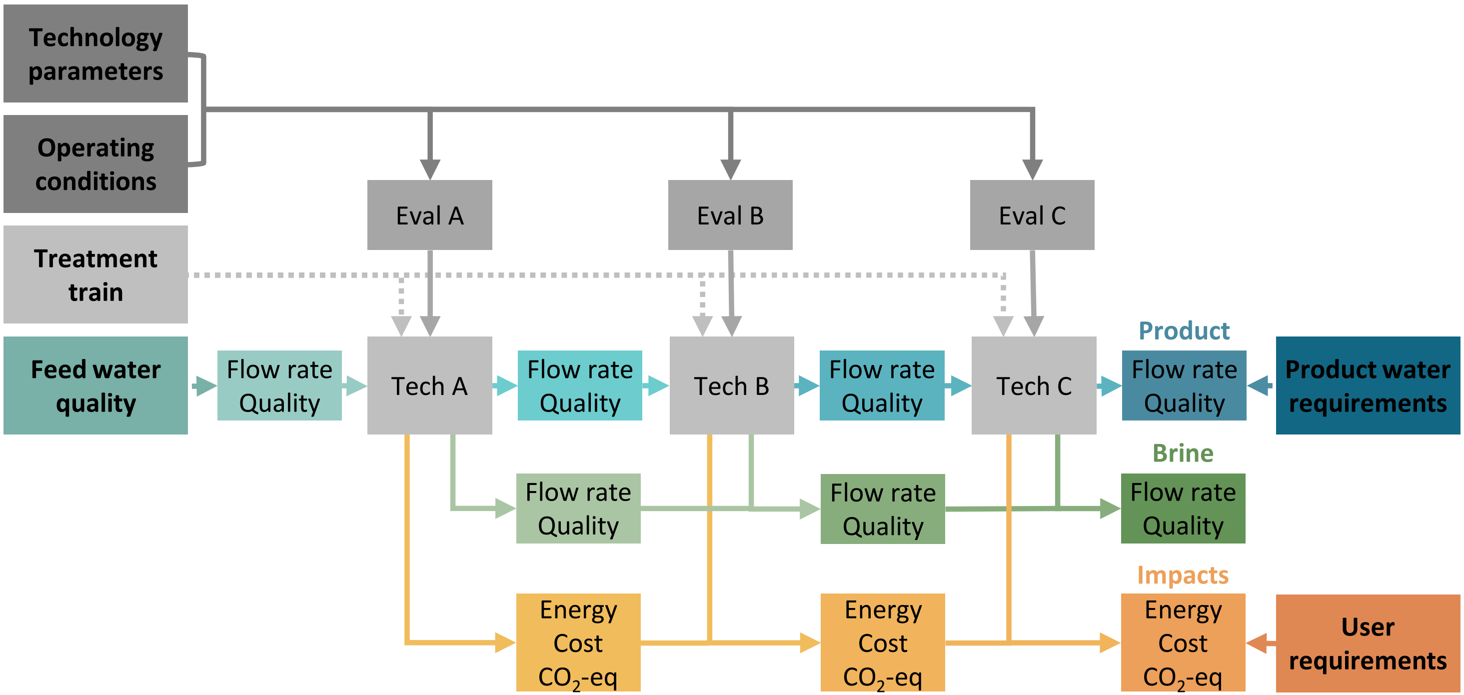

Figure 4.1 Overview of how data is handled in the DESALT treatment train evaluation process.

Finally, the modelling outputs are filtered based on the product water and user requirements. It should be noted that the DESALT method presented in this paper uses a feed-forward approach. This makes it possible for a variety of treatment trains to be more simply evaluated as the incorporation of a brine treatment step or recirculation poses a larger and more complex evaluation process. While it is possible for the model to be expanded to incorporate brine treatment, the scope of this research is limited to treatment trains with consecutive, feed-forward treatment to illustrate the model's design. Since brine treatment is a valuable addition to the model, it is planned to include this feature in future versions of the DESALT model.

4.3.2 DESALT model framework

The DESALT model framework (Figure 4.2) was developed to support the treatment train evaluation discussed in Section 4.3.1 while also following the modelling guidelines outlined in Table 4.1. The framework uses a systematic evaluation approach where each treatment train combination is evaluated under all discrete-based operating condition combinations. This approach was selected since, in the initial development of the DESALT model, it was found that the impact of the operating conditions and complexity of technology interactions resulted in a non-linear optimization problem. Therefore, a full evaluation for each treatment train configuration was necessary before narrowing down to the most preferable options.

The hybrid-modelling structure is achieved through a series of Python subscripts which are managed by a main script controlling the order of execution and feedback of information between evaluation levels. The hybrid structure was achieved using a modular modelling method which keeps each process separate. This allows for the model to be kept up to date and expandable without compromising the model. This format also allows for the technology-specific evaluations to be kept separate from each other, allowing for the evaluation methods to be specific to the technology type.

The input criteria, detailed below, is organized in a controllable Excel workbook which allows for simple review of all input criteria without needing to dissect the model. This format is also customizable so that the input criteria can be reflective of the actual scenario and technology parameters.

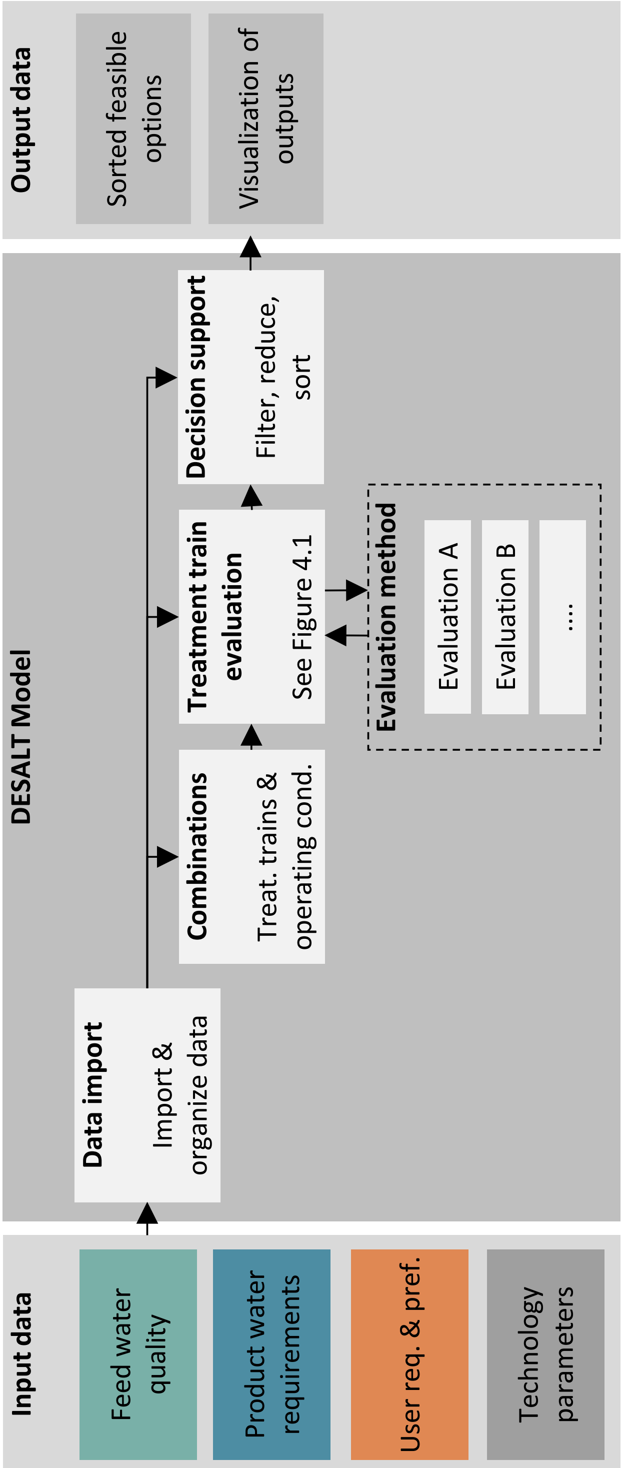

Figure 4.2 Overview of the DESALT model and programming framework.

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Within each evaluation method, key impacts are calculated and then passed to the final decision support script. Within the decision support script, the final modelling outputs are filtered, reduced, and refined to provide a manageable list of options for user consideration.

4.3.2.1 Input criteria and data import

The first step of the DESALT model is to import and organize all the input criteria. This is done separately to facilitate processing speed and data reliability. The input criteria for the DESALT model includes multiple data points which break down into four categories: feed water quality, product water requirements, technology parameters, and user information (Table 4.2). For both the feed water quality and product water requirements, 11 criteria were selected based on expert interviews and literature reviews. Water quality criteria were selected based on their impact on fouling, corrosion, or scaling. Water condition criteria were selected based on their impact on technology performance [28]. In addition, an osmotic pressure conversion factor is needed as the osmotic pressure is dependent on the feed water composition. Osmotic pressure is the amount of force needed to prevent a solvent from passing from one solution to another by osmosis. It is dictated based on the water composition, therefore an osmotic pressure calculator provided by Dow Benelux was used and a correction factor was determined which converted the water composition to an osmotic pressure value. This value has a particular impact on membrane processes such as RO.

User information criteria are broken into three parts: information, preferences, and requirements. User information allows the model to account for site-specific conditions, user preferences are used to help guide the decision support, and user requirements are used to filter out options which do not meet the users operating needs.

The technology parameters are the most extensive aspect of the input criteria. This includes the driving force and operating condition variable range, both of which directly effect a technologies performance. Meanwhile, technology limitations prevent the technology evaluation from operating out of scope and the technology parameters provide information for the technology-specific evaluation. Examples of technology parameters can be found in the supplementary material for both brackish water reverse osmosis (BWRO) (S12) and electrodialysis (ED) (S13).

Table 4.2 Input criteria necessary for the DESALT model.

Feed water specifications	Product water requirements	User information	Technology parameters	
Quality	**Quality**	**Information**	**General**	**Test conditions**
Bicarbonate [mg/L]	Bicarbonate [mg/L]	CO_2-eq conv. for [kg/kWh]	Technology: name, type	Feed salinity [mg/L]
Calcium [mg/L]	Calcium [mg/L]	Local energy cost [$US/kWh]	Driving force: type, min, max	Flowrate [m^3/hour]
Chloride [mg/L]	Chloride [mg/L]	Working hours per day [hours]	Variable A: type, min, max	Pressure [Pa]
Iron [mg/L]	Iron [mg/L]		Variable B: type, min, max	Product salinity [mg/L]
Magnesium [mg/L]	Magnesium [mg/L]	**Preferences**		Recovery ratio [%]
Salinity [mg/L]	Salinity [mg/L]	1st priority [UPC, energy use, ...]	**General performance**	TDS removal rate [%]
TOC [mg/L]	TOC [mg/L]	2nd priority [UPC, energy use, ...]	Availability [%]	Temperature [K]
		Train length [1, 2, 3, ...]	Technology lifetime [years]	TOC removal rate [%]
Condition	**Condition**	Evaluation period [years]		
Flowrate [m^3/hour]	Flowrate [m^3/hour]		**Feed limits**	**Impact factors**
Pressure [Pa]	Pressure [Pa]	**Requirements**	Bicarbonate: min, max [mg/L]	Capital: UPC coefficient b [-]
Temperature [K]	Temperature [K]	Max investment cost [$US]	Calcium: min, max [mg/L]	Capital: UPC coefficient m [-]
		Unit production cost [$US/m]	Chloride: min, max [mg/L]	CO2 conversion factor [kg/m^3]
Other			Flowrate: min, max [m^3/h]	O&M: UPC coefficient b [-]
Osm. press. conv. [Pa mg/L]			Iron: min, max [mg/L]	O&M: UPC coefficient m [-]
			Magnesium: min, max [mg/L]	O&M: Share general [%]
			Pressure: min, max [Pa]	
			Salinity: min, max [mg/L]	**Technology-specific parameters**
			Temperature: min, max [K]	....
			TOC: min, max [mg/L]	

4

4.3.2.2 Combinations

DESALT evaluates all possible treatment train combinations in all possible configurations since the same set of technologies may perform differently depending on their order. The treatment train length ranges from standalone to the maximum specified treatment train length, as set by the user. The treatment train combinations are then filtered to remove any illogical treatment train combinations as determined through literature reviews and expert advice (e.g. nanofiltration should not occur after RO).

The set of operating condition values for each technology are then generated based on a user specified step size and operating bounds. The total number of DESALT evaluations is therefore dictated by the treatment train length, number of variable operating conditions, and the operating condition step size.

4.3.2.3 Treatment train evaluation

The accuracy of the model is entirely reliant on the accuracy of the technology evaluation, therefore, guidelines were developed to guide the development of these evaluations (Table 4.3). It was determined that the most effective evaluation method is one based on systems-level physical equations [30], [200], [201]. The level of physical modelling must reflect the effects of the operating conditions but must also be capable of using the same set of common input criteria as the other technology evaluations.

Almost any technology can be included that is able to adhere to these guidelines and is also accurate. As the model does not include feedback loops or recirculation schemes, it is possible for any technology to be included that can be applied to brackish water for the purposes of a feed-forward analysis.

To illustrate the capabilities of the DESALT model, two evaluation methods were developed for two different technology types: BWRO and ED. BWRO is a pressure driven technology that has been extensively researched and modelled. The extensive amounts of available data and modelling approaches allows for the technology evaluation to be easily validated against existing data. ED was selected to test the capability of the model to incorporate a different technology type with a different level of available data. ED is an energy driven technology with limited available data, especially on a systems-level and commercial scale. The evaluation methods are presented in the supplementary material for BWRO (S12) and ED (S13). While these are the only evaluation models presented in

Table 4.3 Evaluation method guidelines for use in the DESALT model and their explanations.

Guideline	Explanation
Common inputs and evaluation outputs	• Must be able to use the same common input criteria regarding feed water specifications, product water requirements, and user information (presented in Table 4.2). • Must be able to produce the same set of information as presented in the feed water specification in Table 4.2 so that the next technology evaluation can continue the treatment train evaluation.
Attainable technology parameters	• Needed technology parameters must be found on a common datasheet • If data points are not easily found, a standard value must be used
Reasonable complexity	• Must reflect changes in feed water quality and operating conditions • Include technology limitations and parameters • Mindful of computation time
Verifiable	• Verifiable through comparison to existing literature or empirical results

this paper, other technologies were tested as well (e.g. nanofiltration). It is expected that the technology evaluations will grow with further modifications of the model.

4.3.2.4 Decision support and modelling output data

The DESALT model can result in thousands of modelling outputs depending on the treatment train length and operating condition step size. For example, given a maximum train length of two including two technologies results in six treatment train combinations, including standalone operation. If each technology has three operating variables with five steps, this would result in 93,750 treatment train configurations. The purpose of the decision support is therefore to filter through these evaluations and provide a reasonable list of options that can be efficiently reviewed.

The decision support consists of three steps: filter, reduce, and refine. In the filter step, a treatment train configuration is only considered to be an option after it passes several constraints. If at any point in the evaluation the limits of a technology are exceed (i.e. exceeds maximum feed TDS), the treatment train configuration is discarded. Configurations are also omitted if they are not able to meet the produced water quality and quantity requirements or if the modelling outputs are outside the user specified limits (i.e.

Table 4.4 Decision criteria used in the multi-criteria analysis in the DESALT model.

Decision metric	Symbol	Unit	Objective
Recovery ratio	δ	%	Maximize
Removal rate	R	%	Maximize
Unit production cost	UPC	$US/m^3	Minimize
Specific energy	E_{spec}	kWh/m^3	Minimize
CO_2-equivalent	CO_2-eq	CO_2-kg/m^3	Minimize

exceeds the maximum cost). Once these filters are applied, the filtered set of options are then applied to a multi-criteria analysis.

In the reduce step, the filtered set of options are reduced through a Pareto front analysis. In a Pareto front analysis, eligible options are reduced to only those that are considered Pareto-efficient. Pareto-efficient is defined as options where one objective cannot be improved without worsening at least one other [202]. An objective, in this case, is to either maximize or minimize a given decision criteria, as outlined in Table 4.4 [203], [204]. For each decision criteria, a single-objective problem is defined and these single-objective problems are then optimized so that only options which behave well for all objectives are considered. This removes poor performers and results in a Pareto front which is a set of options that are globally beneficial for all decision criteria [205].

In the refine step, the set of filtered and reduced options are further narrowed through use of data envelopment analysis (DEA). DEA is a non-parametric multi-criteria decision technique that calculates the relative efficiency of each decision criteria as compared with the set of decision criteria [204]. In the DESALT model the classic Charnes, Cooper, and Rhodes multiplier model with constant returns to scale was used with equal weight constraints given to each decision criteria [206]. This mathematical approach normalizes and compares the decision criteria associated with each option, referred to in decision science as a decision making unit (DMU) [207]. The result is an efficiency score for each option between zero and one, where a score of one means the option is considered efficient. The output of the 'refine step' is a set of final options to be used as an intelligent starting point for further discussion on the appropriate desalination approach for a given scenario. While this list is useful to review, a radar chart plotting the best performing options for all five decision criteria is included to visualize the trade-offs between options [208].

4.4 Model results

In this section, an illustration of the model results using BWRO and ED and sample input criteria are presented. This section will first highlight the effects of the feed salinity, recovery ratio, and product salinity on the evaluation outputs generated by the DESALT model. The model will then be applied to an industrial case study to further illustrate the decision support aspect of DESALT. The model was able to execute a high number of evaluations with ranges in both feed water composition and operating conditions. The results showed correlations between operating conditions and performance and the decision support was shown to effectively narrow the list of viable options.

4.4.1 Effect of feed salinity

The model was run for both mildly brackish (1,500 mg/L) and moderately brackish (15,000 mg/L) feed water concentrations. Highly brackish feed water was not tested as this concentration exceeded the limitations of the included technologies and the scope of the DESALT model. To demonstrate the number of evaluations, all modelling outputs before the decision support filter were plotted in Figure 4.3. This large amount of data depicts the full range of treatment train configurations and, as a result, some basic correlations can be seen. With a lower feed salinity, the treatment trains can achieve lower product salinity and lower specific energy values. With a higher feed salinity, the lowest possible product salinity increases. Additionally, the unit production cost (UPC) also increases with the product salinity as compared to the lower feed salinity scenario.

Treatment trains that include ED show a relation between increased salt removal and decreased recovery ratio. This is due the effects of water transport since increased salt removal translates directly to increase water removal from the product stream (see supplementary materials S13.5).

At both very low and very high product salinities, the preferred treatment train is essentially clear. BWRO + BWRO is the only treatment train option for very low product salinities due to its high removal rates, while the less expensive single stage ED performs best for higher product salinities due to its low removal rate but more cost-effective operation. However, between these extremes there is a high density and diversity of options making it unclear which treatment trains are preferred. This is because of the inverse correlations between

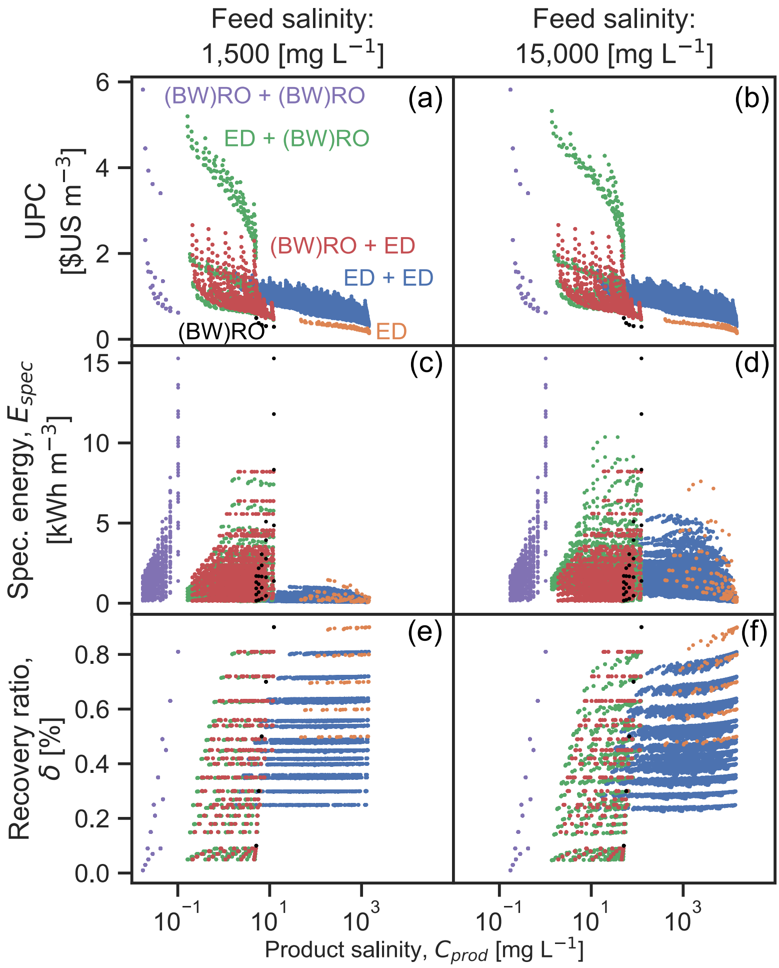


Figure 4.3 The decision criteria performance of all possible treatment train configurations of BWRO and ED are plotted for both high and low feed salinities. Figures a, b, and c represent the model being run with a low feed salinity (1,500 mg/L), while Figure d, e, and f use a moderate feed salinity (15,000 mg/L).

operating conditions on treatment train performance and the counter-relationships between decision criteria.

This large amount of data highlights the need for a systematic facilitation towards decision support so that the best performing options can be identified. Further, there are some options completely unnecessary for a user to consider. For example, in Figure 4.3b and Figure 4.3e the upper right corner of the BWRO + BWRO data represents the highest recovery ratio and the highest applied pressure. This is a non-preferred option since it is more energy-intensive and less effective.

4.4.2 Effect of recovery ratio

The effect of the recovery ratio was reviewed by setting a recovery ratio minimum (δ_{min}) and then reviewing the effects of the product salinity on the specific energy. This was done again for both mildly and moderately brackish feed water scenarios (Figure 4.4).

The plots represent the best operating condition for a given treatment train. The visible steps in the graphs are representative of the change in operating conditions for a new preferred combination. Smoother lines would be achieved with smaller step sizes in the evaluation, however, this would also increase the number of evaluations exponentially. Note that the single phase BWRO line is often hidden behind the two-phase BWRO treatment train.

Low recovery ratios are associated with low specific energy requirements. This is due to lower operating condition requirements because of: i) the inverse relation of salt removal and recovery ratio for BWRO (S12.2); and ii) the direct relation between the quantity of salt being removed from a smaller stream for ED (S13.3). Further, it can also be seen that ED performs worse at higher recovery ratios because higher recovery ratios result in higher velocities which are inversely related to salt removal (S13.4: Equation S13 6).

As expected, for ED treatment trains, the operating conditions must increase with the lower product salinities, therefore resulting in a higher specific energy. For BWRO, the lines are flat since BWRO operates at a very high removal rate and the performance of BWRO treatment trains are dictated by the recovery ratio. While standalone technologies are more energy-efficient than treatment trains, they may not perform best when considering other impacts or requirements.

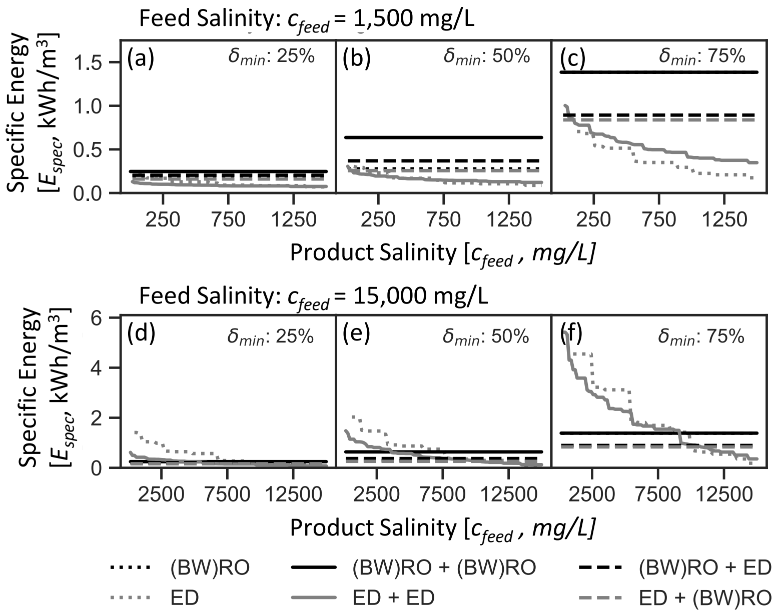


Figure 4.4 Performance of treatment trains in terms of energy based on produced salinity (x-axis) and recovery ratio for a low salinity feed and a high-salinity feed. Figures a, b, and c represent the model being run with a low feed salinity (1,500 mg/L), while Figure d, e, and f use a moderate feed salinity (15,000 mg/L).

4.4.3 Effect of product salinity requirements

The product salinity requirement is one of the most limiting factors for treatment train feasibility. As presented in Figure 4.5, the combination of product salinities and feed water salinities dictate which treatment trains are even possible.

For very low product salinity requirements, BWRO + BWRO is the primary option. However, as the maximum product salinity increases, other treatment trains become both eligible and more competitive. Comparing the third panel to the first it can be seen that as the maximum product salinity increases, ED + ED becomes more competitive and would eventually become the cheapest option.

While ED + BWRO and BWRO + ED are very similar to each other, a difference is seen at the higher removal rates. When ED is first, it shoulders more of the burden for removing salts. Since it operates at a lower cost and reduces the need for BWRO to operate at a higher

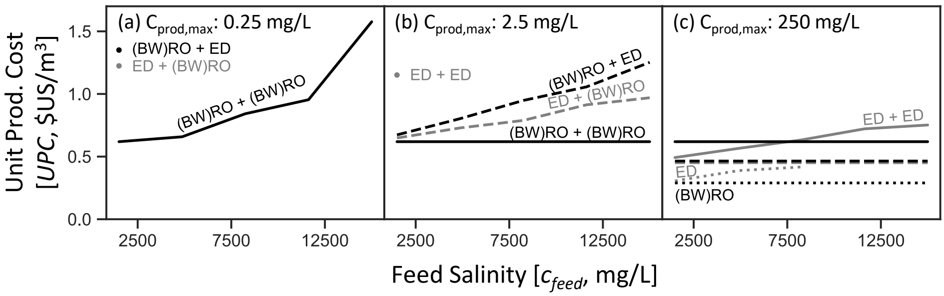


Figure 4.5 UPC performance of treatment trains (excluding standalone technologies) based on the feed salinity and the given product salinity requirement where (a) represents the results with a maximum product salinity of 0.25 mg/L, (b) represents the results with a maximum product salinity of 2.5 mg/L, and (c) represents the results with a maximum product salinity of 250 mg/L.

4

level, it becomes the cheaper option. However, once the product salinity is decreased, the difference in cost becomes negligible.

4.4.4 Case study

The DESALT model was applied to the case study of Dow Benelux [28]. In this case study, the feed water is cooling tower blow down (CTBD) with the produced water requirements based on their internal demi water requirement (Table 4.5) [28].

The DESALT model was run and 22,650 evaluations were completed. Applying the product water requirements, the number of results was immediately decreased to 4,120. Next, the Pareto front analysis was run with equal weight given to each decision metric (see Table 4.4). The resulting Pareto frontier reduced the total options to 365 final results. This translates to a 99.9% reduction from the total initial options. The visualization of the filter and Pareto front analysis as compared to all original options can be seen in Figure 4.6.

The final step in delivering information to stakeholder-based decision support process is sorting the Pareto frontier using the DEA analysis. The DEA was run for each remaining treatment type with equal preference for all decision metrics. The result was the best treatment train configuration for each treatment train type. The best option was then plotted on a radar chart (Figure 4.7) to showcase the differences in performance for each viable treatment train type. Note that the energy, CO_2-eq and, UPC scores are normalized as compared to the other decision metrics. Since the product salinity requirement was

Table 4.5 Feed water specifications and produced water requirements based on CTBD and demi water requirements (respectively) for the Dow Benelux case study [28]

	Feed water specifications: CTBD	Produce water requirements: Demi water
Quality		
Bicarbonate [mg/L]	45	1
Calcium [mg/L]	650	125
Chloride [mg/L]	1538.5	5.78
Iron [mg/L]	0.2	350
Magnesium [mg/L]	60	80
Salinity (NaCl) [mg/L]	2564.1	9.62
Total Organic Carbon [mg/L]	50	20*
Condition		
Flowrate [m^3/hour]	190.26	19.03**
Pressure [Pa]	101.3	101.3
Temperature [̊C]	25	25

* *The actual demi water requirement is 2 mg/L but was modified for comparison purposes*

** *This value was not set as a requirement, so the focus of the results was on water quality.*

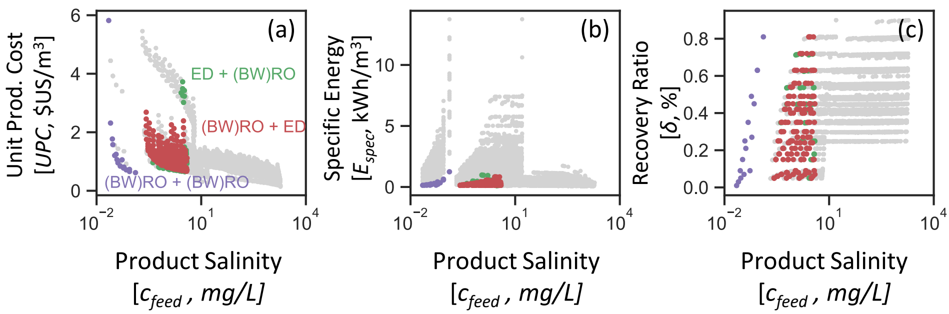
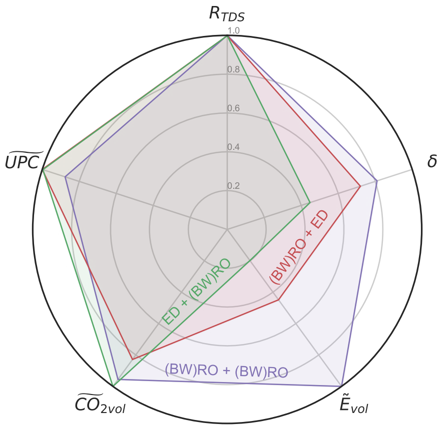


Figure 4.6 Graphical result of the filter and Pareto frontier pairing compared to all original options (grey) where (a) represents the results with respect to the UPC, (b) represents the results with respect to the specific energy, and (c) represents the results with respect to the recovery ratio.



Treatment train	Operating cond. 1	Operating cond. 2
(BW)RO + (BW)RO	P_{app} = 500 kPa δ = 90%	P_{app} = 500 kPa δ = 90%
(BW)RO + ED	P_{app} = 500 kPa δ = 90%	V_{cp} = 0.15 V δ = 80% N_{cp} = 350,000
ED + (BW)RO	V_{cp} = 0.10 V δ = 50% N_{cp} = 250,000	P_{app} = 500 kPa δ = 90%

Figure 4.7 Radar chart of best option per treatment train configuration using a balanced DEA and including changes in operating conditions, as presented in the accompanied table. These options are based on a feed flowrate of 190.26 m^3/hour with a NaCl salinity of 2564.1 mg/L that is treated to meet a product water requirement flowrate of 20 m^3/hour and salinity of 9.62 mg/L.

already applied in the filtering step, all options score similarly for removal rate (good = edge of radar). Since the product salinity requirement was already applied in the filtering step, all options score similarly for removal rate (good = edge of radar).

Regarding the recovery ratio (good = edge of radar), ED treatment trains rely heavily on a smaller product flowrate to achieve higher salinity removal rates. Additionally, the more salt removal required, the more water transport occurs. Therefore, when ED is the first step in the treatment train or when ED is primarily responsible for salt removal, the recovery ratio decreases.

The recovery ratio has a further effect on the graph as the UPC (good = center of radar), specific CO_2-eq (good = center of radar), and specific energy (good = center of radar) are in terms of the product flowrate. Therefore, if the recovery ratio decreases, the product flowrate decreases, and the other impacts increase.

When considering single objectives, the prevailing technology can be clear but when considering all key impacts, the decision process becomes more complicated. This is where the benefit of mixed treatment trains (i.e. including both technologies) is seen. Homogenous treatment trains tend to perform well at the extremes, while mixed treatment trains can achieve a more well-rounded performance. However, choosing the best option involves further consideration including user preferences through stakeholder interactive decision processes and case context dependencies.

4.5 Conclusion

Overall, the DESALT model is an effective modelling approach for reviewing brackish water desalination treatment trains. It is novel in that it uses common input criteria so that all treatment trains are based on the same information. Further, the technology-specific evaluations are based on physical equations and the decision support focus beyond the common technical and economic indicators to include energy and environmental impacts. The model design is also unique since both the input criteria and the evaluation methods are customizable. As such, the DESALT model provides a comprehensive treatment train evaluation that couples detailed assessment methods with general impact considerations.

The development of the model built off the strengths of existing hybrid treatment train models. The result was a set of guidelines for both the treatment train model design and evaluation method development. Two sample evaluation methods were developed to illustrate what is required in an evaluation method and to test the accuracy of the evaluation outputs. In their development it was highlighted both how crucial these evaluations are to the accuracy of the model while also how complex these evaluations can become. Since there are several approaches to this, it is advised that the evaluation be done carefully and that the results should be interpreted with the awareness that deeper investigation of the treatment trains should be done before implementation.

While this exercise included two fairly well-known technologies, this model makes it possible to promote up and coming technologies by providing a platform to test them. All that is required is an evaluation method for the specific technology and input criteria.

The outputs of the model showed that treatment trains were able to achieve a wider range of product salinities. Further, the order of technologies in the treatment train also had an impact on performance. The large number of results and counter-performing impacts confirmed the need for a multi-objective decision support. While this can narrow the number of relevant options, stakeholder interactions, expert input, and case specific contextual effects need to be included in the final decision making process.

The DESALT model can contribute to the development of decentralized water systems by matching supply and demand through testing a large range of treatment trains under varied operations. In future work, it would be relevant to expand upon this model to include sequential treatment on the concentrate streams to better address brine management and increase the overall recovered water. Additionally, inclusion of more technologies would further broaden the applicability of the model to different scenarios.

Reason is the first casualty in a drought.

– Marc Reisner, Cadillac Desert

CHAPTER 5

TREATMENT VS. TRANSPORT

A framework for assessing the trade-offs between on-site desalination and off-site water sourcing for an industrial case study

ABSTRACT

Limited availability of fresh water and growing industrial demand have led to an increased need for alternative water sources. Two common alternative sources are on-site desalination (treatment) and off-site water sourcing (transport). Decision makers managing the integration of these alternative sources need tools to help assess the economic and sustainability impacts, as the combination can result in thousands of options. This research is aimed at developing a modelling framework for Data Envelopment Analysis for Integrated Water Resource Management to enable the comparative analysis of integrated treatment and transport technologies. This framework can assess alternative water supply configurations of treatment and transport and then identify the preferable configuration based on economic and environmental indicators. The framework is comprised of two evaluation modules. First, the performance of treatment and transport are determined using previously developed simulation models. Second, the outputs of these models are analyzed using data envelopment analysis. The framework was applied to an industrial case study in the Netherlands where the best configuration was a combination of 20-30% treatment and 70-80% transport. The outputs of the framework were shown to assist decision-managers in tailoring the configuration for their situation. It was shown that treatment and transport can be complementary measures, since treatment has a greater potential to reduce energy consumption and carbon dioxide emissions while transport is generally more cost-effective.

5

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5.1 Introduction

Freshwater scarcity is rising worldwide due to increasing water demand and limited availability [209], [210]. The available water supply is further impacted by contamination and changes in the hydrological cycle as a result of climate change [211]. It is predicted that by 2025 more than 50% of the world's population could suffer from severe water scarcity making freshwater scarcity one of the major challenges for society [25], [212].

Water availability is a particular challenge for delta regions which attract urban and industrial development but have limited water availability due to saltwater intrusion and salinization of freshwater sources [213]. Saltwater intrusion occurs when seawater infiltrates the groundwater system resulting in non-potable brackish water [214]. The occurrence of saltwater intrusion is increasing due to excessive groundwater withdrawal and sea-level rise [215]. Salinization of surface water occurs when saline water is discharged from agricultural and industrial activities [155], [216].

The industrial sector is focused on reducing the risk of water scarcity by improving processes and shifting towards alternative water sources [16]. The two most common forms of alterative water sourcing are treatment of saline water and transport of fresh water from less water scarce areas [217]–[219]. Desalination is more expensive and energy-intensive while transport is more risky in both development and reliability [217], [220], [221]. While both methods are effective, their eligibility and performance depend on case specific factors.

5.1.1 Desalination treatment

Desalination is the process of removing salt from saline water in order to produce a less saline or fresh water product [222]. Desalination is a reliable solution for supplying fresh water when saline water is present [223]. Desalinated water has the potential to alleviate freshwater demand and can potentially promote circular water use, especially at large water consuming agro- and industrial facilities. As water resources become scarcer, desalination is likely to become a major contributor to water supply, making it necessary to assess the potential impacts of a more substantial use of desalination.

Desalination treatment methods generally fall into one of three categories: membrane, thermal, or electro/chemical [28]. The most common desalination technologies used are reverse osmosis (RO), multi-effect distillation, and multistage flash distillation [45], [224], [225]. Depending on the case specifics, desalination can be cost-prohibitive and its sustainability can be questioned due to its energy consumption, brine production, and CO_2 emissions [226]. The relevance and severity of these issues depend on several factors including treatment technology type, feed water salinity, and product water requirements [227]. Performance and optimization of desalination technologies have been addressed through mathematical modelling which can help determine eligibility and predict performance [149], [228], [229].

Recent technological developments have made desalination more attainable economically resulting in a global expansion of desalination [230], [231]. Now more than 120 countries rely on desalination to either supplement or completely provide their fresh water [230], [231].

5.1.2 Water transport

It is predicted that as water resources become more scarce, water networks will become more decentralized. Water transport can alleviate pressure on local resources and can help balance regional supply with localized demand. Typical water sources used in water transport are lakes, rivers, and aquifers connected by pipelines, aqueducts, or water tankers [215], [232]. The design and evaluation of water transport networks is complex, requiring model-based approaches to explore potential configurations [233], [234]. Several simulation models are available for both design and operation of water transport networks [235], [236]. These simulation models can compare the performance of different networks based on criteria such as economic, environmental, and societal impacts.

While transport can match supply with demand, the withdrawal rate at the source must be considered [139]. Excessive withdrawal can negatively affect the water balance and result in the depletion of a freshwater resource [237], [238]. Building and operating water transport infrastructure can also be expensive and can have significant environmental and societal impacts [239], [240]. The level of impact depends on location specific factors such as the elevation, transport distance, construction materials, and estimated lifetime [241]. Consideration for land use and landscape features in the design phase can help reduce these impacts, especially related to construction costs [234].

5.1.3 Integrated water resources management

Assessing an alternative water source option is typically done independent of other potential options. Combining options using integrated water resources management (IWRM) can uncover additional benefits such as improved economic, environmental, or societal performance [242], [243]. IWRM is valuable in the decision support process since the number of variables associated with combined options are too complex for a decision-maker to intuitively predict and consider future impacts [244].

Processing the performance of a large number of combinations of treatment options, water sources, and available infrastructures can only be achieved through mathematical modelling [245]. It is essential to develop tools in IWRM that present both technical and sustainability indicators in a way that can support the decision making process [246], [247]. This can be achieved by integrating the outputs of simulation models with multi-criteria decision making (MCDM) [10], [248].

5.1.4 Multi-criteria decision making

MCDM is a branch of operations research that finds the best alternatives out of a set of solutions based on multiple objectives or criteria [203], [204]. Assessing alternative water source configurations can benefit from MCDM as there are multiple options and criteria to consider. When there are conflicting objectives and many alternatives, no single solution exists for which all criteria are fully satisfied.

The first step in the MCDM evaluation is to limit the set of solutions by identifying all Pareto-efficient solutions [249], [250]. Pareto-efficient solutions are solutions where one objective cannot be improved without worsening at least one other [202]. Often the remaining number of solutions is still large [251]. In these cases, further differentiation can be done through techniques such as Data Envelopment Analysis (DEA). DEA is a non-parametric MCDM technique that calculates the relative efficiency of each solution within an explicit set of given solutions [204].

Within the water management sector, DEA has been widely applied for the purpose of providing decision support [252], [253]. DEA has not yet been applied within a modelling framework for considering the trade-offs between (or integration of) desalination treatment and water transport systems. Such a modelling framework can assist decision makers in promoting more efficient water supply alternatives based on local availability.

5.1.5 Research aim

In this research a new decision support modelling framework is developed for Data Envelopment Analysis for Integrated Water Resource Management (DEA-IWRM). The aim of the DEA-IWRM framework is to enable the systematic evaluation of integrated desalination and water transport systems as alternative water supply sources.

The proposed DEA-IWRM framework consists of two main phases. In the first phase different combinations of desalination and transport are evaluated to meet a given industrial demand. This is done by integrating the output data of two existing simulation models. In the second phase the modelled data is analyzed using different DEA models to identify the best water supply configuration based on economic and environmental indicators. The framework is tested using an industrial case study provided by Dow Benelux (Dow) in Terneuzen, Netherlands.

To our knowledge, this is the first time that DEA has been applied for assessing the integration of treatment and transport to meet an industrial water demand. The DEA-IWRM framework is unique in that it helps determine what share of water should be internally recycled versus what share of water should be externally sourced based on technical, economical, and environmental indicators.

5.2 Modelling methods and inputs

Two simulation models were selected as inputs for DEA-IWRM. The Desalination Evaluation, Screening, and Learning for Treatment Trains (DESALT) (see Section 5.2.1) evaluates desalination treatment trains and provides a comprehensive output of the available options including technical, economic, and environmental indicators [218]. The Water Supply Network (WSN) model (see Section 5.2.2) evaluates and determines the optimal network configuration of decentralized water sources to meet water demand [219]. DESALT and WSN were selected as they were both built for the purpose of systems-level evaluations and were based on the same set of assumptions as part of the Water Nexus project. DESALT is uniquely relevant as it provides a variety of treatment train scenarios and their related impacts based on a given feed water quality. WSN is unique in its ability to incorporate spatial factors influencing pipeline construction costs with a water balance optimization to generate water network configurations [219]. It should be noted that other models can also be used as input models for DEA-IWRM [31], [233].

Both DESALT and WSN were applied to the Dow case study which aims to meet a portion of their industrial water demand by either recycling brackish cooling tower blowdown or by transporting water from off-site groundwater wells (Section 5.2.3).

5.2.1 Treatment model: DESALT

The DESALT model performs a systematic evaluation of desalination treatment trains operating under the same feed water input [218]. DESALT generates treatment trains based on selected desalination technologies and then evaluates each train under varied operating conditions to determine the optimal configuration. Treatment train combinations consist of multiple desalination technologies operated in sequence and both unique pairings and pairing orders are included. For instance, one treatment train may be technology A followed by technology B while another treatment train would be technology B followed by technology A. The order of the combinations is important as individual technology performance depends on feed salinity and operating conditions. Operating conditions include pressure, temperature, and other variables that can affect technology performance. DESALT then screens the outputs to make sure all options meet product

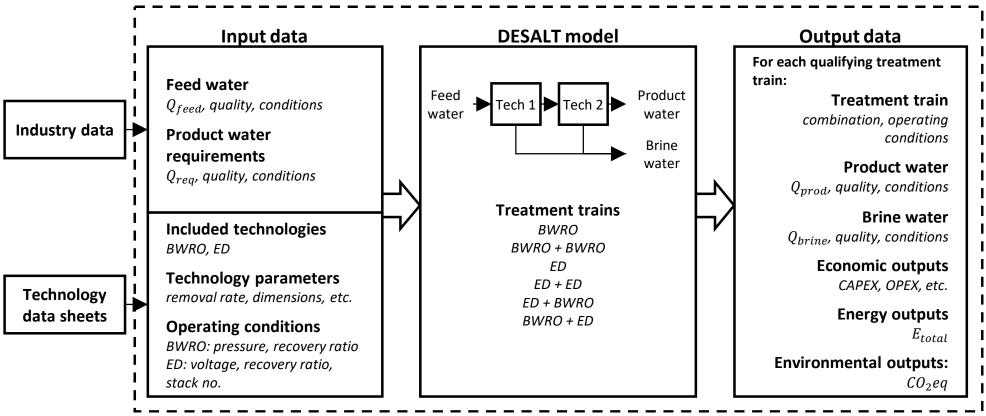

Figure 5.1 DESALT desalination model overview including input data, modelling principle, and output data. Data from industry includes information on the quality and quantity of (waste) water while technology data sheets provide technical information regarding technologies [218].

water quality requirements. An overview of the DESALT model can be seen in Figure 5.1. Note that water quantity is represented by the flowrate (Q).

DESALT inputs include multiple feed water quality data points. Water quality data points include total dissolved solids, relevant minerals, and total organic carbon. Water condition data points include temperature and pressure. The treatment train is then evaluated using a step-wise calculation where the output from one technology is used as the input for the next. Each technology is evaluated using a technology-specific physics-based evaluation method which incorporates the effects of the specified operating conditions. Each technology-specific evaluation method was validated using peer reviewed literature and empirical results.

The output is the performance of the treatment train configuration based on technical, economical, and environmental data points. Both the product and brine quality and conditions are presented in the output. Economic outputs include the capital costs (CAPEX) and the operation and maintenance costs (OPEX) including energy and maintenance. Environmental impacts are captured through energy usage (E_{total}) and CO_2-equivalent (CO_2eq) data.

The DESALT model was run considering two desalination treatment technologies: brackish water reverse osmosis (BWRO) and electrodialysis (ED). BWRO and ED have often been compared to each other in terms of desalination performance and cost effectiveness [159]. There is also an existing research interest in pairing these two technologies [58]. These technologies were also selected for use in DESALT because of their fundamental differences. BWRO is a pressure driven process while ED is an electrically-driven process, each using a different transport mechanism requiring different evaluation methods. The benefit of choosing two fundamentally dissimilar technologies is the ability to uncover possible benefits that may occur when they are integrated.

While these are the only desalination technologies considered in this research, other technologies (e.g. nanofiltration and ion exchange) can be considered in future investigations. Further, including additional technologies in the DESALT model results in an exponential growth of options. It was therefore determined that, for the purposes of illustrating the capabilities of the DEA-IWRM model, the maximum number of included technologies should be two. The operating conditions for BWRO were pressure and recovery ratio while the operating conditions for ED were cell-pair voltage, recovery ratio, and stack number. Specific model inputs and outputs are presented in supplementary materials (S14).

5.2.2 Transport model: WSN

The WSN model generates a preliminary virtual water transport network based on available water sources using geographical information systems and hydrological modelling [219]. The model then optimizes the virtual water network through mixed integer quadratic programming based on cost minimization and quantitative constraints, yielding the optimal route for water transport. The transport network can be represented as a nearly planar mathematical system represented by vertices ($\mathbb{V}$) and edges ($\mathbb{E}$) [254], [255]. Vertices represent water sources with associated water availability while edges represent the pipeline connections and associated transport costs between sources (Figure 5.2). Edges also include an associated size and capacity which reflect specific features of the pipeline section.

The inputs for WSN include technical, economic, and sustainability-focused data points. Technical data points include water demand (Q_{demand}), available water sources ($\mathbb{V}_a$), and pipeline sections ($\mathbb{E}_{a,b}$). Economic data points include both fixed and variable costs related to pipeline installation and the maximum capacity of the network. The cost of owning the water, which could increase the associated costs, is not included. WSN accounts for sustainable water sourcing by limiting the maximum drawdown (D_{max}) for

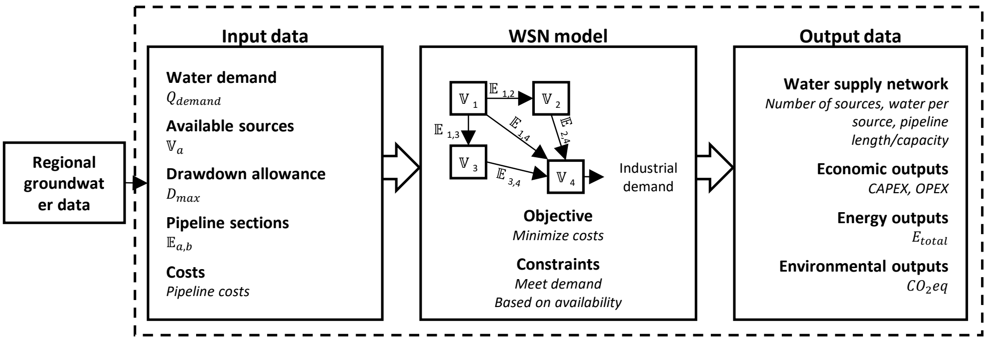

Figure 5.2 Transport model overview including input data, modelling principle, and output data. Data from the industry and water sector includes the water demand and information on available water sources and pipeline infrastructure in the region [219].

each water source. Drawdown is the difference in the groundwater level before and after abstraction and translates into an upper limit to the water withdrawal [256]. The inputs for the WSN model were determined based on expert inputs and policy recommendations. The mass balance for each WSN output was verified to ensure proper accounting of flows.

The WSN model identifies the optimal network configuration based on the specified demand, pipeline capacity, available sources, and drawdown allowance while minimizing costs. The output includes the number of sources used, volume of water withdrawn from each source, water transported over each connection, total pipeline length, and expected cost for the pipeline installation. The economic output is broken into CAPEX and OPEX. CAPEX includes costs for digging, pipeline construction, and pipeline installation. OPEX includes the cost of energy used for pumping.

The WSN model further estimates the associated transport cost, energy consumption, and expected CO_2 emissions. The cost and energy estimates rely on cost and energy functions obtained from hydraulic calculations. These calculations are based on the optimum pipeline diameter, fixed investments per diameter, and fixed volume flow per year. The CO_2 estimate is calculated based on the total pipeline length and the selected pipeline material and associated emission factor. For this case, a ductile iron pipeline with an emission factor of 227 kg CO_2-eq per meter was selected based on expert input. The CO_2 emissions for pumping were calculated based on energy usage, with an average emission factor of 0.5 kg CO_2-eq per kWh. Specific model inputs and outputs are presented in the supplementary materials (S15).

5.2.3 Classic DEA

Classic DEA is a mathematical programming method used for measuring the relative efficiency of a decision making unit (DMU) [257]. In DEA-IWRM, each DMU is a supply-demand-matching option characterized by a specific technology configuration and percentage contribution of treatment and transport. Each DMU is characterized by its inputs ($\mathbb{x}$) and outputs ($\mathbb{y}$) with $\mathbb{x}_{\mathbb{ir}}$ being the amount of input used by DMU $\mathbb{r}$ and $\mathbb{y}_{\mathbb{jr}}$ being the amount of output produced by DMU $\mathbb{r}$. The efficiency score for each DMU ($\boldsymbol{E}_{\mathbb{r}}$) is calculated based on these inputs and outputs. $\boldsymbol{E}_{\mathbb{r}}$ is defined as the ratio of the weighted sum of the outputs to the weighted sum of the inputs, thus becoming a measure of how well a DMU converts inputs into outputs. In classic DEA, $\boldsymbol{E}_{\mathbb{r}}$ is a value between zero and one. DMUs where $\boldsymbol{E}_{\mathbb{r}}=1$ are considered efficient, while DMUs where $\boldsymbol{E}_{\mathbb{r}}<1$ are considered inefficient. The classic DEA model is a linear model (Equation 5.1 through Equation 5.5). The model has an objective function (Equation 5.1) which maximizes the weighted sum of the outputs with four constraints:

- The weighted sum of the inputs must be equal to one (Equation 5.2).
- The efficiency of $\mathbb{r}$ and all other DMUs is limited to one, therefore removing inefficient DMUs (Equation 5.3).
- All weights assigned to the inputs are non-negative (Equation 5.4).
- All weights assigned to the outputs are non-negative (Equation 5.5).

The decision variables are defined as the weights assigned by the DMU to both the inputs and outputs [206]. In this case, $\boldsymbol{V}_{\mathbb{i}\mathbb{r}}$ is the weight assigned by $\mathbb{r}$ to input $\mathbb{i}$ and $\boldsymbol{U}_{\mathbb{j}\mathbb{r}}$ is the weight assigned by $\mathbb{r}$ to output $\mathbb{j}$. These weights are chosen to maximize the efficiency of $\mathbb{r}$. The model is run once for every $\mathbb{r}$ to obtain the set of $\boldsymbol{E}_{\mathbb{r}}$ values for all DMUs.

$$\max \boldsymbol{E}_{\mathbb{r}} = \sum_{\mathbb{j}=1}^{\mathbb{J}} \mathbb{y}_{\mathbb{j}\mathbb{r}} \boldsymbol{U}_{\mathbb{j}\mathbb{r}} \qquad \text{Equation 5.1}$$

$$s.t.$$

$$\sum_{\mathbb{i}=1} \mathbb{x}_{\mathbb{i}\mathbb{r}} \boldsymbol{V}_{\mathbb{i}\mathbb{r}} = 1 \qquad \text{Equation 5.2}$$

$$\sum_{\mathbb{i}=1}^{\mathbb{I}} \mathbb{x}_{\mathbb{i}\mathbb{k}} \boldsymbol{V}_{\mathbb{i}\mathbb{r}} \geq \sum_{\mathbb{j}=1}^{\mathbb{J}} \mathbb{y}_{\mathbb{j}\mathbb{k}} \boldsymbol{U}_{\mathbb{j}\mathbb{r}} \quad for\ \mathbb{k} = 1, \dots, \mathbb{R} \qquad \text{Equation 5.3}$$

$$\boldsymbol{V}_{\mathbb{i}\mathbb{r}} \geq 0 \qquad for\ \mathbb{i} = 1, \dots, \mathbb{I} \qquad \text{Equation 5.4}$$

$$\boldsymbol{U}_{\mathbb{j}\mathbb{r}} \geq 0 \qquad for\ \mathbb{j} = 1, \dots, \mathbb{J} \qquad \text{Equation 5.5}$$

This linear model is referred to as the Charnes, Cooper, and Rhodes multiplier model with constant returns to scale (CCR CRS) [206].

5.2.4 Case study: Dow Terneuzen

Dow Terneuzen is in a delta region of the Netherlands and has an approximate water demand of 10 Mm^3/year. Due to local water scarcity, alternative water sources are being investigated to replace a portion of this demand (2 Mm^3/year, requirements specified in Table S14-1). Dow has been investigating whether to reuse on-site brackish water or transport water from regional sources. The on-site brackish water is a combination of cooling tower blowdown and nearby brackish ground and surface water, amounting to 2 Mm^3/year. The quality and quantity of this brackish water is assumed constant based on the average values over the year (see S14). The transport option uses simulated groundwater resources in the case study area as supply sources.

5.3 DEA-IRWM framework design

5.3.1 DEA-IRWM model framework

The DEA-IRWM modelling framework assesses the performance of alternative supply configurations of treatment and transport based on water availability, costs, and sustainability indicators. Alternative supply configurations are generated by changing the relative contribution of treatment and transport to meet the specified demand. Every configuration of treatment and transport that is evaluated becomes a DMU for application in the DEA evaluation. An overview of the DEA-IRWM framework is presented in Figure 5.3.

The amount of water demand (Q_{demand}) and the total amount of available brackish water (Q_{BW}) are specified as boundary conditions for the simulation. Q_{BW} includes brackish water sourced from wastewater ($Q_{BW,waste}$) and/or other local water ($Q_{BW,local}$). The treatment model then returns all possible treatment train configurations that meet the product water quality requirements based on Q_{BW}. For each treatment train configuration, a portion of Q_{BW} is reusable desalinated product water (Q_{treat}) while the remainder is discharged as brine (Q_{brine}). The transport model is then run for every output generated by the treatment model. The amount of water to be transported ($Q_{transport}$) is defined as the difference between Q_{demand} and Q_{treat}.

Each configuration of Q_{treat} and $Q_{transport}$ that meets Q_{demand} is considered as a possible integrated water resource option. The economic, energy, and environmental performance indicators (Section 5.3.2) for both treatment and transport are combined to create three overall performance indicators for each option. Each set of indicators is a DMU in the DEA evaluation with a unique ID and name reflecting the relative contribution of treatment and transport. For example, a DMU named D40T60 has 40% of Q_{demand} coming from treatment (D) and 60% from transport (T).

The set of DMUs are is then analyzed using six different DEA modelling methods which identify preferred alternatives. The DEA models applied are basic efficiency (Section 5.3.3), weight constraints (Section 5.3.4), cross-efficiency (Section 5.3.5), and super-

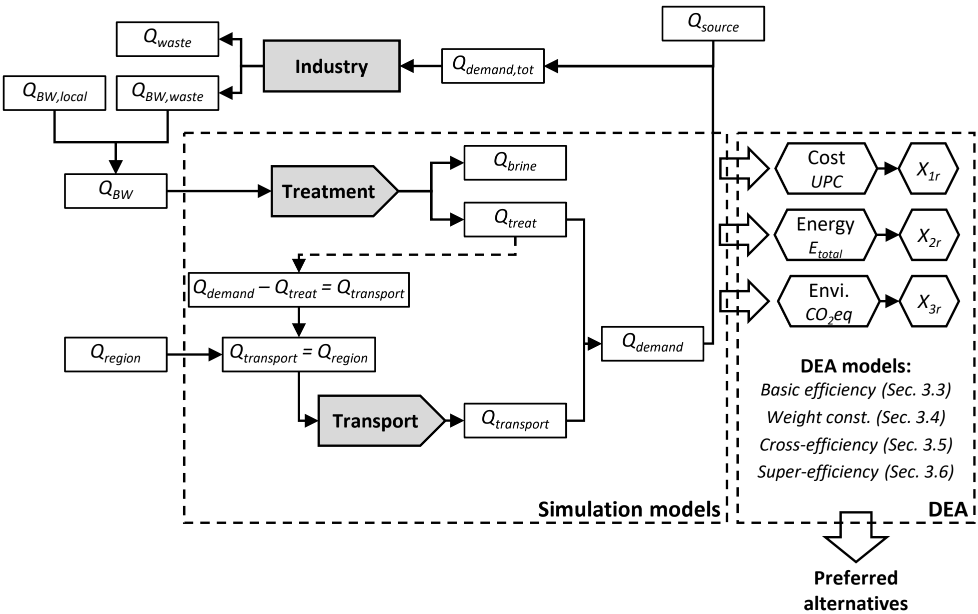

Figure 5.3 The procedure of combining simulation models with DEA to identify preferred designs.

efficiency (Section 5.3.6). The basic efficiency DEA and its extensions were implemented in Python and solved using the Gurobi solver.

5.3.2 Performance indicators

Performance indicators were selected based on existing literature on the performance assessment of water supply systems and with consideration for the treatment and transport model outputs [258]–[261]. Three performance indicators were selected: unit production cost (UPC), specific energy use (E_{spec}), and CO_2-equivalent emissions (CO_2eq) (see Table 5.1). These performance indicators were represented in the DEA analysis as three inputs for a given DMU $\mathbb{r}$: $\mathbb{x}_{1\mathbb{r}}$, $\mathbb{x}_{2\mathbb{r}}$, and $\mathbb{x}_{3\mathbb{r}}$. Normalization of the indicators was needed to prevent differences in magnitude between the indicators from skewing the results.

The UPC is an economic indicator which shows the cost per unit of produced water. The E_{spec} is an energy consumption indicator expressed in kilowatt-hours per cubic meter of produced water and accounts for both installation and operational energy use. The CO_2eq is an environmental indicator representing the total carbon dioxide equivalent

Table 5.1 Overview of the simulation models and the integrated model including identification of performance indicators.

	Treatment model	Transport model	Integrated model
Name	DESALT [218]	WSN [219]	DEA-IWRM
Function	Determine different on-site treatment trains to supply desired water for industrial use based on available water quantity and quality.	Determine the optimal water transport network to supply water for industrial use based on cost minimization demand and availability.	Determine the preferred water supply designs based on desalination and transport, considering economic and environmental objectives.
Study Area	Dow	Zeeland	Dow and Zeeland
Performance Indicators	Unit prod. cost ($US/$m^3$)	Transport costs ($US/$m^3$)	Tot. unit prod. cost ($US/$m^3$)
	Spec. energy use (kWh/m^3)	Spec. energy use (kWh/m^3)	Tot. spec. energy use (kWh/m^3)
	CO_2-eq (kg CO_2-eq/m^3)	CO_2-eq (kg CO_2-eq/m^3)	Tot. CO_2-eq (kg CO_2-eq/m^3)

emissions relative to the entire life cycle of the configuration. The objective for all three performance indicators is minimization.

5

5.3.3 Basic efficiency

The classic DEA is designed to minimize inputs (i.e. 'less is better') and maximize outputs (i.e. 'more is better'). This design, however, is not compatible with the DEA-IWRM framework. While the inputs (performance indicators) are the type 'less is better', there are no outputs with which to maximize. The classic DEA was therefore modified by assigning an artificial output equal to one ($\mathbb{y} = 1$) for all DMUs [262]. This assignment simplifies the classic DEA into the basic efficiency DEA (Equation 5.6 through Equation 5.10). The basic efficiency DEA was validated through comparison to the pyDEA software developed by Raith et al. [263]. This basic efficiency DEA is then used as the foundation for future expansions and modifications of the DEA evaluation in the DEA-IWRM framework.

$$\max \boldsymbol{U}_{\mathbb{r}} \qquad \text{Equation 5.6}$$

$$s.t.$$

$$\textstyle\sum_{\mathbb{i}=1}^{\mathbb{I}} \mathbb{x}_{\mathbb{i}\mathbb{r}} \boldsymbol{V}_{\mathbb{i}\mathbb{r}} = 1 \qquad \text{Equation 5.7}$$

$$\textstyle\sum_{\mathbb{i}=1}^{\mathbb{I}} \mathbb{x}_{\mathbb{i}\mathbb{k}} \boldsymbol{V}_{\mathbb{i}\mathbb{r}} \geq \boldsymbol{U}_{\mathbb{r}} \quad for\ \mathbb{k} = 1, \dots, \mathbb{R} \qquad \text{Equation 5.8}$$

$$\boldsymbol{V}_{\mathbb{i}} \geq 0 \qquad for\ \mathbb{i} = 1, \dots, \mathbb{I} \qquad \text{Equation 5.9}$$

$$\boldsymbol{U} \geq 0 \qquad \text{Equation 5.10}$$

5.3.4 Weight constraints

While the basic efficiency DEA filters the DMU set considerably, the number of remaining DMUs is still too large for decision making purposes. Further, some of the 'efficient' DMUs may not perform well for all criteria. Weight constraints are implemented to distinguish efficient DMUs based on more selective restrictions, resulting in a more balanced DEA model [264]. A balanced model from a decision making context means that all criteria are accounted for instead of just the $\boldsymbol{E}_{r}$. In this research, the balanced model is achieved by filtering the outputs of the basic efficiency DEA model (Section 5.3.3) using the weight constraints presented in Sections 5.3.4.1 and 5.3.4.2.

5.3.4.1 Lower and upper bounds

The first application of weight constraints is focused on the performance of all criteria by setting lower and upper bounds for the multipliers. Multipliers (i.e. relative weights) are the product of the input or output with its associated weight. Multipliers show the relative contribution of each input and output to the final $\boldsymbol{E}_{r}$. These constraints take the form of Equation 5.11 and Equation 5.12, requiring that the individual scores for a given criterion in an efficient DMU should contribute between 0.1 and 0.5 of the total $\boldsymbol{E}_{r}$.

$$x_{ir}\boldsymbol{V}_{ir} \geq 0.1 \qquad for\ i = 1, \ldots, I \qquad \text{Equation 5.11}$$

$$x_{ir}\boldsymbol{V}_{ir} \leq 0.5 \qquad for\ i = 1, \ldots, I \qquad \text{Equation 5.12}$$

5.3.4.2 Preference based

Extreme performers (i.e. DMUs which perform well for a single criterion) can be promoted through preference-based weight constraints. To do so, a weight constraint is applied which states that the preferred multiplier i^* should be m times more important than the other multipliers (Equation 5.13) [207]. To prevent the non-preferred multipliers from being completely excluded, a lower bound for all multipliers is set (Equation 5.14). For this research, the preferred multiplier i^* was set to be three times more important than the other multipliers (m = 3) and a lower bound for other multipliers was set at 0.001.

$$x_{i^*r}\boldsymbol{V}_{i^*r} \geq \frac{m}{m+1}\sum_{i=1}^{I} x_{ir}\boldsymbol{V}_{ir} \qquad i^* = UPC\ or\ E_{spec}\ or\ CO_2eq \qquad \text{Equation 5.13}$$

$$x_{ir}\boldsymbol{V}_{ir} \geq 0.001 \qquad for\ i = 1, \ldots, I \qquad \text{Equation 5.14}$$

5.3.5 Cross-efficiency

The basic efficiency DEA produces an $\boldsymbol{E}_{\mathbb{r}}$ for a specific DMU that does not reflect or consider the performance of other DMUs in the set. This independent evaluation approach coupled with a very flexible weight assignment results in several indistinguishable DMUs. The outputs from the basic efficiency DEA were further processed using a cross-efficiency evaluation to identify the best performing DMUs [265], [266].

Cross-efficiency is a form of peer evaluation between DMUs which produces a cross-efficiency score ($\boldsymbol{E}_{\mathbb{r}}^{cross}$) that measures how well a given DMU performs from the perspective of other DMUs in the set. This is achieved by calculating the performance of a given DMU $\mathbb{r}$ using the optimal weights of the other DMUs ($\mathbb{k}$).

The cross-efficiency analysis begins by calculating the cross-efficiency score from the basic efficiency DEA. In this research only DMUs whose basic efficiency score was between 0.99 and 1 were analyzed. Given the efficiency score for a given DMU ($\boldsymbol{E}_{\mathbb{r}}$) and the associated weights, the cross-efficiencies between DMU $\mathbb{r}$ and DMU $\mathbb{k}$ ($\boldsymbol{E}_{\mathbb{r}\mathbb{k}}$) are calculated (Equation 5.15). $\boldsymbol{E}_{\mathbb{r}\mathbb{k}}$ is the efficiency of DMU $\mathbb{r}$ when judged via the weights of DMU $\mathbb{k}$. $\boldsymbol{E}_{\mathbb{r}}^{cross}$ for DMU r is therefore the average of all calculated $\boldsymbol{E}_{\mathbb{r}\mathbb{k}}$ values (Equation 5.16), where $\mathbb{K}$ is the number of DMUs.

$$\boldsymbol{E}_{\mathbb{r}\mathbb{k}} = \frac{\boldsymbol{U}_{\mathbb{k}}}{\sum_{\mathbb{i}=1}^{\mathbb{I}} \boldsymbol{V}_{\mathbb{i}\mathbb{k}} \mathbb{x}_{\mathbb{i}\mathbb{r}}} \qquad \text{Equation 5.15}$$

$$\boldsymbol{E}_{\mathbb{r}}^{cross} = \frac{1}{\mathbb{K}} \sum_{\mathbb{k}=1}^{\mathbb{K}} \boldsymbol{E}_{\mathbb{r}\mathbb{k}} \qquad \text{Equation 5.16}$$

5.3.5.1 Secondary goal

In the aforementioned cross-efficiency the score is dependent on the weights obtained from the basic efficiency DEA. Since the basic efficiency DEA is a linear program there may be several alternative optimal solutions and therefore the weights $\boldsymbol{U}_{\mathbb{i}\mathbb{r}}$ and $\boldsymbol{V}_{\mathbb{i}\mathbb{r}}$ may not be unique. Different weights can lead to the same $\boldsymbol{E}_{\mathbb{r}}$ but to a different $\boldsymbol{E}_{\mathbb{r}\mathbb{k}}$. To overcome this, a secondary goal cross-efficiency model is applied using outputs from the cross-efficiency to ensure unique $\boldsymbol{E}_{\mathbb{r}}^{cross}$ [265], [266].

After optimizing the efficiency of each DMU, the average cross-efficiency score of the other DMUs should either be maximized (benevolent approach) or minimized (aggressive approach). Secondary goal cross-efficiency, as described in Doyle and Green [265], can be simplified to Equation 5.17 through Equation 5.23.

Depending on the secondary goal, the objective function can use either a benevolent (Equation 5.17) or aggressive (Equation 5.18) approach to determine the weighted sum of the outputs of all other DMUs. The first constraint (Equation 5.19) sets the weighted sum of the inputs of all other DMUs equal to one. The objective function combined with Equation 5.19 ensures that the average cross-efficiency is unique. The second constraint (Equation 5.20) makes sure that the weights chosen will give the highest possible $\boldsymbol{E}_{\mathbb{r}}$ for the given DMU. The third constraint (Equation 5.21) makes sure that none of the DMUs can get a $\boldsymbol{E}_{\mathbb{r}}^{cross}$ >1.

$$benevolent\text{: } \max \boldsymbol{U}_{\mathbb{r}} \left(\textstyle\sum_{\mathbb{k}=1\ \mathbb{k}\neq\mathbb{r}}^{\mathbb{K}} \mathbb{y}_{\mathbb{k}}\right) \qquad \text{Equation 5.17}$$

$$aggressive\text{: } \min \boldsymbol{U}_{\mathbb{r}} \left(\textstyle\sum_{\mathbb{k}=1\ \mathbb{k}\neq\mathbb{r}}^{\mathbb{K}} \mathbb{y}_{\mathbb{k}}\right) \qquad \text{Equation 5.18}$$

$s.t.$

$$\textstyle\sum_{\mathbb{i}=1}^{\mathbb{I}} \boldsymbol{V}_{\mathbb{i}\mathbb{r}} \left(\sum_{\mathbb{k}=1\ \mathbb{k}\neq\mathbb{r}}^{\mathbb{K}} \mathbb{x}_{\mathbb{i}\mathbb{k}}\right) = 1 \qquad \text{Equation 5.19}$$

$$\boldsymbol{U}_{\mathbb{r}} - \boldsymbol{E}_{\mathbb{r}} \textstyle\sum_{\mathbb{i}=1}^{\mathbb{I}} \boldsymbol{V}_{\mathbb{i}\mathbb{r}} \mathbb{x}_{\mathbb{i}\mathbb{r}} = 0 \qquad \text{Equation 5.20}$$

$$\boldsymbol{U}_{\mathbb{r}} - \textstyle\sum_{\mathbb{i}=1}^{\mathbb{I}} \boldsymbol{V}_{\mathbb{i}\mathbb{r}} \mathbb{x}_{\mathbb{i}\mathbb{k}} \leq 0, \qquad for\ \mathbb{k} = 1, \ldots, \mathbb{K};\ \mathbb{k} \neq \mathbb{r} \qquad \text{Equation 5.21}$$

$$\boldsymbol{U} \geq 0 \qquad \text{Equation 5.22}$$

$$\boldsymbol{V}_{\mathbb{i}} \geq 0 \qquad for\ \mathbb{i} = 1, \ldots, \mathbb{I} \qquad \text{Equation 5.23}$$

5.3.6 Super-efficiency

Like cross-efficiency, super-efficiency is a method for distinguishing efficient DMUs to identify the best overall performers [267], [268]. Super-efficiency compares a given DMU with all other DMUs in the set to determine if any input or output multiplier can be improved while keeping the DMU efficient. The super-efficiency score ($\boldsymbol{E}_{\mathbb{r}}^{super}$) is calculated by replacing the basic efficiency DEA constraint presented in Equation 5.8 with Equation 5.24. Equation 5.24 excludes the maximum efficiency constraint for the given DMU making it is possible for a DMU to achieve an efficiency score greater than one. In this case, the super-efficiency operates as a type of sensitivity analysis for the basic efficiency DEA model.

$$\textstyle\sum_{\mathbb{i}=1}^{\mathbb{I}} \mathbb{x}_{\mathbb{i}\mathbb{r}} \boldsymbol{V}_{\mathbb{i}\mathbb{k}} \geq \boldsymbol{U}_{\mathbb{r}} \qquad for\ \mathbb{k} = 1, \ldots, \mathbb{K};\ \mathbb{k} \neq \mathbb{r} \qquad \text{Equation 5.24}$$

5.4 Results and discussion

5.4.1 Simulation model results

To test the DEA-IWRM framework, the model was applied to the Dow case study (see Section 5.2.4). The simulation model portion of the DEA-IWRM framework was run using a Q_{BW} and a Q_{demand} of 2 Mm^3/year. The treatment model was run using incremental feed water flowrates from 5% to 95% of Q_{BW}. Based on the treatment train operating conditions, Q_{treat} ranges between 2% and 65% of the feed water flowrate resulting in 0.02-1.2 Mm^3/year of industrial quality treated water. To bridge the gap between Q_{treat} and Q_{demand}, the transport model simulated water transport between 0.8 and 1.98 Mm3/year. The transport model used simulated regional water sources with a maximum drawdown allowance of 0.05 m to prevent excessive withdrawal of groundwater [269]. The integration of the treatment and transport simulation models under the specified parameters resulted in 15,751 options (i.e. DMUs).

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Both simulation models show an inverse correlation between supply and costs (Figure 5.4) and a direct correlation between supply and energy use (Figure 5.5). Additional simulation result figures are available in the supplementary materials (S16).

The simulation model outputs show that treatment costs are higher than transport costs, which coincides with literature [270]. Treatment requires less energy than transport when less than 1.0 Mm^3/year is transported. This performance turning point indicates that the transport network is more efficient above a certain volume. Case specific factors such as pipeline characteristics and source locations determine this turning point and therefore should not be generalized. The results shown in Figure 5.5 contrasts slightly with existing literature, as it has been found that treatment is almost always more energy-intensive [217]. This difference may be a result of the case study conditions in which the feed water has an exceptionally low salinity resulting in a less intensive desalination requirement.

5.4.2 Basic efficiency results

The results of the basic efficiency were first reviewed related to each simulation model and then as a whole to identify the best performers.

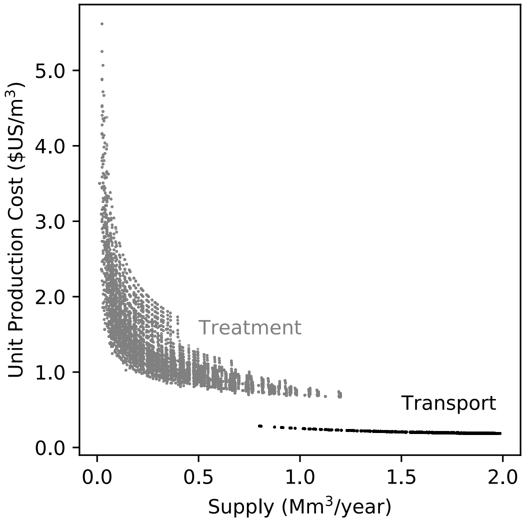

Figure 5.4 Cost performance outputs from the simulation model portion of the DEA-IWRM framework as applied to the Dow case study and plotted against supply.

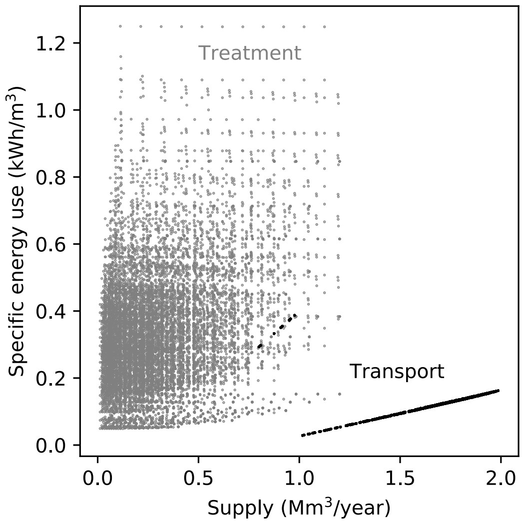

Figure 5.5 Energy performance outputs from the simulation model portion of the DEA-IWRM framework as applied to the Dow case study and plotted against supply.

5.4.2.1 Treatment simulation model evaluation

For the Dow case study, DMUs were found to only be truly efficient ($\boldsymbol{E}_{\mathbb{F}} = 1$) when treatment was equal to 47% or less of the total demand (Figure 5.6). Further, the basic efficiency scores tend to decrease with the increased percentage of treatment.

Plotting the basic efficiency scores by the associated treatment train shows which combination of technologies generally perform best (Figure 5.7). The efficiency score associated with the peak frequency of each treatment train suggests its performance based on all indicators, with higher efficiency scores indicating better performance. BWRO+ED and BWRO+BWRO are identified as the treatment trains associated with the best performance. BWRO+ED shows a better overall performance as compared to ED+BWRO. This is primarily due to the direct relation between water transport and the removal rate in the ED evaluation. In practice this order is less favorable due to the sensitivity and high removal rate of BWRO. This therefore acts as a reminder that the results are reliant on the accuracy of the simulation models and experts should always be consulted before implementation.

5.4.2.2 Transport simulation model evaluation

The transport model generated networks with a distance ranging from 26 to 54 km. Efficient DMUs have network distances between 26 and 27 km (Figure 5.8). An increase in the network distance was shown to lead to lower efficiency scores.

The minimum network length for the Dow case was found to be 26 km (Figure 5.9). While the shortest network distance could supply enough water for all configurations, the outputs of the transport model still included longer network configurations that could also meet the supply needs. The DEA model effectively discards these longer, inefficient, and unrealistic networks which are a result of the tolerance of the WSN solver.

5.4.2.3 Efficient DMU set

The outputs of the basic efficiency evaluation were filtered to present only efficient DMUs (Table 5.2). This reduced the total number of relevant DMUs to 44, a 99.72% reduction from 15,751. The discriminatory power of the DEA increases when indicators are correlated and there are few criteria [271]. Thus, the limited number of indicators for the Dow case helps in reducing the size of the efficient DMU set.

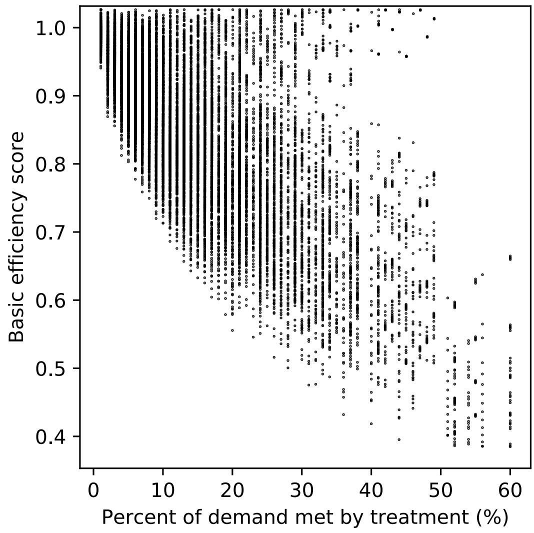

Figure 5.6 Results of the basic efficiency model for the complete DMU set. The x-axis shows the percentage of the demand met by treatment, with the remaining percentage being supplemented by transport. The y-axis shows the efficiency score using basic efficiency

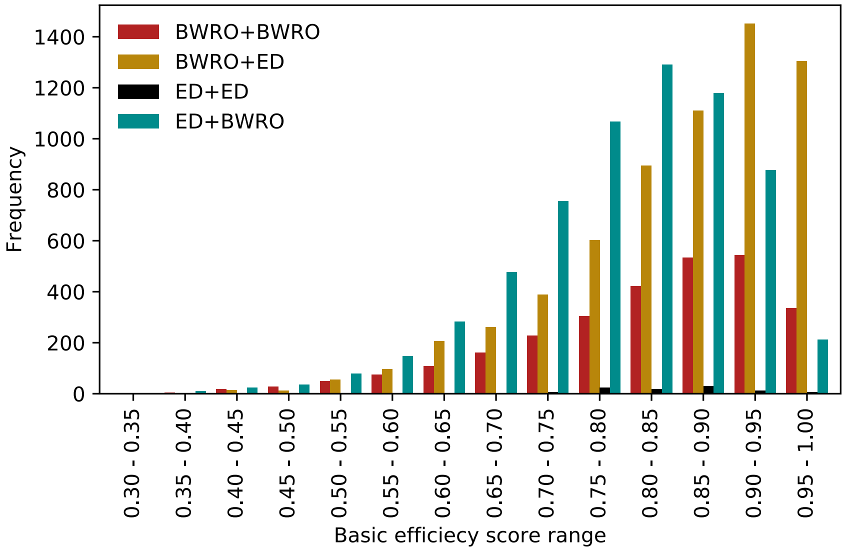

Figure 5.7 Distribution frequency of different treatment trains per efficiency score range.

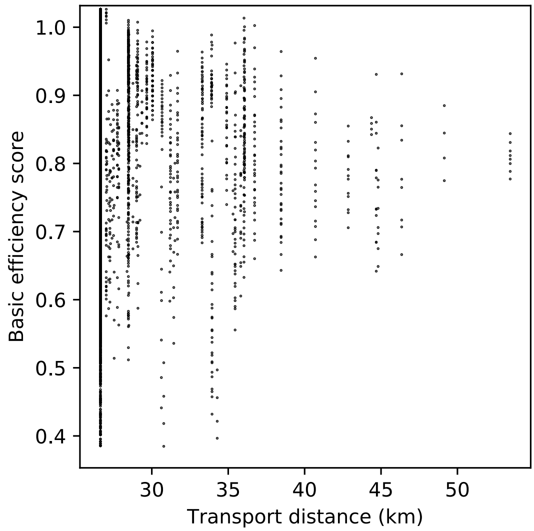

Figure 5.8 Results of the basic DEA model for the complete DMU set; the x-axis shows the transport distance; the y-axis shows the DEA efficiency score.

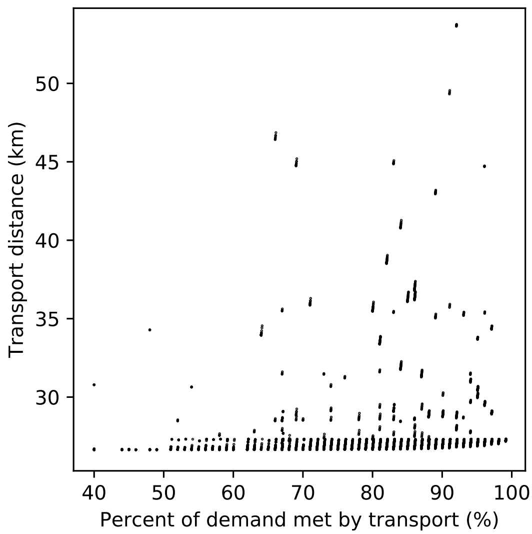

Figure 5.9 Results of the basic DEA model for the complete DMU set; the x-axis shows the transport %; the y-axis shows the transport distance.

Table 5.2 Results of the basic efficiency DEA for all DMUs whose efficiency is equal to one. The DMU column shows the unique identifiers for each DMU. The combination column identifies the percent contribution of treatment (D) and transport (T) to meet the specified demand. The treatment train denotes the associated treatment train provided by DESALT (more information presented in S17). The distance indicates the total length of the pipeline (km) as provided by WSN. The performance per indicator is specified in $\mathbb{x}_{\mathbf{1}\mathbb{r}}$ (cost), $\mathbb{x}_{\mathbf{2}\mathbb{r}}$ (energy), and $\mathbb{x}_{\mathbf{3}\mathbb{r}}$ (environment). The weight associated with each indicator is then represented in $\mathbb{x}_{\mathbf{1}\mathbb{r}}\boldsymbol{V}_{\mathbf{1}\mathbb{r}}$, $\mathbb{x}_{\mathbf{2}\mathbb{r}}\boldsymbol{V}_{\mathbf{2}\mathbb{r}}$, and $\mathbb{x}_{\mathbf{3}\mathbb{r}}\boldsymbol{V}_{\mathbf{3}\mathbb{r}}$.

DMU	Combo	Treatment	Distance	Basic	$\mathbb{x}_{\mathbf{1}\mathbb{r}}$	$\mathbb{x}_{\mathbf{2}\mathbb{r}}$	$\mathbb{x}_{\mathbf{3}\mathbb{r}}$	$\mathbb{x}_{\mathbf{1}\mathbb{r}}\boldsymbol{V}_{\mathbf{1}\mathbb{r}}$	$\mathbb{x}_{\mathbf{2}\mathbb{r}}\boldsymbol{V}_{\mathbf{2}\mathbb{r}}$	$\mathbb{x}_{\mathbf{3}\mathbb{r}}\boldsymbol{V}_{\mathbf{3}\mathbb{r}}$
36	D47 T53	BWRO + ED	26.64	1	0.452	0.067	0.129	0.000	0.180	0.820
92	D42 T58	BWRO + ED	26.64	1	0.431	0.070	0.127	0.000	0.091	0.909
96	D47 T53	BWRO + ED	26.64	1	0.460	0.067	0.129	0.000	0.180	0.820
164	D44 T56	BWRO + BWRO	26.64	1	0.449	0.067	0.129	0.383	0.617	0.000
216	D38 T62	BWRO + ED	26.64	1	0.415	0.075	0.126	0.000	0.080	0.920
352	D38 T62	BWRO + ED	26.64	1	0.423	0.093	0.124	0.063	0.069	0.868
356	D38 T62	BWRO + ED	26.64	1	0.424	0.075	0.126	0.000	0.080	0.920
360	D34 T66	BWRO + ED	26.64	1	0.398	0.081	0.126	0.278	0.145	0.577
384	D33 T67	BWRO + ED	27.02	1	0.393	0.072	0.131	0.335	0.665	0.000
392	D36 T64	BWRO + BWRO	26.64	1	0.413	0.090	0.124	0.100	0.075	0.825
500	D38 T62	BWRO + ED	26.64	1	0.432	0.093	0.124	0.000	0.011	0.989
512	D38 T62	BWRO + ED	26.64	1	0.432	0.075	0.126	0.000	0.080	0.920
548	D30 T70	BWRO + ED	26.64	1	0.380	0.077	0.130	0.270	0.139	0.592
592	D30 T70	BWRO + ED	26.64	1	0.380	0.087	0.126	0.254	0.121	0.626
632	D33 T67	BWRO + ED	26.64	1	0.402	0.098	0.124	0.116	0.064	0.821
644	D31 T69	BWRO + BWRO	26.64	1	0.389	0.096	0.125	0.147	0.079	0.774
764	D28 T72	BWRO + ED	26.64	1	0.372	0.105	0.124	0.136	0.000	0.864
1036	D21 T79	BWRO + ED	26.64	1	0.328	0.097	0.131	0.484	0.308	0.208
1048	D26 T74	BWRO + BWRO	26.64	1	0.364	0.103	0.125	0.186	0.088	0.726
1248	D20 T80	BWRO + ED	26.64	1	0.323	0.096	0.137	0.536	0.464	0.000
1460	D22 T78	BWRO + ED	26.64	1	0.342	0.112	0.126	0.201	0.017	0.783
1512	D18 T82	BWRO + ED	26.64	1	0.312	0.104	0.131	0.310	0.173	0.517
1604	D21 T79	BWRO + ED	26.64	1	0.336	0.103	0.128	0.183	0.082	0.735
1724	D17 T83	BWRO + ED	26.64	1	0.307	0.112	0.129	0.209	0.152	0.639
1916	D16 T84	BWRO + ED	26.64	1	0.301	0.106	0.137	0.444	0.338	0.218
2856	D13 T87	BWRO + ED	26.64	1	0.284	0.122	0.131	0.202	0.059	0.739
4784	D11 T89	BWRO + ED	26.64	1	0.279	0.132	0.131	0.174	0.028	0.798
6808	D6 T94	BWRO + ED	26.64	1	0.238	0.144	0.135	0.157	0.000	0.843
12920	D1 T99	BWRO + BWRO	26.64	1	0.192	0.155	0.140	1.000	0.000	0.000
12921	D1 T99	BWRO + BWRO	26.64	1	0.192	0.155	0.141	1.000	0.000	0.000
12922	D1 T99	BWRO + BWRO	26.64	1	0.192	0.155	0.142	1.000	0.000	0.000
12923	D1 T99	BWRO + BWRO	26.64	1	0.192	0.156	0.142	1.000	0.000	0.000
12924	D1 T99	BWRO + BWRO	26.64	1	0.192	0.156	0.143	1.000	0.000	0.000
12925	D1 T99	BWRO + BWRO	26.64	1	0.192	0.156	0.144	1.000	0.000	0.000
12926	D1 T99	BWRO + BWRO	26.64	1	0.192	0.157	0.144	1.000	0.000	0.000
12927	D1 T99	BWRO + BWRO	26.64	1	0.192	0.157	0.145	1.000	0.000	0.000
12928	D1 T99	BWRO + BWRO	26.64	1	0.192	0.157	0.146	1.000	0.000	0.000
12929	D1 T99	BWRO + BWRO	26.64	1	0.192	0.157	0.147	1.000	0.000	0.000
12930	D1 T99	BWRO + BWRO	26.64	1	0.192	0.158	0.147	1.000	0.000	0.000
12931	D1 T99	BWRO + BWRO	26.64	1	0.192	0.158	0.148	1.000	0.000	0.000
12932	D1 T99	BWRO + BWRO	26.64	1	0.192	0.158	0.149	1.000	0.000	0.000
12933	D1 T99	BWRO + BWRO	26.64	1	0.192	0.158	0.149	1.000	0.000	0.000
12934	D1 T99	BWRO + BWRO	26.64	1	0.192	0.159	0.150	1.000	0.000	0.000
12935	D1 T99	BWRO + BWRO	26.64	1	0.192	0.159	0.150	1.000	0.000	0.000

Among the efficient DMUs, different inputs for cost, energy, and environment ($\mathbb{x}_{\mathbf{1}\mathbb{r}}$, $\mathbb{x}_{\mathbf{2}\mathbb{r}}$, and $\mathbb{x}_{\mathbf{3}\mathbb{r}}$) are observed as well as associated weights ($\mathbb{x}_{\mathbf{1}\mathbb{r}}\boldsymbol{V}_{\mathbf{1}\mathbb{r}}$, $\mathbb{x}_{\mathbf{2}\mathbb{r}}\boldsymbol{V}_{\mathbf{2}\mathbb{r}}$, and $\mathbb{x}_{\mathbf{3}\mathbb{r}}\boldsymbol{V}_{\mathbf{3}\mathbb{r}}$). For some DMUs, positive weights for all three multipliers can be seen (i.e. DMU 92). This means that all three criteria are reflected in the efficiency score. Alternatively, some DMU efficiency scores are entirely reliant on the performance of a single criterion. For example, DMU 12920 performs well for one indicator but not the other two, resulting in an unbalanced performance.

5.4.3 Weight constraint results

Further analysis was done using weight constraints (Section 5.3.4). Both the lower and upper bound method (i.e. balanced) and the preference method (i.e. cost, energy, and environment) were applied and are presented in the supplementary materials (S18).

The balanced weight constraint identified that ten of the 44 efficient DMUs performed well when considering all three performance indicators. The cost preference weight constraint identified eight efficient DMUs, all of which were comprised of 99% transport and 1% treatment. This reaffirms that transport performs better with regards to costs. The energy preference weight constraint returned only one DMU (DMU 164), which indicates that the remaining DMUs do not perform well from an energy perspective. The environmental preference weight constraint, meanwhile, returned 19 DMUs, 18 of which combined treatment and transport.

The results confirm that treatment is associated with lower energy use and better environmental performance while transport is associated with lower costs. Therefore, the weight constraint model is a found to be a valuable addition to the basic efficiency model [271].

5.4.4 Cross-efficiency results

The cross-efficiency model (Section 5.3.5) was applied to the set of efficient DMUs generated by the basic efficiency model presented in the supplementary material (S18). The aggressive approach minimizes $\boldsymbol{E}_{\mathbb{r}\mathbb{k}}$ and results in more pronounced discrimination, therefore, it was selected for further analyses (Figure 5.10). In the aggressive approach, the best performing DMUs (i.e. cross-efficiency score > 0.94) had somewhere between 15% and 34% of their demand met through treatment. The cross-efficiency was also binding for inefficient units, meaning that inefficient DMUs (efficiency score < 1) can have a higher cross-efficiency score than efficient DMUs.

5.4.5 Super-efficiency results

The added benefit of the super-efficiency analysis is shown by comparing the results with the basic efficiency model (Figure 5.11). The super-efficiency model highlights the better performing DMUs by allowing their efficiency to increase above one. In the Dow case, DMUs with super-efficiency scores above one were found to have between 20% and 45% of their demand met through treatment. The scores of the super-efficient DMUs remain close to one. While they do perform better, the difference in performance is minimal and therefore does contribute much to the decision making process for this specific case.

5.4.6 Best performing options

The efficient DMU set was then filtered based on the different DEA models. A DMU was considered preferred if it met at least one of the weight constraints and had a relatively high cross-efficiency score (>0.935) or a relatively high super-efficiency score (>1.005). This resulted in 17 preferred DMUs for the Dow case study which are presented in Table 5.3. Treatment and transport appear to be complementary measures rather than alternative solutions.

Transport maintains a substantial contribution (> 56%) for the total demand in all preferred options. The results from the DEA analyses confirm that transport is the preferred option from a cost perspective. This is partially due to the expensive nature of desalination and by the landscape in the case study which includes very little elevation change. Changes in elevation can contribute to higher costs and energy use if the transported water must be pumped up hill.

The lowest energy use and CO_2 emissions can be achieved by combining treatment and transport. Supplying specific portions of demand with treated water results in lower energy use and CO_2 emissions. This is especially true for the Dow case study, in which the amount of desalination required is small and therefore needs only low energy-intensive treatment. If the amount of desalination were to increase, such as desalinating seawater, the energy-intensity as well as the costs and CO_2 emitted would increase significantly.

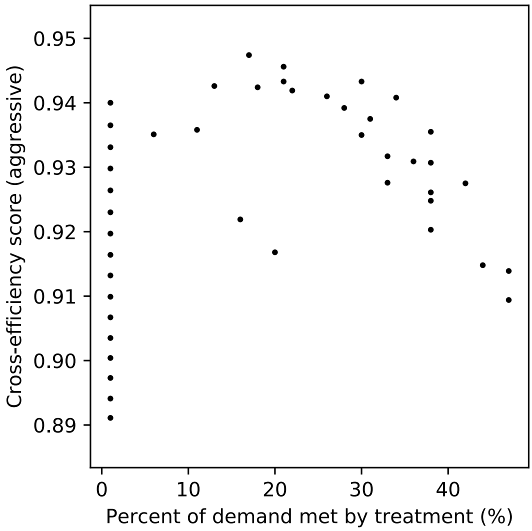

Figure 5.10 Results of the aggressive cross-efficiency evaluation. The x-axis shows the percentage of the demand met through treatment while the y-axis shows the aggressive cross-efficiency score for the efficient DMUs.

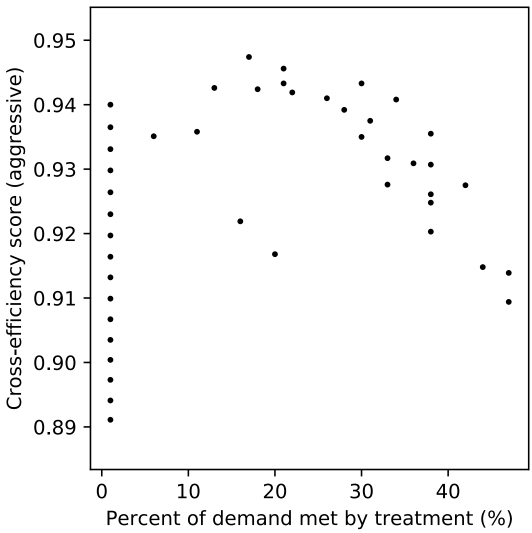

Figure 5.11 Results of the super-efficiency analysis compared to the CCR CRS efficiency which depict the ability for DMU's to have a score exceeding one. The x-axis shows the desalination percentage; the y-axis shows the cross-efficiency score.

Table 5.3 Summary of results including different methodologies used for the Dow case study. x_{1r} is the economic indicator; x_{2r} is the energy indicator; x_{3r} is the environmental indicator; a dot (•) means DMU is efficient; the empty cells indicate that the DMU is not efficient.

DMU	Combo	x_{1r}	x_{2r}	x_{3r}	Basic	Weight-constraints				Cross-eff. (Aggr.)	Super-Eff.
						Bal.	Cost	Energy	Envi.		
92	D42 T58	0.431	0.070	0.127	•	•			•	0.928	1.004
164	D44 T56	0.449	0.067	0.129	•	•		•	•	0.915	1.006
216	D38 T62	0.415	0.075	0.126	•				•	0.936	1.002
360	D34 T66	0.398	0.081	0.126	•				•	0.941	1.002
384	D33 T67	0.393	0.072	0.131	•	•				0.928	1.012
548	D30 T70	0.380	0.077	0.130	•	•				0.935	1.003
592	D30 T70	0.380	0.087	0.126	•				•	0.943	1.002
644	D31 T69	0.389	0.096	0.125	•				•	0.938	1.001
764	D28 T72	0.372	0.105	0.124	•				•	0.939	1.003
1036	D21 T79	0.328	0.097	0.131	•	•				0.943	1.005
1460	D22 T78	0.342	0.112	0.126	•				•	0.942	1.003
1512	D18 T82	0.312	0.104	0.131	•	•				0.942	1.001
1604	D21 T79	0.336	0.103	0.128	•	•				0.946	1.001
1724	D17 T83	0.307	0.112	0.129	•				•	0.947	1.004
2856	D13 T87	0.284	0.122	0.131	•				•	0.943	1.000
12920	D1 T99	0.192	0.155	0.140	•	•	•		•	0.940	1.004
12921	D1 T99	0.192	0.155	0.141	•		•			0.937	1.000

The possible advantages for combining treatment and transport extend beyond the selected performance indicators. First, treatment allows (re)use of readily available brackish water at the industrial site and therefore reduces pressure on freshwater sources. Second, combining treatment and transport can lower the final energy consumption as well as CO_2 emissions. Third, choosing the appropriate ratio between treatment and transport may prevent the need for longer networks which require more construction and may be less manageable long term.

The results of the DEA-IWRM framework are based on modelled data with inherent uncertainty. Therefore, the uncertainty and sensitivity in the models should be considered beforehand. While the results of the DEA-IWRM framework is a clear list of preferred alternatives, any further interpretation of these options should be done by relevant stakeholders and decision makers. Decision makers may use the set of preferred alternatives as a reference to support future planning of projects for regional water supply-demand matching based on their goals and preferences.

5.5 Conclusion

This research presents the DEA-IWRM modelling framework which evaluates and identifies preferred combinations of treatment and transport to meet an industrial water demand. The DEA-IWRM model first uses existing simulation models to determine the performance of treatment and transport for various demands. The model then determines the preferred combination of treatment and transport based on multiple objectives and variations of the DEA analysis.

This unique approach of integrating different simulation models makes it possible to evaluate integrated water supply alternatives while accounting for altered operating conditions. The DEA-IWRM model applies a variety of DEA methods making it possible to processes multiple water supply alternatives and filter based on cost, energy, and environmental criteria. The result is a refined list of options which meet the requirements of the user and can further support decision makers.

Application to the Dow case study found that treatment generally remains more expensive than transport. In specific configurations, treatment performs better in terms of energy use and CO_2 emissions. The overall best configurations for the Dow case study combined treatment (20%–30%) and transport (70%–80%). DEA-IWRM shows that treatment and transport can be complementary measures for ensuring future water supply-demand matching while considering all potential impacts.

Though the results presented in this research are case specific, the framework is designed to be customized for other situations and cases. Users should consider this framework as a tool for decision support, not decision making. Several non-quantifiable aspects, such as risk, policy, societal impact, and resource use, should also be considered in design and water management network.

It is expected that both treatment and transport will become increasingly important as water scarcity rises. The scope of future research, therefore, should extend to larger industrial or regional demands with different water qualities. The DEA-IWRM can be expanded by increasing the number of included treatment technologies and by accounting for changes in groundwater availability. Including more decision criteria by incorporating non-quantitative performance indicators (e.g. social and risk criteria) is recommended to further improve the DEA-IWRM framework.

Young people are always asking what kind of artist should they be.

They always say, "Do you think I should be a writer or a filmmaker?"

And I always think, "If I were your age, I'd look for water".

– Fran Liebowitz, Pretend It's a City

CHAPTER 6

DISCUSSION

6.1 Introduction

The benefits of an alternative water use scheme include reduced demand on freshwater sources, reduced contamination of resources, and improved water security for non-potable applications [12]. Transitioning from the more conventional water use scheme, however, can be quite complex. To do so without posing health risks, financial risks, or impacts to public perception requires that this transition be done with as much transparency and information as possible. This research, therefore, provides the foundation for identifying the potential sources and applications and the criteria and standards which must be considered. In addition, a thorough exploration of the methods of connecting sources and end uses through non-conventional treatment configurations was also explored. The result is a framework which can be used for evaluating alternative non-potable water use schemes from source to application.

This research began by first critically reviewing the current state of alternative water use in literature with a focus on non-potable water (Chapter 2). This provided an understanding of the state of alternative water use while also identifying key sources, end uses, criteria, and standards that are relevant to its implementation. Next, the potential for treatment technologies to connect alternative sources and applications was explored. This was achieved by first developing systems-level models of select treatment technologies (Chapter 3) and then integrating these technologies into treatment train configurations (Chapter 4). The output was performance predictions for a variety of treatment technologies and trains under various operating conditions. In addition, the effects of these configurations on the technical, economic, and environmental impacts were also included. This resulted in a large number of results which were difficult to differentiate based on the non-linear relation of the impact outputs. Therefore, a decision support framework was developed to help determine which options were the most appropriate based on the scenario and stakeholder interests (Chapter 5). A summary of the objectives, main findings, and conclusions for each chapter, including the outputs of this chapter, are presented in Table 6.1.

This chapter will be divided into three sections. Section 6.1 will provide an overview of the conclusions based on the previous chapters. This will be presented within the context of the main aspects of the water use scheme (i.e. sources, methods of connection, and

Table 6.1 Summary of main findings for each chapter

Chapter	Research objective	Method
Chapter 2: Alternative Water Use *A critical review of reclaimed water sources, applications, criteria, standards, and overlooked opportunities*	Assess the state of existing literature on the topic of reclaimed water and provide a comprehensive overview of the state of alternative water use.	Systematic literature review
Chapter 3: Electrodialysis Modelling *Continuous mode electrodialysis modelling methods for brackish water desalination*	Inventory the existing systems-level modelling methods for continuous mode electrodialysis and identify which models are most accurate and applicable for implementation in a comparative desalination model.	Systematic literature review Modelling
Chapter 4: Treatment Train Analyses *Modelling framework for desalination treatment train comparison applied to brackish water sources*	Investigate and design a comprehensive systems-level model that can evaluate and evaluate different brackish water desalination treatment train configurations and compare their performance.	Desk research Interviews Modelling
Chapter 5: Treatment vs. Transport *A framework for assessing the trade-offs between on-site desalination and off-site water sourcing for an industrial case study*	Develop a decision support framework that can combine and compare alternative water sources (i.e. desalination treatment and transportation of water) and help determine the best configuration for a given scenario.	Modelling Data Envelopment Analyses
Chapter 6: Discussion	Assess and review what is needed to modify typical water use schemes to account for alternative non-potable water use and what changes are necessary to promote alternative water use schemes	Desk research Modelling

Main Findings	Conclusions
• Majority of literature focuses on municipal sources and domestic applications • Available source data does not often address end-user concerns • Environmental and industrial applications often overlooked but have a great potential • Freshwater demand can be offset by using alternative sources for overlooked applications	Reclaimed water use is a reliable, flexible, and efficient alternative water source. However, implementation must consider several perspectives and criteria to mitigate risk and prevent improperly designed reclaimed water systems.
• Theoretical and semi-empirical models were the most comprehensive methods • Operating conditions play an important role on the severity of systems-level impacts • Additional phenomena (e.g. boundary layer and water transport) should be included in future research	Semi-empirical methods can achieve the desired accuracy for systems-level understanding of continuous mode electrodialysis. However, attention must be paid to both the bounds of the evaluations and the included phenomena to assure relevance and accuracy.
• Treatment train modelling requires accurate and technology-specific evaluations • The order of technologies plays a significant role in treatment train performance • Using a discrete-based approach results in a large number of results • Decision support is needed and must include environmental and sustainability indicators	Treatment trains have the potential to widen the possibility of reclaimed water reuse, allowing for a broader input salinity and achieving a higher quality product water. Using the DESALT model allows for this to be seen, though the results are reliant on the accuracy of the technology-specific evaluation methods.
• The DEA method makes it possible to evaluate integrated water supply alternatives • The output of the DEA method is a refined list of options which can support decision makers • Treatment and transport were found to be complimentary measures for supplying water • Users should consider this framework as a tool for decision support, not decision making	The model was able to capture the general benefits and constraints of both treatment and transport. It is expected that both alternative water sources will become increasingly important as water scarcity rises, therefore, more investigation into their comparison and integration should be pursued.
• All options for alternative sources, treatment methods, and applications need to be accessible • Transparency of data and inclusion of non-quantitative criteria should be further investigated • Reframing alternative water use from the brine requirement perspective can improve options and reduce impacts	Research needs to support the educated implementation of alternative water reuse to mitigate potential risks and improve the image of this source. Further, shifting focus from product water requirements to brine water requirements can potentially improve feasibility and reduce potential impacts.

6

applications). Section 6.2 will apply the developed framework using a novel objective, namely, a targeted brine requirement. This is done to illustrate both how the framework can be implemented in future research and how shifting the objective from product water to brine can impact potential options. Finally, section 6.3 will present the future outlook for alternative water use based on this research and provide recommendations for future research.

6.2 Transitioning from standard water use to alternative water use

In conventional water use schemes, water is sourced from potable or near-potable sources, used for an application, and then discharged. This linear application of and heavy reliance on freshwater sources has led to worsening water scarcity issues [20]. This problem is typically addressed through soft path approaches such as improving internal water use efficiency or internal water reuse and recycling [10], [11]. However, these methods for reducing water use are not always feasible nor are they always the most sustainable option [49]. For example, improving the efficiency of potable water use for non-potable applications neglects the fact that the use of potable water is not actually needed at all [39]. Therefore, it is necessary to explore other alternative options for water use that can reduce the reliance on potable water and consider sustainability on a larger scale.

Through this research, it is recommended that the boundaries of conventional water use be broadened to include alternative non-potable water use schemes. The points of expansion are illustrated in Figure 6.1 where the white icons depict modifications to the conventional water use scheme. It is proposed that by identifying and accounting for all alternative water use options and assessing their associated impacts, mitigation of risks can be achieved early on and the most educated alternative water use schemes can be implemented. The developed framework discussion will be structured into three parts coinciding with the three primary aspects of alternative water use: alternative sourcing (Section 6.1.1), novel methods of connection (Section 6.1.2), and non-potable applications (Section 6.1.3). The topic of brine management will be discussed in more detail in Section 6.2.

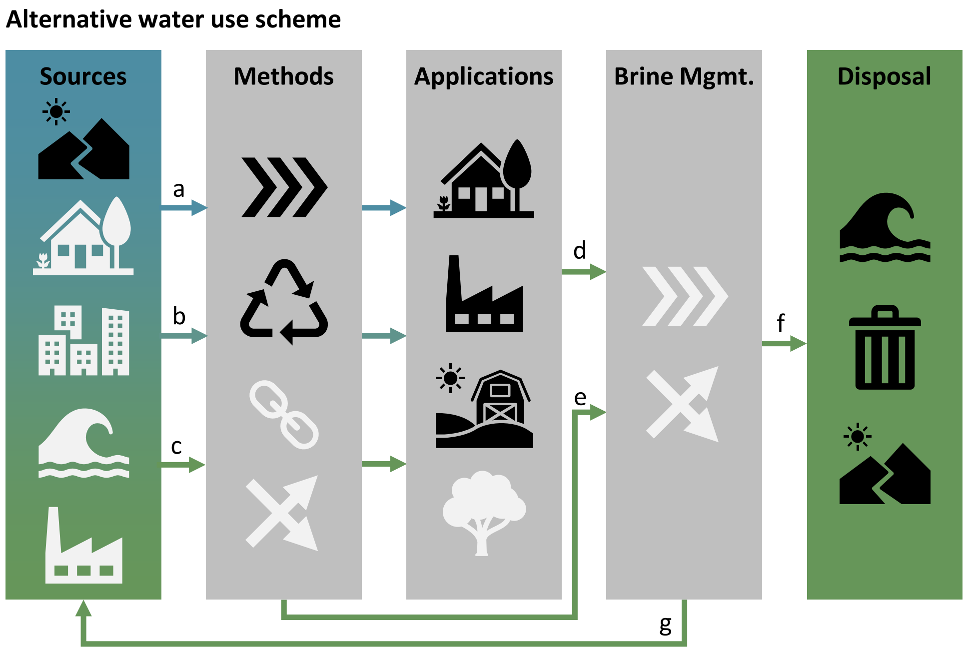

Figure 6.1 Overview of the proposed modifications to the conventional water use scheme to transition to an alternative water use scheme. Items in black denote the existing aspects of a conventional water use scheme while those in white are the additions recommended through this research. The flows are defined as the following: a) potable water; b) near-potable water; c) non-potable water; d) non-potable water output from applications; e) non-potable water output from treatment methods; f) brine / heavily contaminated wastewater; g) reclaimed non-potable water. Note that the color scheme will be use throughout this chapter to distinguish the water quality (blue = freshwater, bluish green = brackish water, green = heavily saline or brackish).

Sources: Environment, residential, municipal, saline surface water, or industrial. Methods: Direct use, recycling, treatment (train), or cross-sectoral use. Applications: Residential, industrial, agriculture, or environment. Brine Mgmt.: Direct use or cross-sectoral use. Disposal: Surface water, disposal, or environment.

6.2.1 Alternative sources

Conventional water schemes typically omit non-potable sources since the main focus is on meeting potable demand [12]. However, not all applications require potable water [39]. In these cases, non-potable sources can not only be applicable but also preferred based on their proximity, availability, or reliability [22]. Further, some applications can benefit from the presence of nutrients in these alternative non-potable sources [97], [98]. The first step in transitioning from the conventional water use scheme is to identify and include these alternative non-potable sources within the water scheme, as shown in Figure 6.1 [37].

Though there is research on the topic of alternative sources, these are almost exclusively focused on municipal and residential sources (i.e. human-based) [68], [102]. Human-based sources always contain some level of pathogens which can pose serious health risks [79]. This risk is amplified when used for applications that have any level of human exposure [98]. Instead of using treatment to mitigate these risks, it is recommended that alternative water reuse research begin to focus on non-human-based sources (e.g. environmental or industrial sources). These alternative sources may actually present more novel opportunities for reuse that have the potential to be implemented without extensive treatment [272]. In order to better understand this potential, however, it is important that a better representation of all non-potable sources be included in alternative water use schemes. Without this information readily available, end users may not know what is truly feasible and may make uneducated decisions that have alternative impacts [273]. Improperly implemented alternative sources can cause a ripple effect which can significantly impact an end-user's willingness to accept future alternative water use schemes [274]. It is, therefore, necessary that the image of alternative water use be managed and also elevated by ensuring that only efficient, appropriate, and safe applications are pursued.

6.2.2 Novel methods of connection

In addition to identifying what alternatives are available, it is also important to know what methods of connection are available and how they perform beyond just technical feasibility [275]. Modelling is shown to be an effective method for evaluating different methods of alternative water sourcing and application connections [189]. The modelling used in this research, for example, was able to predict performance, visualize feasible connections, assess potential impacts, and provide guidance in filtering through the available options. With that said, modelling is heavily reliant on the evaluation method accuracy and available data. Therefore, it should be stressed that the outputs of models such as the ones presented in this research be viewed as a starting point in the decision making process and not the final solution.

Conventional water schemes often promote internal reuse methods, however, this is not necessarily the safest nor the most sustainable approach [49]. For example, in the case of reusing greywater for toilet flushing, treatment is still required to mitigate health risks even though this is seen as the safest form of reuse with the lowest potential human exposure [60]. However minimal the impacts may be internal to the operations, this treatment may have adverse environmental impacts outside of the internal reuse scope [53]. It is therefore recommended that the narrow focus of internal reuse be elevated and expanded to include other options for connecting sources and applications such as cross-sectoral reuse (6.1.2.1), treatment trains (6.1.2.2), and transportation of water (6.1.2.3). These three alternative methods were investigated in this research and a summary of the discussion points are presented in the following sub-sections.

6.2.2.1 Cross-sectoral reuse

Cross-sectoral water use is the method of using the effluent from one location or sector as the influent for another. In this case it is still the promotion of water reuse but with the bounds of reuse applying to an area or region rather than a single location [181]. By connecting available alternative water sources with applications, costly treatment methods or over-extraction potentials can be avoided. The connection of sources and applications, however, can only be pursued when these are clearly identified and the relevant information is presented. This can be difficult as different sectors have different criteria considered relevant. Additionally, criteria that are important to end users may not be easily measurable by potential providers. For example, a commonly measured criteria in source water quality is electroconductivity. This is because it gives a general idea of the water composition and is easy to measure and monitor. This value, however, does not address end-user concerns regarding pathogens or heavy metals [9], [89], [98]. In order to approach cross-sectoral water management, some level of standardization is required where the measured criteria is both achievable for potential source providers and relevant for potential end users.

6.2.2.2 Treatment trains

Treatment trains combine individual treatment technologies to try and achieve a desired water quality. The aim is that the strengths of each technology are utilized while the impacts are minimized [187]. In the treatment train model presented in Chapter 4, it was found that indeed treatment trains have the potential to capitalize off the strengths of the individual technologies and minimize their potential impacts. This method was shown to have the potential to achieve the same product water quality requirements as individual technologies but with reduced economic or environmental impacts. Treatment trains also allowed for a larger range of eligible feed water salinity. With that said, treatment trains were also shown to be potentially costly and the repeated rounds of treatment could lead to very small quantities of effluent. Therefore, particular attention must be given to the decision making process in order to determine the most optimal and feasible configuration.

The scope of the treatment train modelling should also increase to provide a more accurate picture of what is possible. The DESALT model presented in Chapter 4 was limited to two technologies for the purposes of illustrating its potential. However, it is recommended that multiple technologies, both mature and novel, should be included in future research to further examine the potential performance of treatment trains. Additionally, the scope of the model was reliant on the available data. Therefore, the focus of the evaluations was on TDS and TOC as these were the most commonly present criteria in the available data and literature. However, other criteria are also relevant in determining eligibility and should be included to both improve the relevance to end users and legitimacy of the model outputs [2].

6.2.2.3 Transport of water

Transporting water using intelligent networking was shown to help balance the water table by improving the connection between water availability and demand [219]. The use of an intelligent networking model when outsourcing water resources allows for standard water use operations to continue while efficiently minimizing the reliance on nearby resources. However, the logistics of transport can be complex as theoretical pathways may actually be infeasible depending on permitting and land use restrictions. Additionally, the reliance on the transportation of water must also be mindful of the sustainable extraction rate at the resource. Over-extraction of a resource can limit the reliability of the source and may contribute to water scarcity outside of the investigation bounds. Further, changes to the hydrological system may impact the long-term reliability of this method. Therefore, this method can be seen as an approach for maintaining the existing water use operations but may be less preferrable in the long term.

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While each alternative method was found to be successful at connecting sources and applications on their own, it was also found that these methods were not necessarily mutually exclusive. This is because cross-sectoral reuse and transport are more relevant at a regional level while treatment trains are considered a more localized method. However, the integration of these methods can potentially address a regional water challenge on a comprehensive level. To accurately compare and contrast, however, requires that the applied modelling methods be of a similar level (e.g. systems-level) and consider the same impacts with the similar assumptions. When this is achieved, the developed decision support was shown to effectively rectify the different scales of application to refine the options to those most applicable with minimized impacts. When integrating and comparing treatment trains and the transportation of water, for example, it was found that these could actually be complimentary measures which reduced regional environmental impacts. When one method reached the bounds of its sustainable operation, the other could be used to supplement. With that said, this approach remained from the perspective of meeting a specific product requirement and only considered economic and environmental indicators. In future developments on this topic it is recommended that the impacts of infrastructure (re: transport) and brine production (re: treatment) be further investigated as these are crucial aspects that can completely undermine an approach.

6.2.3 Non-potable applications

As mentioned in Section 6.1.1, water reuse schemes typically focus on potable sources and applications. This is because water scarcity issues are often presented from the perspective of potable water scarcity, thus non-potable applications are not recognized as a relevant demand [12], [37]. Non-potable environmental applications, in particular, are often entirely omitted from consideration because they are seen as both irrelevant to human needs and are assumed to be met through natural hydrological cycles [38]. However, non-potable environmental applications can also experience water demand and quality issues. Coastal estuaries, for example, provide coastline protection and ecosystem support but also have a long history of droughts [2]. Ignoring these demands can have devastating impacts to coastal resilience and ecosystem stability. Making these non-potable applications more visible is the first step in meeting and protecting their water demand. Additionally, the identification of these non-potable applications increases the visibility and potential of alternative non-potable water use which can indirectly address potable water scarcity issues.

Use of non-potable sources for non-potable applications were also overlooked due to infrastructure limits (e.g. one pipe providing one quality of water) [67]. The close proximity of some non-potable applications to potable applications and the limits of conventional infrastructure often forces potable water to be used for non-potable applications [276]. Therefore, the primary barrier in matching non-potable sources and applications is proper infrastructure that allows for these different water flows to be delivered to the necessary applications [68]. Though intensive, the implementation of dual-reticulation systems has proven feasible in Australia, especially in new builds [277]. Existing infrastructure has also been modified in Hong Kong and parts of California to allow for salt water toilets [278], [279]. While this is logistically daunting, it has proven doable especially in locations experiencing extreme water stress. To validate and argue for these alterations to infrastructure, however, a better accounting of non-potable applications is needed to justify its purpose.

Once infrastructure is modified to allow for reuse, the potential for non-potable reuse can expand even further and the availability of non-potable application standards can help promote these opportunities. Based on the literature presented in Chapter 2, an example set of standards was generated (Table 6.2). While this table provides some general guides on water standards for non-potable applications, the most important thing to see is the lack of consistent information. There are both missing applications (e.g. environmental) and missing data which makes it difficult to truly say if a source and application are an acceptable match. It should also be noted that the presented values are based on estimations and ranges that can vary between countries and locations. This is partially because standards are context specific but also because the formation of standards requires lots of research and monitoring to formalize. The formalization of data and standards is necessary for truly assessing all options and preventing improperly implemented alternative water use schemes.

Table 6.2 Standard ranges based on the standards available in the literature review from Chapter 2. Note that these are the ranges present in the literature which spans multiple countries. Therefore, these do not necessarily state what the standards should be for all applications in all countries.

Application	EC (dS/m)		TDS (mg/L)		TSS (mg/L)		TP (mg/L)		TOC (mg/L)		BOD (mg/L)		COD (mg/L)	
	Min	*Max*	*Min*	*Max*	*Min*	*Max*	*Min*	*Max*	*Min*	*Max*	*Min*	*Max*	*Min*	*Max*
A1 - Crop irrigation (edible)	0.7	7.0	450	2,000	2.0	200	-	2.0	-	40.0	10	70	-	90
A2 - Crop irrigation (non-edible)	0.2	3.0	500	3,500	5.0	45	-	5.0	-	-	20	70	-	-
A3 - Livestock	-	-	2,000	6,000	-	-	-	-	-	-	-	-	-	-
D1 - Landscape (restricted)	1.6	4.2	-	500	10	150	-	30.0	-	-	60	300	-	500
D2 - Landscape (unrestricted)	-	8.8	-	500	10	60	-	30.0	-	-	10	200	-	150
D3 - Recreation	-	-	-	-	-	30	-	-	-	-	-	30	-	-
D4 - Residential (non-potable)	-	-	-	1,500	-	20	-	-	-	-	-	20	-	50
D5 - Residential (potable)	-	-	-	-	-	0	-	-	-	-	-	-	-	-
D6 - Urban uses	-	4.7	-	1,000	-	35	-	2.0	-	16.3	-	30	-	100
E1 - Groundwater (non-potable)	-	1.4	-	-	-	35	-	-	-	2	-	-	70	100
E2 - Groundwater (potable)	-		-	-	-	10	-	-	-	-	-	-	-	-
E3 - Irrigation	-	3.0	-	500	10	60	-	8.0	10	15.0	10	33	70.0	100
E4 - Surface water (non-potable)	-	2.2	-	-	-	-	-	-	-	-	-	-	-	750
E5 - Surface water (potable)	-	-	-	-	-	30	-	0.2	-	-	-	30	-	70
I1 - Boiler feed water	-	5.4	-	3,500	-	10	-	-	-	-	-	-	-	-
I2 - Cooling water	-	4.7	-	1,000	10	30	-	0.2	10	15.0	-	30	-	40
I3 - Process water	-	1.0	75	500	-	500	-	7.0	-	0.7	-	30	-	80

The final modification recommended for alternative use schemes is to prevent improper categorization of non-potable water applications. Often, the application of non-potable water to non-potable locations is termed disposal. This term can both reduce the protection of the location and tarnish the image of non-potable sources. When the term 'disposal' is used, the attention to water quality may be less respected. By reframing non-potable applications as applications with specific demands, the standards of these applications can be better protected and respected. Further, the use of disposal can also perpetuate the negative image associated with reclaimed water which further impacts public perspective. When this is instead framed as meeting a non-potable demand, it is possible that this can help reduce improper disposal and preserve the image of non-potable sources.

6.3 Reframing brine management

Alternative water use optimization has primarily focused on the optimal configuration for meeting a specific quality of product water [29]. While the primary focus has been on improving technology performance for this specific target, the result can be secondary by-products such as brine which cannot be easily mitigated [280]. Desalination, for example, is often regarded for its daily production of 95 million m^3 of freshwater. However, the resulting 142 million m3 of brine produced is rarely mentioned [25]. When scaled at this level it is clear that brine management is not a minor issue and should be thoroughly considered in the initial design of a sustainable water use scheme.

Unfortunately, the urgency to deliver product water can lead to hastily implemented treatment schemes that do not fully vet the impacts of the produced brine [281]. When brine management is considered so late in the planning stage, the options for disposal are limited and the long-term feasibility of the treatment plant may become compromised [13]. In extreme cases, the narrow focus on product water has led to fully implemented treatment plants that did not consider a long-term brine management plan. Haphazard brine mitigation is then pursued, sometimes including disposal to landfills, which has negative consequences both economically and environmentally.

The most common brine management method is disposal, even though this has a considerable environmental impact [13]. Other conventional disposal methods such as deep well injections, zero liquid discharge, and land applications were once acceptable brine mitigation approaches. However, the long-term effects are proving that these are unsustainable methods that undermine the feasibility and sustainability of the treatment process as a whole [44]. Even the most passive discharge method, discharging to the sea, has now been linked to the increasing rate of deoxygenated dead zones in seas and oceans, negatively impacting an estimated 245,000 km2 of marine ecosystems and disrupting food chains [23].

Due to the large and considerable impact of poorly managed brine, it is proposed to reframe alternative water use to focus on this aspect of alternative water treatment rather than manage it after the fact. It is theorized that by addressing brine management from the beginning, one of the largest barriers to water reuse can be removed improving the feasibility of alternative water use schemes. To explore this idea, a small exercise will be carried out that will build upon the case study presented in Chapter 4.

To begin this exercise, the case study for a cooling tower will be reintroduced as the baseline scenario (Section 6.2.1). Next, the baseline scenario will be modified to include the conventional goal of internal reuse with a product water focus (Section 6.2.2). The same baseline scenario will then be modified but with the alternative goal of meeting a brine requirement instead (Section 6.2.3). The application options for the resulting product water will then be assessed using the cross-sectoral method. Since this will be investigated in such a brief and limited exercise, the limits to this exercise will be discussed in Section 6.2.4 with the intent of being addressed in future research.

6.3.1 Baseline water use scheme

The baseline case used for this exercise is a cooling tower with a potable freshwater input and a non-potable brackish cooling tower blow down (CTBD) output (Figure 6.2) [28]. The CTBD quality is not good enough to be immediately reused, though it is conceivable that with proper treatment it could be. The CTBD is instead discharged to nearby surface water in accordance with local disposal requirements. In this baseline scenario, the end-user is aware that the freshwater source relied upon for operation is unstable and is looking to find a more reliable and sustainable replacement. In addition, it is known that the discharged CTBD contributes to an already heavily salinized water table and once discharged to the environment the potential for reclaiming this resource is lost.

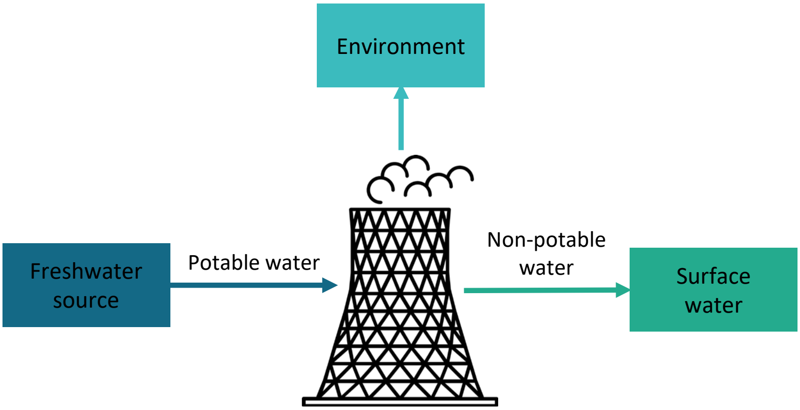


Figure 6.2 Baseline water flow scheme for the cooling tower case study

6.3.2 Internal reuse scheme

Since there is pressure to both reduce reliance on the freshwater source and reduce disposal, the initial instinct is to investigate internal reuse. This internal reuse approach is further supported since the reuse of CTBD is a commonly implemented method in industrial parks [19], [54]. Using the DESALT model in Chapter 4, the most optimal configuration is determined based on the product water requirements as well as three economic and environmental indicators. These indicators include the unit production cost (UPC, $US/m^3), the volumetric energy usage (E_{vol}, kWh/m^3), and the volumetric CO_2-equivalent ($CO_{2,vol}$, kg/m^3). These are all calculated based on the quantity of product water produced.

As shown in Figure 6.3, the DESALT model found that it is feasible to internally reuse the CTBD, though this is based purely on the TDS and TOC criteria which is major limitation and is discussed further in Section 6.2.3.5. However, the high water quality requirement for the product water results in an expensive UPC and a high $CO_{2,vol}$. In addition, the brine resulting from this treatment may no longer be eligible for being discharged to surface water. To investigate other brine management options, the standards presented in Table 6.2 are reviewed to see if there are any non-potable applications that could use this quality of water.

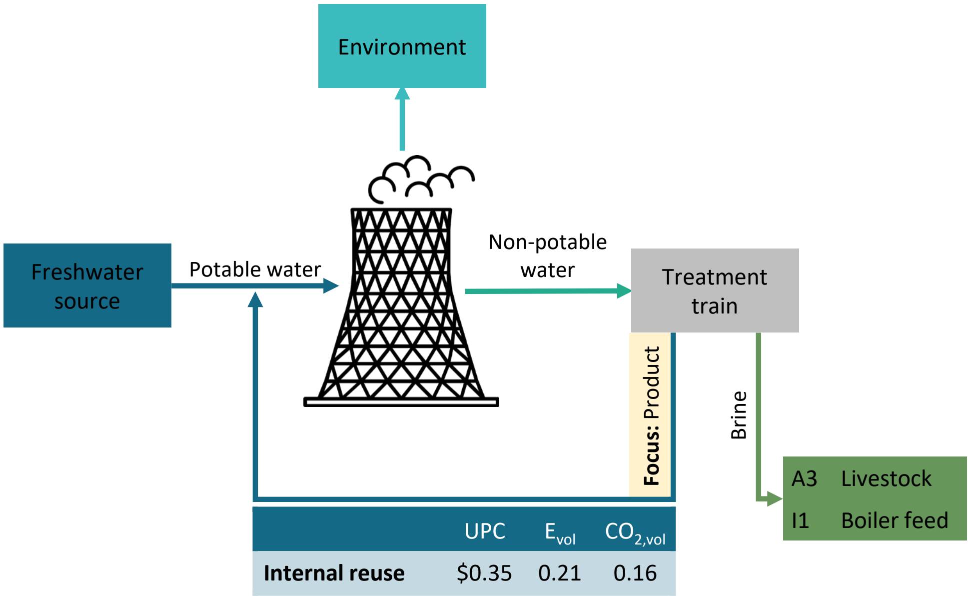


Figure 6.3 The baseline water use scheme is altered to include internal reuse. This is optimized based on the product water requirements and the preferred configuration was determined based on the unit production cost (UPC, $US/m^3), the volumetric energy usage (E_{vol}, kWh/m^3), and the volumetric CO_2-equivalent ($CO_{2,vol}$, kg/m^3). The result is a high UPC and $CO_{2,vol}$ as well as only two brine management options.

Two options were found to be viable applications of this brine: livestock (A3) and industrial boiler water (I1). The livestock standard, presented in Table 6.2, refers to the upper bound of the standards used for livestock watering, as presented in Horner et al. [129]. In this case the water would be used for irrigating crops that cattle would consume, with special attention that the cattle would not ingest the soil irrigated with this water. The industrial boiler water standard is based on the American Water Works Association standard for low to moderate pressure boilers, as presented in Jami et al. [282].

It must be noted that only the TDS and TOC standards from Table 6.2 were used in this evaluation as these were the only available inputs for the DESALT model in its current state. However, it is important to note that the concentration of other components (e.g. NaCl) are also pivotal to the feasibility of these schemes. While the brine produced in the internal reuse scheme indeed meets the required TDS and TOC quality, the presence of only two possible brine management options leaves this configuration vulnerable. Due to the limited scope of the evaluation method, it is quite possible that at least one if not both options would no longer be eligible once including other contaminants. For example, the livestock application may be adversely impacted by high concentrations of NaCl, as this can be detrimental to crop growth and have long-term impacts to the soil quality. Therefore, a limited number of options increases the chances that this brine will end up defaulting to disposal. In order to develop a secure water management scheme, it is important to have as many options as possible to increase the chance of at least one option being truly feasible and implementable.

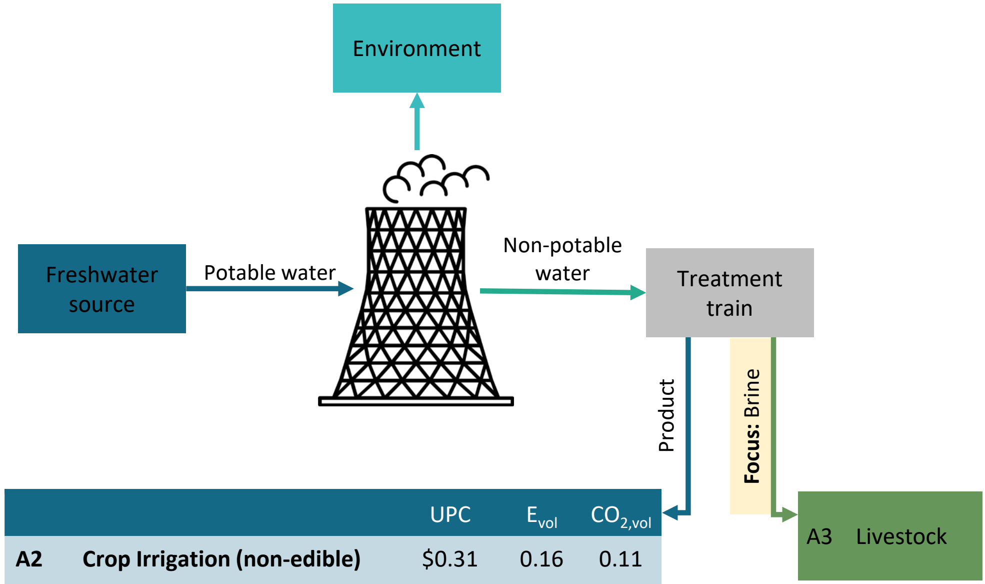
6.3.3 Alternative reuse with a brine focus

The baseline scenario is again revisited but this time with the target of meeting a maximum brine requirement. This is completed using the framework developed in this research. To begin, a non-potable application is selected from the information provided in Chapter 2. For the purpose of illustration, the livestock application discussed in Section 6.2.2 is used as the target brine requirement [129]. The DESALT model developed in Chapter 4 was then run using the maximum brine quality requirement as listed in Table 6.2. The output of the DESALT model was a large range of feasible configurations with various product water qualities. The resulting options were then processed using the decision support tool presented in Chapter 5 for each product water application listed in Table 6.2. The result was eight feasible product water applications with various economic and environmental impacts as shown in Figure 6.4.

When compared to the internal reuse scenario, the brine focus approach shows a potential to improve on multiple aspects which are discussed in detail in the following sub-sections. These include offsetting water demand (6.2.3.1), minimizing economic and environmental impacts (6.2.3.2), reducing disposal (6.2.3.3), and improving feasibility (6.2.3.4).

6.3.3.1 Offsetting freshwater demand

Seven of the eight product water options in the brine focused scheme were applications that would otherwise rely on freshwater sources. By supplying these applications with the resulting product water, this is in turn offsetting the demand on local freshwater sources. While this approach may not necessarily resolve the reliability issue of the freshwater source internally, the decreased demand on the freshwater sources should reduce the competition for this water which would improve the overall water security in the area.



		UPC	E_{vol}	$CO_{2,vol}$
A2	**Crop Irrigation (non-edible)**	$0.31	0.16	0.11
D1	**Landscape (restricted)**	$0.31	0.16	0.11
D2	**Landscape (unrestricted)**	$0.31	0.16	0.11
D4	**Residential (non-potable)**	$0.19	0.16	0.06
D6	**Urban uses**	$0.55	0.19	0.19
E3	**Irrigation**	$0.55	0.22	0.23
E4	**Surface water (non-potable)**	$0.19	0.17	0.06
I2	**Cooling water**	$0.55	0.22	0.23

Figure 6.4 The baseline water use scheme is altered to focus on a maximum brine quality requirement. This is optimized based on the livestock requirements. The resulting product water was then reviewed to see where it could be applied based on Table 6.2. The result was eight possible applications which could use the resulting product water with varying effects on the unit production cost (UPC, $US/m^3), the volumetric energy usage (E_{vol}, kWh/m^3), and the volumetric CO_2-equivalent ($CO_{2,vol}$, kg/m^3). The result is an increased number of potential options which can also potentially decrease the economic and environmental impacts.

It should also be noted that for the higher water quality options (e.g. landscape irrigation) the quantity of produced water may be much lower than those with lower water quality requirements (e.g. non-potable surface water). This is a result of less intensive treatment needs to meet the lower quality requirements. A low removal rate, in this case, typically results in a higher product water recovery ratio. While the quantity of water was not included in this exercise, it is important that this be addressed and considered in future investigations of reframing brine management so that indeed the best option is selected.

6.3.3.2 Minimizing economic and environmental impacts

With regards to potential impacts, six of the eight options resulted in a lower energy demand. Further, five options were able to lower all three economic and environmental indicators. Since these five options at a reduced impact level are still more than the two options presented in the internal reuse scheme, it shows that the brine focused scheme can potentially improve the feasibility of the water use scheme while also reducing the potential impacts.

6.3.3.3 Reducing disposal

By approaching the scenario with a brine focus, the issue of brine management is addressed from the beginning. This means that, once the brine application is secured, the feasibility of the project greatly improves. In this scenario, the brine is already allocated for the livestock application, therefore the industrial plant is eliminating its brine disposal and reducing its impact on the environment. While it could be argued that this is "passing the buck" to the next application to manage the waste, this framework could be used again at the next location to optimize the brine there as well. In addition, this use of non-potable water is typically for applications that are already managing their own outputs. In the case of livestock wastewater, treatment technologies have been implemented to both remove pathogens and recover nutrients that can be repurposed nearby [283]. Therefore, the collection of these non-potable sources could potentially improve the yield of nutrients in this system while also reducing the demand on freshwater. Though possible, the effects of the additional contaminants (e.g. increased salt concentrations) should be further assessed before implementation as the effectiveness of wastewater treatment and nutrient removal can be effected by factors such as increased salinity [284].

6.3.3.4 Feasibility

In general, the brine focused scenario can be considered more feasible than the internal reuse scheme since it removes the risk of brine management complications. In addition, there are more options for the product water application and there is a potential that this configuration can reduce economic and environmental impacts. While it can be argued that this exercise is incomplete since Table 6.2 has missing options and data (e.g. maximum concentration of NaCl), it is seen as a representative sampling of the water applications identified in the literature. While the actual number of viable options may vary, the relative difference in representation of internal product focused scenarios vs. alternative brine focused scenarios should be similar. This also reinforces the previous sentiment that it is important for all applications (potable and non-potable) to be clearly identified with available standards so they can be represented in these types of evaluations.

6.3.3.5 Limits to this exercise

Though this exercise helps illustrate the impact of reframing brine, there are several considerations that must be taken into account. These are outlined as follows:

Limited inclusion of criteria: Due to data availability, these scenarios were based almost entirely on TDS and TOC requirements. However, in the standards it is clear that there is concern for other contaminants including but not limited to TSS, TP, and heavy metals. As an example, the livestock application used in this exercise actually has 14 other standards as presented in Horner et al. [129]. As previously mentioned, these other criteria (e.g. NaCl) can have determinantal and long-term impacts (e.g. crop yields and soil quality) if not properly assessed. Similarly, the boiler feed standard included five other criteria specified in Jami et al. including hardness, pH, and alkalinity limits [282]. Due to the limits of this evaluation method, however, these were not able to be taken into account. Therefore it is important that before implementation, these factors also be considered. Further, it is expected that if these other criteria were monitored and presented, the list of eligible product water applications may be different than what is shown in this exercise. This underscores the need for an approach such as the brine focused scheme that starts with a large number of options which leaves room for options to fall out.

Missing applications: As previously stated, this exercise is limited to the applications presented in Table 6.2. Notably missing are environmental applications such as salt water marshes and other non-potable applications that are discussed further in Section 6.1.3. If these applications were included, the potentials for both brine and product water applications could increase considerably.

Limits to economic considerations: The presented costs for the brine focus approach do not include the cost to deliver product water and brine to the specified locations. Therefore, the savings seen should consider that additional costs for transport may need to be included. Integration of this approach with water networking programs can be a starting point for estimating the cost of transport and presenting a more accurate picture.

Inaccurate standards: Since the standards used are based on a range of situations from a variety of countries, it is possible the implemented standards are not reflective of specific locations. While these provide a starting point to understand what is possible, it is necessary that future evaluations incorporate more accurate and specific standards for different locations and sectors.

6.4 Outlook

6.4.1 Integrated framework for alternative water use

This research intended to evaluate the state of alternative non-potable water use and determine what modifications are necessary to consider and promote alternative water use schemes. While the initial purpose of this research was to investigate the feasibility of achieving internal water reuse based on a product water requirement, it was shown in Section 6.2.3 that this same methodology can be modified and expanded to account for other perspectives and targets. This implementation from two different perspectives proves the relevance of the foundational framework developed for assessing alternative water use schemes. The structure of the framework is outlined as follows:

Step 1: Identify source and application options

In Chapter 2, the basis of the existing alternative water sources and non-potable applications are identified as well as the relevant standards and water quality data. This investigation highlights why this information is necessary to collect and which information is relevant so that future investigations can build off of this foundation. In future investigations, this information can provide a starting point and the lessons learned can help guide the identification of other neglected sources and applications.

Step 2: Develop a systems-level understanding of treatment technologies

With the sources and applications identified, Chapter 3 provides insight into how these can be connected through a treatment technology. In this chapter, the development of a systems-level model is outlined, emphasizing the necessary connection between operating conditions and impacts. This level of understanding is necessary so that the outputs are reflective of the operating conditions and a general understanding of the technology's performance can be seen. With this knowledge in hand, technologies can then be more easily evaluated and compared within integrated models and the capabilities of these technologies can be more clearly understood. Future research should account for both economic and environmental impacts as well as be expanded to include other relevant criteria and indicators.

Step 3: Apply an integrated modelling method to evaluate all options

Chapter 4 presents a modelling framework which can integrate these systems-level modelling evaluations developed in Chapter 3 with the possible source and relevant applications identified in Chapter 2. This approach makes it possible to view all options and while also considering the impacts of these configurations. Since the source data, application standards, and included technologies can all be changed or modified, this systematic evaluation framework allows for novel treatment configurations and source-application connections to be discovered that may been previously overlooked.

Step 4: Use decision support methodologies to intelligently select the most appropriate option

The output of the previous steps can result in an overwhelming and confusing array of options. Therefore, the decision support methodology presented in Chapter 5 can be used to help decipher and narrow the potential options to those that are both relevant and cognizant of having minimal impacts while also being feasible. This methodology can also be used to compare different alternative water use options outside of treatment and transport such as cross-sectoral reuse, if their performance and impacts are captured in a similar way.

Step 5: Consider alternative perspectives, methodologies, and impacts

The final step of this framework is to reflect on the process, as done in Chapter 6. Once the evaluation portion of the framework is complete, it is necessary to review and evaluate the outputs to include relevant points of concern or risk. This can even lead to finding a new perspective on the alternative water use scheme which can encourage a novel approach to this topic, such as the reframing brine approach. In this final stage, it is important to remember that this framework is the starting point for the continued discussion and investigation into alternative pathways for addressing water scarcity and that decision makers should build from these results the most appropriate and comprehensive water scheme.

6.4.2 Future research

Future research on the topic of alternative non-potable water should explore and expand upon each aspect of the alternative water use scheme. Approaches to this topic should continue to focus on aspects which improve its implementation but it is also necessary to address its public perception issues as well. Therefore, it is recommended that future research keeps this in mind in scoping and address the public perception issue when possible.

To begin, more transparency is needed on what the available non-potable sources and non-potable end uses are. While Chapter 2 provided an overview of what has been presented in the literature to date, a more thorough categorization of all potential sources and applications is needed so that the possibilities can be more clearly seen and accounted for. This could be done through expert interviews as well as an inventory of all current water applications and then a follow up assessment of which applications can utilize non-potable water. As discussed in Chapter 2, it appears that some applications have received more attention than others, therefore a true overview of all possibilities to stimulate further investigations would be beneficial. A specific focus on non-potable environmental applications should also be completed to make sure this category is more properly represented and accounted for in assessing water use possibilities. Doing so will help broaden reuse options as well as increase their protection.

In this same vein, a standardization of the relevant criteria is needed so that the monitored criteria and tailored standards for specific applications are better aligned. As previously stated this should include considerations for what is accessible for source providers and what is of concern for end users. By including and addressing all relevant criteria, end users may improve their trust of alternative non-potable sources and this limiting social factor may allow for an increased pursuit of this topic.

Once this information is available, proper connections between non-potable sources and applications can begin from a point of technical feasibility. In future research this could be done from a modelling perspective or in a more in-depth qualitative review. From a modelling perspective, this could be done by either directly matching sources with applications based on quality and quantity information or via technology models, as presented in Chapter 3 and 4.

With regards to the models presented in Chapter 3 and 4, there are several aspects that can be improved upon in the future. Specifically, expanding the treatment train modelling platform to include additional and more novel technologies would be the first step in deepening the understanding and benefits of treatment trains. By incorporating these into the DESALT model, it may be possible to discover new treatment trains or new configurations (e.g. different recovery ratios). Additionally, expanding the technology evaluations to address additional contaminants is also pivotal for improving the accuracy of the evaluations and making a more realistically feasible list of options. While the focus on TDS and TOC helped illustrate the modelling methodologies in these chapters, a much wider range of criteria is necessary for more accurate and realistic evaluations in the future.

Reframing the approach of alternative water use to focus on brine requirements was shown to open up opportunities for cross-sectoral water reuse while also reducing economic and environmental impacts. This brief exercise shows promise for both management of brines and reviewing options from a novel perspective. It also proves that it is both pivotal and beneficial to address these complex issues first (i.e. before designing technological applications in a specific case or context) rather than waiting to address them as an afterthought (i.e. trying to improve a certain desalination technology installed in practice, which is bound to lead to a marginal reduction in environmental impact).

Finally, the participation and acceptance of stakeholders from different sectors is necessary for the success of alternative water use to be fairly researched and properly implemented. While existing research has helped grow this topic, input and knowledge from those in the field is necessary for research to develop solutions that are both attractive and feasible.

Further, the focus on alternative sources and applications requires the boundary of the investigations to cover multiple sectors with varying needs and concerns, all of which need to be in alignment for cross-sectoral water use to occur. Therefore, the integration and co-creation of solutions with participation from all stakeholders is necessary. It is proposed that stakeholders such as those from industrial and agricultural sectors are encouraged to widen their concerns to include regional water use impacts and create comprehensive solutions that improve water security as a whole and not just internally.

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R

NOMENCLATURE

Variables	Description	Units
α	Permeate selectivity	-
$\mathfrak{a}$	Constant for resistance calculations	-
A	Area	m^2
$\mathbb{A}$	Availability	%
β	Pressure conversion factor	-
$\mathfrak{b}$	Constant for resistance calculations	-
$\mathcal{B}$	Cost coefficient	-
c	Concentration	mg/L
$\mathbb{c}$	Conversion factor	kg/m^3
$\mathbb{C}$	Costs	$US or $US/year
$CAPEX$	Capital costs	$US
CO_2eq	CO_2-equivalent	kg CO_2
δ	Recovery ratio	%
d	Diameter	m
D	Diffusion coefficient	m^2/s
ε	Porosity	%
ϵ	Void fraction	-
ξ	Empirical coefficient for mechanical dispersion	-
$\mathbb{e}$	Current efficiency	%
E	Energy use	kWh
$\mathbf{E}$	Efficiency score	-
$\mathbb{E}$	Edges (i.e. pipeline sections)	-
f	Darcy friction coefficient	-
F	Faraday constant (96,485)	s A/mol
γ	Activity coefficient estimation	-
h	Channel height	m
i	Current density	A/m^2
$\mathbb{i}$	Index for input	-
I	Current	A
$\mathbb{I}$	Total number of inputs	-
$\mathbb{j}$	Index for output	-
J	Ionic flux	mol/m^2 s
$\mathbb{J}$	Total number of output	-
J_{ave}	Average permeate flux	m^3/m^2 hour
k_m	Mass transfer coefficient	-
$\mathbb{k}$	Index for DMUs	-
$\mathbb{K}$	Total number of DMUs including the given DMU r	-

Variables	Description	Units
λ	Water permeability coefficient	m^3/Pa s m^2
Λ_{chan}	Equivalent conductivity	S cm^2/mol
ℓ	Length	m
l	Expected lifetime	year
L	Channel length	m
μ	Chemical potential of an ion species	J/mol
m	Molarity of the electrolyte	mol/L
M	Molar mass	kg/mol
$\mathcal{M}$	Capital cost coefficient	-
η	Non-ohmic voltage drop	V
$\varkappa$	Efficiency	%
$\mathbb{m}$	Preferred multiplier for preference-based weight constraints	-
N	Total number	-
NDP	Net driving pressure	kPa
ω	Boundary layer thickness	m
$OPEX$	Operations and maintenance costs	$US/year
π	Osmotic pressure	kPa
ϕ	Potential drop	
p	Overall pressure drop	kPa
P	Pressure	kPa
q	Water flux	m^3/m^2 s
Q	Flowrate	m^3/hour
ρ	Density	kg/m^3
$\mathbb{r}$	Index for a given DMU	-
R	Resistance	Ω m^2
$\mathbb{R}$	Total number of DMUs	-
$\mathcal{R}$	Removal rate	%
$\mathbb{Re}$	Reynolds number	
R_g	Universal gas constant	m^3 Pa/K mol
$\mathbb{Sc}$	Schmidt number	
$\mathbb{Sh}$	Sherwood number	-
φ	Voltage drop	V
τ	Transport number for ions	-
t	Time	s
T	Temperature	K
TCF	Temperature correction factor	-
t_{res}	Residence time	s

N

Variables	Description	Units
u	Velocity	m/s
$\boldsymbol{U}$	Weight used for efficiency score calculation	-
UPC	Unit production cost	\$US/m^3
ν	van't Hoff coefficient	-
v	Dynamic viscosity	kg/m s
V	Voltage	V
$\boldsymbol{V}$	Weight used for efficiency score calculation	-
$\mathbb{V}$	Vertices (i.e. available water sources)	-
W	Channel thickness	m
x	Location along the length of the channel	m
$\mathbb{x}$	Common input	-
$\mathbb{x}_1$	Input for the economic indicator	-
$\mathbb{x}_2$	Input for the energy indicator	-
$\mathbb{x}_3$	Input for the environmental indicator	-
$\mathbb{X}$	Total number of inputs	-
y	Location across the thickness of the channel	-
$\mathbb{y}$	Output or artificial output	-
ζ	Shadow factor	-
z	Ion charge number for an ion species	-

N

Subscript	Description
a	Location a
adj	Adjusted
AEM	Anion exchange membrane
app	Applied
ave	Average
b	Location b
$bound$	Boundary layer
$brine$	Brine
BW	Brackish water
$BWRO$	Brackish water reverse osmosis
cap	Capital
cp	Cell-pair
$cell$	ED unit cell
CEM	Cation exchange membrane
$chan$	Channel
Cl^-	Chloride ions
$conc$	Concentrate
$cond$	Conductive
$counter$	Counter ions
$cross$	Cross-efficiency
day	Day
$demand$	Demand
$diff$	Diffusion
dil	Diluate
e	Effective
EC	Electroconductivity
ED	Electrodialysis
$elec$	Electricity
$eosm$	Electroosmotic
exp	Experiment
f	Filament
$feed$	Feed water
gen	General operations
h	Hydraulic
$hour$	Hour
i	Ion species i
$\mathbb{i}$	Index for input

N

Subscript	Description
IEM	Ion exchange membrane
in	Inlet
$installed$	Installed
j	Ion species j
$\mathbb{j}$	Index for output
$\mathbb{k}$	Index for DMUs
lim	Limiting
$local$	Local
max	Maximum
md	Membrane interface
mem	Membrane
min	Minimum
Na^{+}	Sodium ions
$NaCl$	Sodium chloride
OM	Operations and maintenance
osm	Osmotic
out	Outlet
$prod$	Product water
$pump$	Pumping
$\mathbb{r}$	Index for a given DMU
req	Required
$region$	Region
sec	Seconds
sol	Solution
$source$	Source
sp	Spacer
$spec$	Specific
$stack$	ED stack
sub	Subcell
sup	Superficial
$super$	Super-efficiency
sys	System
$test$	Test
$trans$	Transport
$treat$	Treatment
$total$	Total
w	Water

Subscript	Description
$waste$	Wastewater
x	Location along the length of the channel
$\mathbb{x}$	Common input
y	Location along the thickness of the channel
$\mathbb{y}$	Output or artificial output
$year$	Annual
0	Initial

N

Acronym	Description
AEM	Anion Exchange Membrane
BWRO	Brackish Water Reverse Osmosis
CAPEX	Capital Costs
CCR CRS	Charnes, Cooper, and Rhodes Multiplier Model with Constant Returns to Scale
CEM	Cation Exchange Membrane
CFD	Computational Fluid Dynamics
CTBD	Cooling Tower Blow Down
DEA	Data Envelopment Analysis
DEA-IWRM	Data Envelopment Analysis of Integrated Water Resource Management
DESALT	Desalination Evaluation, Screening, and Learning for Treatment trains
DMUs	Decision Making Unit
Dow	The Dow Chemical Company
EC	Electroconductivity
ED	Electrodialysis
EVALEAU	Evaluation Tool of Environmental and Economic Performance for Drinking Water
GDP	Gross Domestic Product
IEM	Ion Exchange Membrane
IWRM	Integrated Water Resources Management
MCDM	Multi-Criteria Decision Making
MINLP	Mixed Integer Nonlinear Programming
NDP	Net Driving Pressure
O&M	Operations and Maintenance
OPEX	Operation and Maintenance Costs
RO	Reverse Osmosis
ROSA	Reverse Osmosis System Analysis
TDS	Total Dissolved Solids
TOC	Total Organic Carbon
VRS	Variable Returns to Scale
WSI	Water Scarcity Index
WSN	Water Supply Network
WWAP	World Water Assessment Programme

SUPPLEMENTARY MATERIAL

S1 Results of the systematic literature review on reclaimed water sources and applications

Table S1-1 Systematic literature search results for the reclaimed water applications.

Authors	Scope	Aim	Environment	Residential	Municipal	Industrial	Agriculture	Domestic	Environment	Industrial
Abou-Shady (2017)	Specific Source	Apply Tech.			•		•			
Aiken et al. (2010)	Specific Source	Feasibility			•		•			
Alcaide Zaragoza et al. (2020)	Specific Application	Optimization	•		•		•			
Al-Hamaiedeh & Bino (2010)	Specific Connection	Assessment		•				•		
Aybuğa & Yücel Işıldar (2017)	Specific Source	Feasibility	•	•				•		
Bakare et al. (2019)	Specific Connection	Feasibility		•				•		
Becerra-Castro et al. (2015)	Specific Application	Assessment			•			•		
Bertone & Stewart (2011)	Specific Connection	Decision Making	•					•		
Brissaud (2008)	General Overview	Assessment			•		•	•		
Chanan et al. (2009)	General Overview	Assessment			•			•		
Chang & Ma (2012)	General Overview	Public Perception			•		•	•		•
Chen & Chen (2014)	Specific Connection	Optimization			•					•
Chen et al. (2012a)	General Overview	Assessment					•	•		•
Chen et al. (2012b)	Specific Application	Decision Making			•			•		
Chen et al. (2013a)	General Overview	Assessment								
Chen et al. (2013b)	General Overview	Feasibility								
Chen et al. (2013c)	General Overview	Decision Making			•			•		
Chen et al. (2014a)	General Overview	Decision Making			•		•	•		
Chen et al. (2014b)	Specific Connection	Feasibility			•			•		
Chiou et al. (2007)	Specific Source	Feasibility			•		•	•	•	•
Chowdhury et al. (2015)	Specific Connection	Feasibility		•				•		
Darwish et al. (2007)	Specific Application	Feasibility			•		•			
Das & Kumar (2009)	Specific Connection	Feasibility				•	•			
Ernst et al. (2007)	Specific Connection	Apply Tech.			•			•		
Garcia-Cuerva et al. (2016)	General Overview	Public Perception		•	•		•	•		
Ghisi & Mengotti de Oliveira (2007)	Specific Connection	Optimization	•	•	•			•		
Jang et al. (2008)	Specific Connection	Feasibility			•		•			
Jang et al. (2010)	Specific Source	Feasibility			•			•	•	
Kalavrouziotis (2011)	Specific Connection	Feasibility			•		•		•	
Lawhon & Schwartz (2006)	Specific Connection	Assessment			•		•			
Lazarova et al. (2012)	Specific Source	Assessment			•			•	•	•
Leffert et al. (2008)	Specific Connection	Feasibility				•			•	
Lozier & Ortega (2010)	Specific Source	Apply Tech.			•		•	•	•	•
Mainali et al. (2011)	Specific Connection	Feasibility			•			•		
Mainali et al. (2013)	Specific Connection	Public Perception			•			•		
Ngo et al. (2009)	Specific Connection	Public Perception			•			•		
Ntibrey et al. (2021)	Specific Application	Public Perception			•			•		
Oliveira-Esquerre et al. (2011)	Specific Application	Feasibility	•		•	•				•
Oviedo-Ocaña et al. (2018)	Specific Application	Feasibility	•	•	•			•		
Page et al. (2012)	Specific Source	Feasibility			•			•	•	
Pan et al. (2018)	General Overview	Decision Making			•		•	•		
Perulli et al. (2019)	Specific Connection	Feasibility			•		•			
Peterson (2016)	Specific Source	Feasibility	•					•		
Pham et al. (2011)	Specific Application	Public Perception		•	•			•		
Roshan & Kumar (2020)	General Overview	Assessment								
Stevens et al. (2008)	Specific Application	Assessment			•			•		
Styczen et al. (2010)	Specific Connection	Decision Making			•		•			

S1

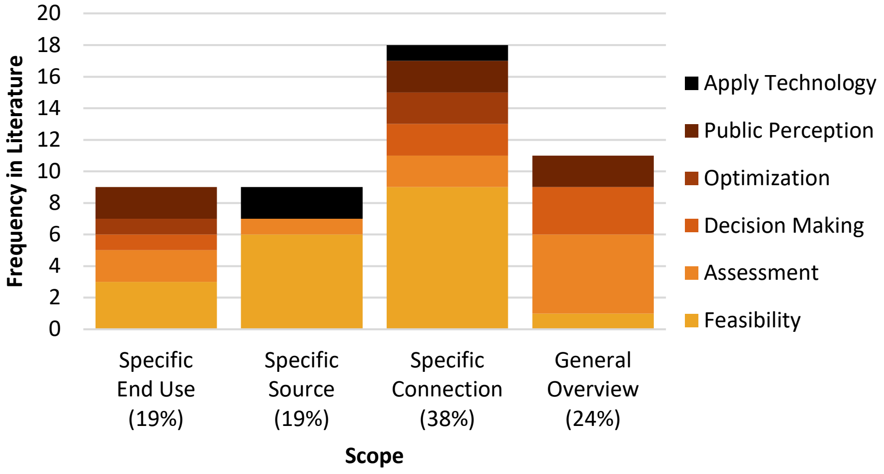


Figure S1-1 Presentation of the application literature based on the research scope and aim.

S2 Results of the systematic literature review on reclaimed water criteria, data, and standards

Table S2-1 Systematic literature search results for criteria literature.

Authors	Scope	Aim	Technical	Economic	Environmental	Social	Agriculture	Domestic	Environment	Industrial
Abdulbaki (2017)	Presents	Optimization	•	•	•		•	•		•
Adewumi et al. (2010)	Applies	Decision Making	•	•	•	•	•	•	•	•
Anane et al. (2012)	Applies	Decision Making	•	•	•	•	•			
Aydin et al. (2015)	Applies	Decision Making	•		•					
Balfaqih et al. (2017)	Presents	Assessment		•	•					
Behzadian et al. (2015)	Presents	Assessment	•	•	•	•	•	•		•
Ben Brahim-Neji et al. (2014)	Applies	Decision Making		•	•	•	•			
Chen et al. (2012a)	Applies	Assessment		•	•	•	•	•		•
Chen et al. (2012b)	Applies	Decision Making	•	•	•	•		•		
Chen et al. (2013c)	Identifies	Assessment	•	•	•	•	•	•		•
Chen et al. (2014a)	Applies	Decision Making	•	•	•	•	•	•		
Chen et al. (2014c)	Identifies	Decision Making	•	•	•	•	•	•	•	•
Chhipi-Shrestha et al. (2019)	Presents	Decision Making		•	•	•	•	•	•	
Chowdhury & Al-Zahrani (2013)	Applies	Assessment		•	•	•	•			
Coutts (2006)[113]	Identifies	Feasibility	•	•	•	•	•	•		
Das & Radhakrishnan (2019)	Identifies	Decision Making	•	•	•	•				
Domènech et al.(2013)	Identifies	Assessment	•	•	•	•		•		
dos Santos Amorim et al. (2020)	Applies	Decision Making	•	•	•	•				
Fooladi Dehaghi & Khoshfetrat (2020)	Applies	Decision Making	•	•	•	•				
Friend & Coutts (2006)	Identifies	Public Perception	•	•	•	•	•	•		
Gdoura et al. (2015)	Presents	Decision Making	•	•					•	
Gual et al. (2008)	Identifies	Apply Tech.	•	•		•		•		
Hadipour et al. (2016)	Applies	Decision Making	•	•	•	•	•	•	•	•
Horner et al. (2011)	Applies	Assessment	•			•	•			
Hyde et al. (2017)	Identifies	Public Perception	•			•		•		
Ilemobade et al. (2009)	Presents	Assessment	•	•	•	•		•		•
Joksimovic et al. (2006)	Presents	Assessment	•	•	•	•	•	•		•
Kumar et al. (2016)	Presents	Decision Making	•	•	•		•	•		•
Mariano-Romero et al. (2007)	Presents	Optimization	•	•	•		•	•		•
Naji & Lustig (2006)	Applies	Assessment	•	•	•	•	•	•		
Newcomer et al. (2017)	Identifies	Feasibility	•			•	•	•		
Oertlé et al. (2019)	Presents	Decision Making	•	•	•					
Oertlé et al. (2020)	Presents	Decision Making	•	•	•	•				
Opher et al. (2019)	Presents	Assessment	•	•	•	•		•		
Paranychianakis et al. (2015)	Identifies	Assessment	•	•	•					
Rezaei et al. (2019)	Applies	Assessment	•	•	•	•				
Rygaard et al. (2014)	Applies	Assessment		•	•	•		•		
Sa-nguanduan & Nititvattananon (2011)	Presents	Decision Making	•	•	•	•		•		•
Sapkota et al. (2015)	Presents	Assessment	•		•			•		
Stathatou et al. (2017)	Identifies	Public Perception	•	•		•				
Urkiaga et al. (2008)	Identifies	Assessment	•	•	•	•		•		
Wade Miller (2006)	Presents	Assessment	•	•	•	•				
Wilcox et al. (2016)	Identifies	Assessment		•	•	•		•	•	•
Woltersdorf et al. (2018)	Applies	Assessment	•	•	•	•				
Zolfaghary et al. (2021)	Applies	Decision Making	•	•	•					

S2

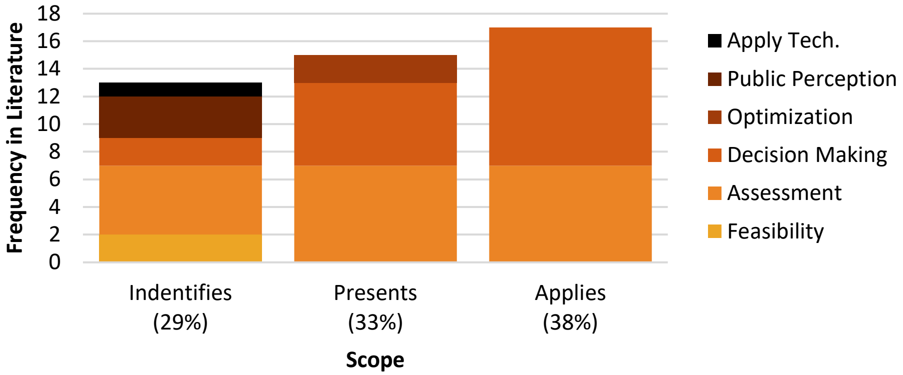


Figure S2-1 Presentation of the criteria literature based on the research scope and aim.

S3 Overview of source sub-categories

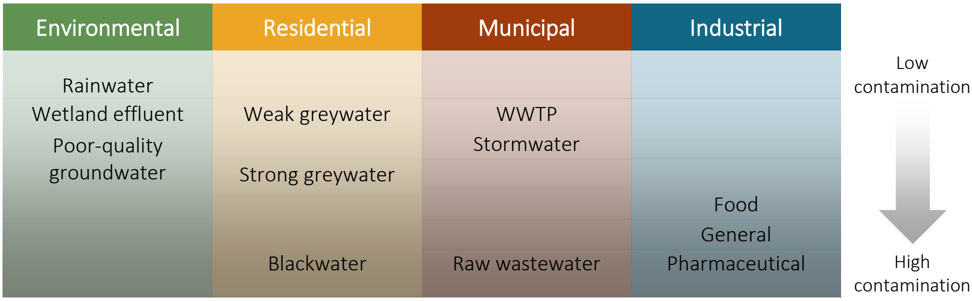


Figure S3-1 Overview of water reuse source categories and sub-categories arranged based on their general contamination levels. It should be noted that the actual quality within these sub-categories can vary greatly and that this is just a general understanding of how different source relate to each other from a contamination perspective.

Table S3-1 Overview of the sub-category sources and examples.

Environmental	
Rainwater	*Small scale, Large scale*
Wetland effluent	*Natural, Constructed*
Poor-quality groundwater	*Brackish, Saline, Contaminated*
Residential	
Weak greywater	*Baths, Showers, Sinks, Laundry, Other residential*
Strong greywater	*Dishwashers, Kitchen sinks*
Blackwater	*Toilet flushing*
Municipal	
WWTP	*Treatment effluent*
Stormwater	*Street runoff, Drainpipes, Gutters*
Untreated wastewater	*Domestic, Commercial, Industrial, Other effluents*
Industrial	
Food processing	*Crop refining, Processing*
General industrial	*Livestock, Tannery, Refinery, Commercial laundry, Mining, Paper and Pulp*
Pharmaceutical	*Processing, Cleaning*

S4 Overview of application sub-categories

		Environment	Agriculture	Domestic	Industry
Potable	Direct			Residential *(potable)*	
	Indirect	Groundwater *(potable)* Surface water *(potable)*			
Non-potable	Direct	Irrigation Surface water *(non-potable)*	Livestock	Residential *(non-potable)* Landscape *(unrestricted)* Recreation	
	Indirect	Groundwater *(non-potable)*	Crop irrigation *(edible)* Crop irrigation *(non-edible)* Frost protection	Commercial Landscape *(restricted)* Urban uses	Boiler feed water Cooling water Process water

Figure S4-1 Overview of water applications categories and sub-categories based on their (a) needed quality (potable or non-potable) and application type (direct or indirect) and (b) presence in the literature.

Table S4-1 Explanation of water use applications and examples of these applications.

Agriculture	
Crop irrigation (edible)	*Fiber Crops, Grains, Grapes, Lemon Trees, Mandarin Trees, Nectarines, Rice, Sugar, Vegetables*
Crop irrigation (non-edible)	*Cotton, Decorative Plants, Horticulture, Flowers, Nurseries, Trees*
Frost protection	*Edible crops, Non-edible crops*
Livestock	*Dairy Farming, Fisheries, Feedlots, Paddocks, Pastures*

Domestic	
Commercial	*Commercial Car washing, Laundry Services, Office Buildings*
Landscape (restricted)	*Cemeteries, Greenbelts, Non-Residential Golf Courses, And Industrial Landscaping*
Landscape (unrestricted)	*Athletic fields, Common areas, Fountains / Water Features, Gardens, Parks, Playgrounds, Public and Commercial Facilities, Residential Golf Courses, Residential Landscaping, Schools*
Recreation	*Artificial Snow Making, Swimming Pools, Recreational Lakes*
Residential (non-potable)	*Air Conditioning, Aquariums / Fishponds, Gardening, Laundry, Toilet Flushing*
Residential (potable)	*Bathing / Showering, Dishwashing, Sinks / Taps*
Urban	*Construction, Dust Control, Fire Protection, Road Cleaning / Maintenance, Sewer Flushing, Snow Melting, Transport Washing, Treatment Plants, Urban Cleaning*

Environment	
Groundwater (non-potable)	*Seawater intrusion protection*
Groundwater (potable)	*Replenishment*
Irrigation	*General irrigation, Forestry, Marsh enhancement, Riverbanks, Subsidence Control, Stream Augmentation, Wetlands*
Surface water (non-potable)	*Reservoir dilution, Surface water dilution*
Surface water (potable)	*Fisheries, Lakes, Stream flow augmentation, Water traps*

Industrial	
Boiler feed water	*Normal, High Pressure*
Cooling water	*Evaporative, Non-evaporative*
Process water	*Chemical Dilution, Cleaning and Washing, Construction, Dust Control, Fire Control / Suppression, Friction Reduction, Lubrication, Pollution Management*

S5 Overview of all identified criteria and their classifications

Table S5-1 Categorization of all technical criteria derived from the criteria literature review.

Infrastructure

Energy	*Facilities*	*Transport*	*Treatment*
Availability	Existing Infrastructure	Distance to Application	Post-treatment
Efficiency	Failure / Leakage	Distance to Source	Pre-treatment
Seasonal Demand	Feasibility / Viability	Distance to WWTP	Treatment Technologies
Total Demand	Flexibility / Upgradability	Elevation	
	Implementation Time	Existing Distribution Sys.	
	Lifetime / Longevity	Piping Risks	
	Maintenance Needs	Topography	
	Management Needs		
	Monitoring		
	Needed Infrastructure		
	Operability		
	Reliability		
	Resilience		
	Robustness		
	Storage Capacity		

Water

Demand	*Effluent*	*Influent*
Quality	Heavy Metals	Quality
Quantity	Ions	Quantity / Availability
Supply / Demand Rel.	Metrics & Char.	Reliability / Vulnerability
	Micropollutants	
	Pathogens	
	Quantity (Current)	
	Quantity (Expected)	
	Reliability	
	Storage Capacity	

Table S5-2 Categorization of all economic criteria derived from the criteria literature review.

Market considerations

Financing	*Factors*	*Risks*
Affordability	Cost Savings	Contamination Event
Financing Fees	Crop Yield	New Regulations
Financing Rate	Fertilizer Use	Public Relations
Funding Availability	Health Savings	
Internal Rate of Return	Potential Income	
Life Cycle Costs	Water Use	
Market		
Net Present Value		
Net Unit Cost		
Payback Period		
Profits		
Return on Investment		
Subsidies		

Implementation

Capital	*Operations & Maintenance*	*Transport*
Construction	Effluent cost	Disposal
Infrastructure / Equipment	Effluent price	Pumping
Land Value	Energy costs	Storage
Total Capital	Maintenance	Transport
	Operations	
	Overhead / Staffing / Labor	
	Replacements	
	Source cost	
	Taxes	
	Training	

Table S5-3 Categorization of all environmental criteria derived from the criteria literature review.

Existing Conditions

Existing Land Use	*Climate Type*
Flood mitigation	Saltwater Intrusion
Landscape	Water Scarcity
Soil composition	Water Security
Urbanization	Water Stress Index
	Water Supply Index

General

Climate	*Contaminants*	*Miscellaneous*
Environmental Impacts	Biogeochemical Impacts	Ecology Impacts
Global Warming Potential	Carbon Monoxide	Effect on Waste(water)
Greenhouse Gases	Chemical Requirements	Fertilizer red. / nutrient savings
Ozone Depletion Potential	Ecotoxicity	Footprint
	Nitrogen Oxide	
	Particulate Matter	
	Photo Chemical Oxidation	
	Sulphur Oxide	
	Volatile Organic Compounds	

Local

Plants	*Soil*	*Species*	*Water*
Impact to Wetlands	Abiotic Resources	Habitat Impact	Acidification
Quality	Biotic Resources	Health Impacts	Downstream Effects
Safety	Ecosystem		Eutrophication
Yield	Erosion		Water Quality Impact
	Heavy Metal Accumulation		Water Supply Impact
	Long-term Impacts		
	Quality		
	Scouring		

Table S5-4 Categorization of all social criteria derived from the criteria literature review.

Institutional

Legal	*Political*	*Stakeholders*
Institutional Framework	Economy	Acceptance
Institutional Support	Empowerment / Capacity	Agricultural Support
Liability / Risk	Existing Issues	Community Involvement
Regulations / Policies / Guidelines	Improvement Needs / Local Cond.	Hierarchy
Standards	Job Creation	Industrial Support
	Preferences / Agenda	Preferences / Agenda
	Risk	Staff Health Risk
	Socio-Economic Effects	Stakeholder Support
	Support	
	Sustainability	
	Urbanization	

Public

End Users	*General Public*
Availability	Construction Disruption
Color	Cultural Views
Convenience	Degree of Human Exposure
Cost impacts	Displacement
Effect on uses (cloth, machines, etc.)	Education
Health Risks	Application
Perception	Health Risk
Taste	Noise
Yuck factor	Odor
	Perception
	Risk Assessment
	Risk Control
	Support
	Traffic Disruption
	Trust
	Willingness

S6 Technical criteria related to source data and application standards

Table S6-1 Overview of all technical criteria related to source data and application standards as found through the literature review.

Metrics & Characteristics	Ions & Molecules	Heavy Metals	Pathogens	Micropollutants
Alkalinity ($CaCO_3$)	Aluminum (Al^{3+})	Antimony (Sb)	Bacteria	Antibiotics
Anionic detergents (ABS)	Ammonium (NH^{4+})	Arsenic (As)	E. coli	Pharmaceuticals
Basicity (pH)	Barium (Ba^{2+})	Cadmium (Cd)	Fecal Coliform (FC)	
Biological Oxygen Demand (BOD)	Beryllium (Be^{2+})	Chromium (Cr)	Giardia	
Chemical Oxygen Demand (COD)	Bicarbonate (HCO_3^-)	Cobalt (Co)	Intestinal Helminths	
Color	Boronic acid ($RB(OH)_2$)	Copper (Cu)	Parasites	
Dissolved Oxygen (DO)	Bromide (Br^-)	Iron (Fe)	Protozoa	
Electroconductivity (EC)	Calcium (Ca^{2+})	Lead (Pb)	Total Coliform (TC)	
Hardness ($CaCO_3$)	Carbonate (CO_3^{2-})	Manganese (Mn)	Viruses	
Odor	Chloride (Cl^-)	Mercury (Hg)		
Oil	Cyanide (CN^-)	Molybdenum (Mo)		
Sodium Adsorption Ratio (SAR)	Fluorine (F^-)	Nickel (Ni)		
Temperature (T)	Lithium (Li^+)	Selenium (Se)		
Total Dissolved Solids (TDS)	Magnesium (Mg_{2+})	Silver (Ag)		
Total Nitrogen (TN)	Nitrate ($NO_{3-}N$)	Vanadium (V)		
Total Organic Carbon (TOC)	Phenol (C_6H_6O)	Zinc (Zn)		
Total Phosphorous (TP)	Phosphate (PO_4^{3-})			
Total Suspended Solids (TSS)	Potassium (K^+)			
Turbidity (NTU)	Silicon Dioxide (SiO_2)			
	Sodium (Na^+)			
	Strontium (Sr^{2+})			
	Sulfate ($SO^{2-}{}_4$)			

Table S6-2 Overview of technical criteria present in the source data and application standards. Dark blue denotes criteria that occurs most in application standards. Dark green denotes criteria that occurs most in source data. The criteria are organized based on the difference between the application standards and source data.

Criteria	Presence in Source Data	Presence in End Use Stand.	Difference
FC	1%	37%	36%
E. coli	1%	25%	24%
Helminths	1%	22%	21%
TC	1%	15%	14%
NTU	18%	27%	8%
ABS	1%	6%	6%
Color	1%	6%	6%
Be^{2+}	1%	4%	3%
Se	1%	4%	3%
Li^{+}	1%	3%	2%
Bacteria	1%	3%	2%
As	3%	5%	2%
F^{-}	0%	2%	2%
Al^{3+}	3%	5%	2%
Odor	0%	1%	1%
SiO_2	3%	3%	1%
Co	3%	3%	1%
V	3%	3%	1%
Oil	4%	5%	1%
Hg	4%	5%	1%
TSS	58%	58%	1%
Br^{-}	0%	0%	0%
Giardia	0%	0%	0%
Sb	1%	1%	0%
$CaCO_3^{2}$	5%	5%	0%
BOD	51%	50%	-1%
Parasites	1%	0%	-1%
Protozoa	1%	0%	-1%
Viruses	1%	0%	-1%
Mo	5%	4%	-1%
Cr	6%	5%	-1%
T	3%	2%	-2%
Ag	3%	2%	-2%
Sr^{2+}	3%	0%	-3%
C_6H_6O	3%	1%	-3%
CN^{-}	4%	2%	-3%
Ba^{2+}	5%	2%	-3%
$CaCO_3$	4%	1%	-3%
NH_4^{+}	8%	5%	-3%
Cd	10%	6%	-4%
Ni	10%	6%	-4%
PO_4^{3-}	5%	0%	-5%
TOC	9%	4%	-5%
DO	20%	14%	-6%
Mn	8%	2%	-7%
Cu	13%	6%	-7%
SO^{2-}_4	18%	10%	-8%
Zn	18%	8%	-10%
Fe	22%	10%	-12%
CO_3^{2-}	13%	0%	-13%
HCO_3^{-}	18%	3%	-14%
$RB(OH)_2$	20%	4%	-16%
Pb	23%	6%	-16%
SAR	29%	13%	-16%
Mg^{2+}	27%	10%	-17%
Cl^{-}	31%	13%	-18%
TP	38%	19%	-19%
COD	38%	18%	-20%
TDS	29%	9%	-20%
Na^{+}	28%	3%	-24%
TN	43%	18%	-25%
Ca^{2+}	28%	1%	-27%
K^{+}	28%	0%	-28%
NO_3-N	38%	10%	-29%
pH	77%	41%	-36%
EC	53%	14%	-39%

S7 Systematic literature review results

Table S7-1 List of literature identified in the systematic literature review and selected for the review and analyses. The 'included' column refers to the final set of papers investigated.

Reference	Included	Reference	Included
Alizadeh et al. (2019)		Kwon et al. (2015)	
Al-Karaghouli et al. (2009)		La Cerva et al. (2019)	Yes
Aponte & Colón (2001)		Largier et al. (2017)	
Atlas & Suss (2019)		Lee et al. (2002)	Yes
Bawornruttanaboonya et al. (2015)		Li et al. (2013)	
Bitaw et al. (2016)		Liu & Wang (2017)	
Bladergroen & Linkov (2001)		Liu et al. (2017)	
Borges et al. (2009)		Liu et al. (2019)	
Brauns (2009)		McGovern et al. (2014)	
Brauns et al. (2009)		Mishchuk et al. (2001)	
Brauns et al. (2012)	Yes	Mitko & Turek (2014)	
Camacho et al. (2017)		Myint (2014)	
Campione et al. (2018)	Yes	Nakayama et al. (2017)	Yes
Campione et al. (2019)	Yes	Nayar et al. (2019)	
Catrini et al. (2017)		Nezungai & Majozi (2016)	Yes
Charcosset (2009)	Yes	Nikonenko et al. (2008)	
Chehayeb et al. (2017)	Yes	Nikonenko et al. (2014)	
Chehayeb et al. (2017)	Yes	Ortiz et al. (2005)	Yes
Chen et al. (2019)	Yes	Ortiz et al. (2006)	
Choi et al. (2019)		Ortiz et al. (2008)	
Dara et al. (2017)		Pellegrino et al. (2007)	
de Schepper et al. (2019)		Pérez-González et al. (2015)	
Demircioglu et al. (2003)		Pismenskiy et al. (2006)	
Ding et al. (2018)		Qasem et al. (2018)	Yes
Dydo (2012)		Qureshi & Zubair (2016)	
Dydo (2013)		Qureshi & Zubair (2018)	Yes
Fan & Yup (2019)		Ratanasanya et al. (2018)	
Farrell et al. (2017)		Ruiz et al. (2006)	
Fernandez-Gonzalez et al. (2017)		Ryabtsev et al. (2001)	
Fidaleo & Moresi (2005)		Ryabtsev et al. (2001)	Yes
Fidaleo & Moresi (2010)		Sadrzadeh et al. (2007)	Yes
Fidaleo & Moresi (2011)		Sadrzadeh et al. (2008)	
Fidaleo & Moresi (2013)		Saleem et al. (2017)	
Galama et al. (2014)		Scarazzato et al. (2018)	
Galvanin et al. (2016)		Shah et al. (2019)	
Ghassemi & Danesh (2013)		Siddiqui et al. (2016)	
Gómez-Coma et al. (2019)		Sistat et al. (2015)	
Gong et al. (2005)		Tado et al. (2016)	Yes
Grigorchuk et al. (2005)		Tanaka (2009)	Yes
Gurreri et al. (2017)	Yes	Tedesco et al. (2016)	Yes
Han et al. (2017)		Tedesco et al. (2017)	Yes
Honarparvar et al. (2019)	Yes	Tsiakis & Papageorgiou (2005)	Yes
Ibáñez et al. (2013)		Turek & Mitko (2014)	
Jalili et al. (2019)		Turek (2003)	Yes
Jiang et al. (2015)	Yes	Uche et al. (2013)	
Karimi & Ghassemi (2016)	Yes	Veza et al. (2001)	
Karimi et al. (2015)		Wang et al. (2014)	
Kim et al. (2011)	Yes	Welgemoed & Schutte (2005)	
Kim et al. (2012)		Woźniak & Prochaska (2014)	
Kim et al. (2017)		Wright & Winter (2019)	
Kodým et al. (2019)		Wright et al. (2018)	Yes
Kraaijeveld et al. (1995)	Yes	Zhao et al. (2017)	
Kürklü et al. (2017)		Zornitta & Ruotolo (2018)	
Kwak et al. (2013)		Zourmand et al. (2015)	Yes

Table S7-2 Summary of the final paper set and their reason for being included or excluded from the implementation portion of this research.

Publication	Summary	Transport Phenomena	Status	Notes
Campione et al. (2019)	Semi-empirical model for a multistage system with empirically fitted membrane parameters	Electromigration Diffusion Electroosmosis Osmosis	Included	Versatile model that also includes batch operation mode and is validated for a wide range of feed salinities (3,500 - 30,000 mg/L)
Gurreri et al. (2017)	Theoretical 2D model-based on the finite element method	Electromigration Diffusion Convection	Out of scope	Commercial software needed
Kraaijeveld et al. (1995)	Theoretical model-based on Maxwell-Stefan for feed water containing NaCl, HCl, and two amino acids	Electromigration Diffusion Electroosmosis Osmosis Convection	Out of scope	Model validated for only a limited feed salinity
Lee et al. (2002)	A lumped model to be used for preliminarily design	Electromigration	Out of scope	Model is less accurate with feed salinities over 5,000 mg/L
Nakayama et al. (2017)	Theoretical model for determining the stack voltage drop operating under the limiting current density	Electromigration Diffusion	Included	Continuous mode operating under the limiting current
Qasem et al. (2018)	Modification on the Lee model to include the Donnan potential	Electromigration	Out of scope	Model is limited to feed salinities under 9,000 mg/L
Qureshi & Zubair (2018)	Modification of the Lee model to include an empirically based conductivity equivalent	Electromigration	Out of scope	Model is limited to feed salinities under 9,000 mg/L
Tado et al. (2016)	Theoretical model for ion transport process analysis operating under the limiting current density.	Electromigration Diffusion Osmosis Convection	Out of scope	Model cannot be used to calculate the stack voltage drop
Tedesco et al. (2017)	2D model including water transport through the membrane for a wide range of feed salinities.	Electromigration Diffusion Electroosmosis Osmosis Convection	Included (comparison)	Validation included, but not for steady state.
Wright et al. (2018)	Semi-empirical model for slightly brackish water with empirically fitted membrane parameters	Electromigration Diffusion	Out of scope	Model is limited to concentrations up to 5,850 mg/L

S8 Campione et al. additional equations

S8.1 Ion flux

The conductive flux is viewed as the most dominant transport phenomena, occurring as a result of conduction and expressed as:

$$J_{cond}(x) = \frac{[\tau_{counter}^{CEM} - (1 - \tau_{counter}^{AEM})]i(x)}{F} \qquad \text{Equation S8-1}$$

where $\tau_{counter}^{AEM}$ and $\tau_{counter}^{CEM}$ are the transport numbers of the counter-ions inside the IEMs [151]. It should be noted that the non-ideal permselectivity of the membranes is included in the form of the $\tau_{counter}^{CEM}$ - (1 - $\tau_{counter}^{AEM}$).

The back-diffusive fluxes are caused by the concentration gradient at the membrane surfaces. This transport phenomena can be calculated through Fick's law written as:

$$J_{diff}^{IEM}(x) = -\frac{D_{IEM}}{\omega_{IEM}}\left(c_{conc}^{IEM}(x) - c_{dil}^{IEM}(x)\right) \qquad \text{Equation S8-2}$$

where J_{diff}^{IEM} is the diffusive flux for a given IEM, D_{IEM} is the diffusion coefficient of the solute for the IEM, ω_{IEM} is the membrane thickness, and c_{dil}^{IEM} and c_{conc}^{IEM} are the concentrations at the membrane interfaces in both the diluate and concentrate channels, respectively [151].

The salt concentration at the membrane surfaces (Equation S8-3 through Equation S8-6) are be obtained by applying the electro-neutrality condition in the polarization layer. In this way the concentration of positive ions is balanced by the concentration of negative ions. The concentrations at the membrane – solution interfaces can be calculated as:

$$c_{dil}^{AEM}(x) = c_{dil}(x) - \frac{i(x)(\tau^{AEM} - \tau_{-}^{sol})}{Fk_m} \qquad \text{Equation S8-3}$$

$$c_{dil}^{CEM}(x) = c_{dil}(x) - \frac{i(x)\left(\tau^{CEM} - \tau_{+}^{sol}\right)}{Fk_m} \qquad \text{Equation S8-4}$$

$$c_{conc}^{AEM}(x) = c_{conc}(x) + \frac{i(x)(\tau^{AEM} - \tau_{-}^{sol})}{Fk_m} \qquad \text{Equation S8-5}$$

$$c_{conc}^{CEM}(x) = c_{conc}(x) + \frac{i(x)\left(\tau^{CEM} - \tau_{+}^{sol}\right)}{Fk_m} \qquad \text{Equation S8-6}$$

where $c_{dil}(x)$ and $c_{conc}(x)$ are the concentrations in the bulk solution depending on the position along the ED channel, k_m is the mass transfer coefficient related to the Sherwood number which is a function of the Reynolds number. For more information on the calculation of the dimensionless number, see S13.4.

S8.2 Water transport

Osmosis occurs due to the osmotic pressure difference across the membrane and is expressed as:

$$q_{osm}^{IEM} = \lambda_w^{IEM}\left(\pi_{conc}^{IEM} - \pi_{dil}^{IEM}\right) \qquad \text{Equation S8-7}$$

where λ_w^{IEM} is the water permeability coefficient for a given IEM, and π_{dil}^{IEM} and π_{conc}^{IEM} are the osmotic pressure for the diluate and concentrate channels, respectively [151]. The osmotic pressure can be calculated using the van't Hoff equation, written as:

$$\pi_{chan}^{IEM} = \nu R_g T \varphi_{chan}^{IEM} c_{chan}^{IEM}(x) \qquad \text{Equation S8-8}$$

where ν is the van't Hoff coefficient [151].

Electroosmosis is caused by the friction between the water and ions. Electroosmosis can be calculated as:

$$q_{eosm}(x) = \frac{\tau^w M_w J_{total}(x)}{\rho_w} \qquad \text{Equation S8-9}$$

where τ^w is total water transport number, M_w is the molar mass of water, and ρ_w is the water density [151]. Though in theory the water transport number is specific to each ion (e.g. τ_{Na^+} = 6 and τ_{Cl^-} = 8), where it has been assumed that τ_{NaCl} = 7 [174].

S8.3 Resistance

The resistances across the membranes can be calculated as

$$R_{IEM}(x) = R_{IEM}^{HIGH} + \frac{a}{c_{dil}(x)^b} \qquad \text{Equation S8-10}$$

where R_{IEM}^{HIGH} is the resistance of membrane at the standard concentration of 0.5 M NaCl, and a and b are constants with values 7 x 10^{-3} and 1.25, respectively [290]. The resistances in the channel can be expressed as:

$$R_{chan}(x) = \frac{\zeta_{chan}\omega_{chan}}{\Lambda_{chan}(x)c_{chan}(x)} \qquad \text{Equation S8-11}$$

S8

where ζ_{chan} is the shadow factor, ω_{chan} is the channel thickness, and Λ_{chan} is the equivalent conductivity as calculated from the Islam et al. correlation [151], [173]. The shadow factor, which represents the increase in resistance due to a non-conductive spacer, can be expressed as $\frac{1}{\epsilon^2}$ where ϵ is the void fraction [291], [292].

The resistance of the boundary layer is represented as:

$$R_{bound} = \frac{0.31 t_{res,dil} \omega_{chan}}{L} + \frac{0.31 t_{res,conc} \omega_{chan}}{L} + 0.05 \quad \text{Equation S8-12}$$

where $t_{res,dil}$ and $t_{res,conc}$ is the residence time of the diluate and concentrate, respectively.

S8.4 Pressure drop in channels

This pressure drop can be calculated via:

$$\Delta p_{chan} = \frac{1}{2} f_{chan} L \frac{\rho_{chan} {u_{chan}^{sup}}^2}{d_{chan}^2} \quad \text{Equation S8-13}$$

where f_{chan} is the Darcy friction coefficient, ρ_{chan} is the density of the solution in the channel, and u_{chan}^{sup} is the superficial velocity in the channel. The superficial velocity is defined as:

$$u_{chan} = \frac{Q_{chan}(x)}{W\, \omega_{sp}} \quad \text{Equation S8-14}$$

where ω_{sp} is the spacer thickness.

S8.5 Coupling mass transfer to flow

The mass transfer coefficient can be calculated from the following relation:

$$k_m = \frac{\mathbb{Sh}\, D}{d_h} \quad \text{Equation S8-15}$$

where $\mathbb{Sh}$ is the Sherwood number and d_h is the hydraulic diameter.

The hydraulic diameter can be assumed to be equal to two times the thickness of spacer [151]:

$$d_h = 2\omega_{sp} \quad \text{Equation S8-16}$$

Another definition of the hydraulic diameter is presented by Pawlowski et al. which is:

$$d_h = \frac{4\epsilon}{\frac{2}{\omega_{sp}} + (1-\epsilon)\left(\frac{8}{\omega_{sp}}\right)} \qquad \text{Equation S8-17}$$

where the void fraction is defined as:

$$\epsilon = 1 - \frac{\pi d_f^2}{2 l_f \omega_{sp}} \qquad \text{Equation S8-18}$$

Where d_f and ℓ_f are the diameter and the length of the filament, respectively [149].

The Sherwood number can be obtained from CFD that enables to perform simulation of the mass transfer in ED channels with overlapped or woven spacers. These kind of simulations were carried out by Gurreri et al.. Woven spacers promote a higher Sherwood number that results in a better mass transfer and a lower shadow effect [294]. The obtained values of Sherwood number from CFD can be used in Equation S8-15 to determinate the mass transfer coefficient and the limiting current density defined as:

$$\epsilon = 1 - \frac{\pi d_f^2}{2 l_f \omega_{sp}} \qquad \text{Equation S8-19}$$

For the solution including only ion spices such as Na^+ and Cl^-, the limiting current is chosen based on the lower transport number in the solution. Therefore, in Equation S8-15 the transport number for Na+ in the solution is chosen since $\tau_+^{sol} < \tau_-^{sol}$ and $i_{lim} = i_{lim}^+$ [149].

It is worthwhile to underline that the diffusion coefficients of the ions in the solution are about 1,000 times lower than that in the membrane. Therefore, in the membrane the migration flux is much higher than the diffusive flux [295]. Additionally, the transport of counter-ions from the dilute to the concentrate compartment causes an increase in the resistance of electrolyte in the dilute part and decrease in the concentrate compartment. However, an increment in the resistance of the dilute solution is higher than a drop in the resistance of the concentrate solution. This phenomenon leads to higher energy consumption [295].

The Donnan potential is calculated at each membrane interface, for left- and right-hand side ($\Delta\varphi_{Don^L}$, $\Delta\varphi_{Don^R}$). The derivation procedure of the Donnan potential is expressed as:

$$\eta_{IEM}(x) = \frac{\alpha_{IEM}\left(R_g\,T\right)}{F} ln\left[\frac{\gamma_{conc}^{int,IEM}(x)c_{conc}^{int,IEM}}{\gamma_{dil}^{int,IEM}(x)c_{dil}^{int,IEM}}\right] \qquad \text{Equation S8-20}$$

where γ is the activity coefficient estimated from the Pitzer correlation. For a cell-pair voltage drop, the sum of Donnan potential at AEM and CEM interfaces is needed as shown in Equation S8 21.

$$\eta(x) = \eta_{CEM}(x) + \eta_{AEM}(x) \qquad \text{Equation S8-21}$$

S9 Doornbusch et al. inputs

Table S9-1 Feed water parameters used for Doornbusch et al. evaluation.

Variable	Value	Unit	Description
Inputs			
N_{sub}	100	-	Number of subcells
Feed water specifications			
c_{feed}	500	mg/L	Feed concentration
Λ_{chan}	126.5	S cm^2/mol	Islam: Equivalent conductance at infinite dilution
P_{feed}	1E5	Pa	Feed pressure
$\mathbb{Sh}$	10	-	Sherwood number
T_{feed}	298	K	Feed temperature
u_{chan}	0.01	m/s	Velocity of water in the channel

Table S9-2 Technology parameters used for Doornbusch et al. evaluation.

Variable	Value	Unit	Description
Membrane properties			
D_{IEM}	1E-12	m^2/s	Diffusion coefficient
D_{AEM}	2.00E-09	m^2/s	Diffusion coefficient for AEM
D_{CEM}	1.30E-09	m^2/s	Diffusion coefficient for CEM
ω_{AEM}	0.000146	m	Membrane thickness AEM
ω_{CEM}	0.000155	m	Membrane thickness CEM
λ_w^{AEM}	2.22E-14	m^3/Pa s m^2	Water permeability AEM
λ_w^{CEM}	2.22E-14	m^3/Pa s m^2	Water permeability CEM
α_{AEM}	0.96	-	Permeate selectivity AEM
α_{CEM}	0.976	-	Permeate selectivity CEM
$R_{0,AEM}$	0.000129	Ω m^2	Membrane resistance AEM
$R_{0,CEM}$	0.000202	Ω m^2	Membrane resistance CEM
Spacer properties			
ω_{sp}	0.000155	m	Spacer thickness
ϵ	0.79	%	Void fraction
ED stack properties			
W	0.1	m	Channel thickness
L	0.1	m	Channel length
l	20	year	Lifetime of technology
N_{cp}	10	-	Number of cell-pairs
N_{stack}	4	-	Number of stacks
Other properties			
ɑ	0.007	-	Constant for resistance calculations
ɓ	1.25	-	Constant for resistance calculations
$i_{y,0}$	0	A/m^2	Initial ionic density
R_0	0	Ω m^2	Initial membrane resistance
D_e	1.575E-09	m^2/s	Effective diffusion coefficient
ξ	0.000015	-	Empirical coefficient for mechanical dispersion

S9

S10 Tedesco et al. inputs

Table S10-1 Feed water parameters used for Tedesco et al. evaluation.

Variable	Value	Unit	Description
Inputs			
N_{sub}	100	-	Number of subcells
Feed water specifications			
c_{feed}	500	mg/L	Feed concentration
Λ_{chan}	126.5	S cm^2/mol	Islam: Equivalent conductance at infinite dilution
P_{feed}	1E5	Pa	Feed pressure
$\mathbb{Sh}$	10	-	Sherwood number
T_{feed}	298	K	Feed temperature
u_{chan}	6.67E-08	m/s	Velocity of water in the channel

Table S10-2 Technology parameters used for Tedesco et al. evaluation.

Variable	Value	Unit	Description
Membrane properties			
D_{IEM}	1E-12	m^2/s	Diffusion coefficient
D_{AEM}	1E-10	m^2/s	Diffusion coefficient for AEM
D_{CEM}	1E-12	m^2/s	Diffusion coefficient for CEM
ω_{AEM}	0.00008	m	Membrane thickness AEM
ω_{CEM}	0.00008	m	Membrane thickness CEM
λ_w^{AEM}	2.78E-13	m^3/Pa s m^2	Water permeability AEM
λ_w^{CEM}	2.78E-13	m^3/Pa s m^2	Water permeability CEM
α_{AEM}	0.85	-	Permeate selectivity AEM
α_{CEM}	0.94	-	Permeate selectivity CEM
$R_{0,AEM}$	0.00008	Ω m^2	Membrane resistance AEM
$R_{0,CEM}$	0.00012	Ω m^2	Membrane resistance CEM
Spacer properties			
ω_{sp}	0.0002	m	Spacer thickness
ϵ	0.77	%	Void fraction
ED stack properties			
W	0.1	m	Channel thickness
L	0.1	m	Channel length
l	20	year	Lifetime of technology
N_{cp}	10	-	Number of cell-pairs
N_{stack}	4	-	Number of stacks
V_{cp}	0.3	V	Cell-pair voltage
Other properties			
a	0.007	-	Constant for resistance calculations
b	1.25	-	Constant for resistance calculations
$i_{y,0}$	0	A/m^2	Initial ionic density
R_0	0	Ω m^2	Initial membrane resistance
D_e	1.575E-09	m^2/s	Effective diffusion coefficient
ξ	0.000015	-	Empirical coefficient for mechanical dispersion

S11 Campione et al. model results with voltage as input

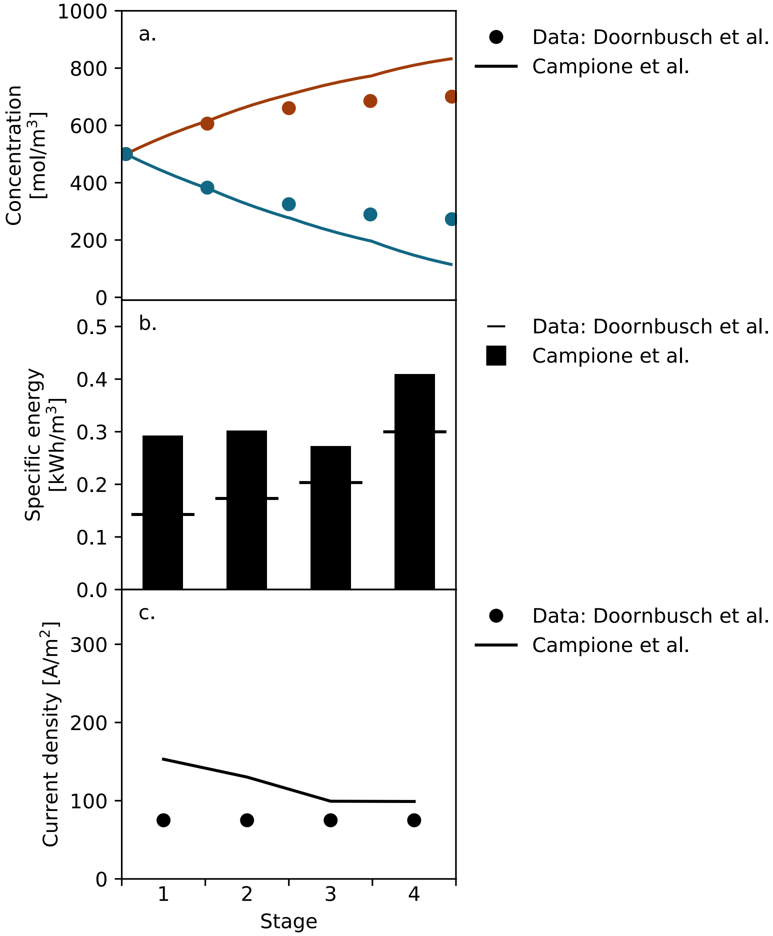


Figure S11-1 Concentration, specific energy, and cell-pair voltage results for the voltage-based Campione et al. model as compared to the Doornbusch et al. experimental outputs.

S12 Brackish water reverse osmosis evaluation method

S12.1 Technology parameters

Table S12-1 Technology parameters used for the BWRO evaluation [297].

BW30XFR-400/34i technology parameters				
General	*Min*	*Max*	**Impact factors**	
Driving force: P_{app}	500 kPa	4,000 kPa	Capital: UPC coefficient b	6,756.50
Variable A: δ	25%	75%	Capital: UPC coefficient m	-0.22
			CO_2 conversion factor	0.62 kg/m^3
General performance			O&M: UPC coefficient b	2.31
Availability	90%		O&M: UPC coefficient m	-0.26
Technology life-time	10 years		O&M: Share general	50%
Feed limits	*Min*	*Max*	**Technology-specific parameters**	
Bicarbonate	- mg/L	- mg/L	Unit area	37 m^2
Calcium	- mg/L	- mg/L	Pump efficiency	80%
Chloride	- mg/L	- mg/L	Average permeate flux	0.08 m^3/hour m^2
Flowrate	- m3/hour	- m^3/hour	Product pressure	100 kPa
Iron	0 mg/L	35,000 mg/L	Membrane unit cost	1000 $US
Magnesium	mg/L	mg/L	Osmotic pressure conversion factor	1 kPa/mg/L
Pressure	100 kPa	4,000 kPa		
Salinity	0 mg/L	16,025.64 mg/L		
Temperature	0°C	45°C		
TOC	0 mg/L	35,000 mg/L		
Test conditions				
Feed salinity	2,000 mg/L			
Flowrate	1.79 m^3/hour			
Pressure	15.50 Pa			
Product salinity	7 mg/L			
Recovery ratio	15%			
TDS removal rate	99.7%			
Temperature	25°C			
TOC removal rate	66%			

S12.2 Technology evaluation method

BWRO is one of the most common and fastest growing desalination technologies in the world [27], [298]. Its benefits are a small physical foot print, modular design, automated control, and relatively low cost [27], [30], [31]. Since this technology is well researched, there are abundant amounts of literature on the topic of BWRO modelling. However, many of these evaluations are either too detailed for the scope of the DESALT model [57], [200], [299] or were not in a format that could be easily included in the DESALT model [201], [300]–[305]. As a result, it was necessary to develop a custom evaluation method.

The BWRO evaluation method was adapted from existing models where the given parameters determine the required membrane area [31], [306], [307]. In this approach, the primary driving force is the hydraulic pressure while the recovery ratio operates as a secondary variable.

To begin, the product water flowrate (Q_{prod}) is determined through its direct relation to both the recovery ratio (δ) and the feed water flowrate (Q_{feed}) [306]–[308].

$$Q_{prod} = \delta Q_{feed} \qquad \text{Equation S12-1}$$

The removal rate of the system ($\mathcal{R}_{sys}$) is also directly related to δ [307]. $\mathcal{R}_{sys}$ is typically found in BWRO data sheets, however, this value is only valid under the specified test conditions [307]. It is therefore necessary to use the test conditions in combination with Equation S12-2 to determine the removal rate of the membrane ($\mathcal{R}_{mem}$). Equation S12-2 is then reapplied using the given operating conditions to determine the actual $\mathcal{R}_{sys}$.

$$\mathcal{R}_{sys} = 1 - \frac{1 - (1 - \delta)^{1-\mathcal{R}_{mem}}}{\delta} \qquad \text{Equation S12-2}$$

The $\mathcal{R}_{sys}$ under the given operating conditions is then used to determine the concentration in the product water (c_{prod}) based on the feed water concentration (c_{feed}) [154], [307]. Note that this method is used for all TDS components listed in Table 4.2. Additionally, the same methodology is used for TOC, however, the corresponding $\mathcal{R}_{sys}$ and $\mathcal{R}_{mem}$ need to be used.

$$c_{prod} = (1 - \mathcal{R}_{sys})c_{feed} \qquad \text{Equation S12-3}$$

As stated previously, δ is treated as a secondary variable thus it is a given value per evaluation. With this approach, Q_{prod} remains constant in the evaluation. However, the transport of water across the membrane per area of membrane (i.e. the average permeate flux) is not fixed since it is directly related to the applied pressure and feed water temperature [154], [200], [309]. These are reflected in the calculation of the average permeate flux (J_{ave}) through the water permeability coefficient (λ_w), the net driving pressure (NDP) as explained in S12.3, and the temperature correction factor (TCF) as explained in S12.4.

$$J_{ave} = \lambda_w \times NDP \times TCF \qquad \text{Equation S12-4}$$

Next, a mass balance approach is applied which is based on dividing the parallel flow of water along the membrane into sub-sections. These sub-sections are then used for mass balances of both the flowrate and salt flux. The flowrate mass balance states that the amount of water crossing the membrane for a given subsection is based on both J_{ave} and the surface area of the membrane subsection (A_{mem}).

$$\frac{dQ}{dx} = -J_{ave}A_{mem} \qquad \text{Equation S12-5}$$

The salt flux mass balance follows a similar relation in which the concertation of salt entering the subsection ($c_{conc,x}$) in combination with the flowrate relation (Equation S12-5) is directly related to the concentration of the product stream at given point x ($c_{prod,x}$). It should be noted that for the purposes of the mass balance, the concentration of salt entering the first subsection ($c_{conc,1}$) is equal to the feed concentration entering the BWRO system, while the output from the first subsection would be the input to the next subsection.

$$\frac{d\left(Qc_{conc,x}\right)}{dx} = -J_{ave}A_{mem}c_{prod,x} \qquad \text{Equation S12-6}$$

S12

The equation for the required membrane area (A_{req}) is then developed through the derivation of both Equation S12-5 and Equation S12-6. This equation is then expanded to show the correlation between A_{req} and TCF, applied pressure (ΔP), osmotic pressure

(π_{feed}), feed water conditions, and the technology parameters. The equation is evaluated over the length of channel from the input ($feed$) to the output (con)

$$A_{req} = \frac{1}{-\lambda_w TCF} \int_{Q_{feed}}^{Q_{conc}} \frac{1}{\Delta P - \mathcal{R}_{mem} \pi_{feed} \left(\frac{Q_{feed}}{Q_{conc,x}} \right)^{\mathcal{R}_{mem}}} dQ \quad \text{Equation S12-7}$$

The installed capacity ($Q_{installed}$) is then determined based on the number of units required and the test conditions. The number of units are determined by dividing A_{req} by the area for one membrane as applied in testing (A_{test}). This ratio is rounded up as it is assumed that only whole membranes are to be installed. This is then multiplied by the test installed capacity (Q_{test}) to arrive at $Q_{installed}$.

$$Q_{installed} = Q_{test} \left\lceil \frac{A_{req}}{A_{test}} \right\rceil \quad \text{Equation S12-8}$$

BWRO energy use is assumed to be only the electrical energy required for the hydraulic pump. Therefore, the total energy use per hour ($E_{total,hour}$) is simplified to the pumping power which is based on the needed pump pressure (P_{pump}), feed flowrate per second ($Q_{feed,sec}$), and pump efficiency ($\varkappa_{pump}$: 80%) [193], [310], [311].

$$E_{total,hour} = \frac{\Delta P_{pump} Q_{feed,sec}}{\varkappa_{pump}} \quad \text{Equation S12-9}$$

Abdulbaki et al. developed a cost function based on technology type and plant capacity [114]. This method breaks down the UPC into capital and yearly operations and maintenance (O&M) [114]. The capital UPC correlation determined by Abdulbaki et al. (first term in Equation S12 10) matches with other publications such as Wittholz et al. who found that the larger the installation capacity, the smaller the UPC [312]. The total capital costs ($\mathbb{C}_{Cap}$) are then calculated using this correlation with the installed capacity ($Q_{installed,day}$) and the expected daily production of water ($Q_{prod,day}$). Note that the given constants ($\mathcal{B}_{cap}$ and $\mathcal{M}_{cap}$) are presented in Abdulbaki et al. and are also given in S12.2.

$$\mathbb{C}_{Cap} = \left(\mathcal{B}_{cap} Q_{installed}{}^{\mathcal{M}_{cap}} \right) Q_{prod,day} \quad \text{Equation S12-10}$$

The annual O&M costs ($\mathbb{C}_{OM,pump}$) must be broken out to account for changes in operating conditions (i.e. energy use) and site-specific information (i.e. cost of energy).

Three aspects of O&M costs were identified. Specifically, membrane replacement costs ($\mathbb{C}_{OM,mem}$), pumping costs ($\mathbb{C}_{OM,pump}$), and general costs ($\mathbb{C}_{OM,gen}$). The method for calculating each is presented in S12.5.

$$\mathbb{C}_{OM,year} = \mathbb{C}_{OM,mem} + \mathbb{C}_{OM,pump} + \mathbb{C}_{OM,gen} \qquad \text{Equation S12-11}$$

The total adjusted UPC (UPC_{adj}) is then determined using the aforementioned $\mathbb{C}_{Cap}$ and $\mathbb{C}_{OM,year}$ as well as the annual product water flowrate ($Q_{prod,year}$), plant availability ($\mathbb{A}$: 90%), and expected lifetime (l) [114], [312]. In this case the UPC is defined as the total cost per cubic meter produced.

$$UPC_{adj} = \frac{\mathbb{C}_{Cap}/_{l} + \mathbb{C}_{OM,year}}{Q_{prod,year}\mathbb{A}} \qquad \text{Equation S12-12}$$

The final step of the BWRO evaluation method is calculating the CO_2-equivalent (CO_2eq). This is achieved using Tarnacki et al.'s conversation rate method where it was found that 0.624 kg of CO_2eq is created for every cubic meter of product water produced by BWRO [313]. The total CO_2eq of the system over its lifetime is then based on the given conversion factor ($\mathbb{C}_{CO_2}$: 0.624 kg/m^3) and $Q_{prod,year}$.

$$CO_2eq = \mathbb{C}_{CO_2} Q_{prod,year} l \qquad \text{Equation S12-13}$$

S12.3 Net driving pressure

The net driving pressure (NDP) is the driving force behind the transport of water and salt through the membrane [154], [200]. The NDP is the difference of the applied pressure difference (ΔP) and the osmotic pressure difference ($\Delta\pi$) [154], [200], [307]. Though the NDP varies across the length of the membrane, the aim of the evaluation method is the overall result. Therefore Equation S12-14 is based on the averages over the length of the channel.

$$NDP = \Delta P - \Delta\pi = P_{feed} - P_{prod} - \pi_{feed} + \pi_{prod} \qquad \text{Equation S12-14}$$

There are three methods for calculating π: physics-based, general relation, and hybrid. The physics-based equation is derived from the van 't Hoff equation based on the gas constant (R_g), temperature (T), and the sum of the molarities of ions and non-ionic compounds (m_i) [154], [200].

$$\pi = R_g \mathrm{T} \sum m_i \qquad \text{Equation S12-15}$$

The general relation is that π will increase by 77 kPa for every 1,000 mg/L increase in salt concentration (β:0.077 kPa L / mg) [154], [200]. The hybrid approach uses a similar relation, however, the conversion factor (β) is non-fixed and instead defined by the feed water composition [154], [200].

$$\pi \approx \beta c \qquad \text{Equation S12-16}$$

In keeping with the reasonable complexity guideline from Table 4.1, the hybrid approach is used. In this research, β is determined using the DuPont Manual for the Calculation of Osmotic Pressure which includes several inputs including (but not limited to) pH, salinity, and temperature.

S12.4 Temperature correction factor

The effect of the feed water temperature is represented as the TCF [200], [307], [314]. The general relation accepted in literature is that for every degree above the standard temperature (T_{std}: 20°C) the TCF will increase by 3% [154], [309], [315]. This is represented in Equation S12-17, where α is between 2,500 - 3,000 [154], [309], [315]. Through empirical based testing, Dow Chemical Company determined more specific values for α based on T being above T_{std} (α: 2640) or below (α: 3020) [316].

$$TCF = exp\left[\alpha\left(\frac{1}{T_{std}} - \frac{1}{T}\right)\right] \qquad \text{Equation S12-17}$$

S12.5 Operation and maintenance costs

$\mathbb{C}_{OM,mem}$ is determined by the number of membranes (n), their expected lifetime (l_{mem}) vs. the plant lifetime (l), and the cost of the membranes (c_{mem}).

$$\mathbb{C}_{OM,mem} = \frac{n l_{mem} \mathrm{c}_{mem}}{l} \qquad \text{Equation S12-18}$$

$\mathbb{C}_{OM,pump}$ are based on the local cost of electricity (c_{energy}) and the amount of energy consumed (E).

$$\mathbb{C}_{OM,pump} = \mathrm{c}_{energy} E \qquad \text{Equation S12-19}$$

$\mathbb{C}_{OM,gen}$ is based on the relations presented in Abdulbaki et al. (first term in Equation S12-20), the product flowrate per day ($Q_{prod,day}$), and a general O&M conversion factor ($\mathfrak{c}_{OM,gen}$) [114], [312], [317]. This conversion factor is the percentage of O&M costs that do not include membrane replacement or energy consumption. Per existing literature this value is estimated to be 50% [26], [312], [317], [318].

$$\mathbb{C}_{OM,gen} = Q_{prod,day}\mathfrak{c}_{OM,gen}\mathcal{B}_{OM}Q_{installed,day}{}^{\mathcal{M}_{OM}} \quad \text{Equation S12-20}$$

S12.6 Validation

The technical performance of the BWRO evaluation method was compared to the expected general relations found in the support documentation for the Reverse Osmosis System Analysis software (ROSA) [311]. Per ROSA documentation, it is expected that the removal rate will decrease rapidly as the recovery ratio approaches 100%, and the average permeate flux has a linear relation with the feed pressure. As can be seen in Figure S12-1a, both general relations occur through the BWRO evaluation method.

The accuracy of the BWRO evaluation method was first tested by comparing the specific energy performance to Sarai Atab et al. [30]. This was done by first applying the same inputs found in Sarai Atab et al. and then comparing. As shown in in Figure S12-1b, the results of the evaluation method are similar with that in Sarai Atab et al. The same method was used for evaluating the accuracy of the UPC as compared to Wittholz et al. [312]. In this case, Wittholz et al. only provided an average non-pressure dependent cost curve. As can be seen from Figure S12-1c, this evaluation method is more accurate at higher product flowrates, thus this methodology should not be relied upon at lower product flowrates with higher applied pressures.

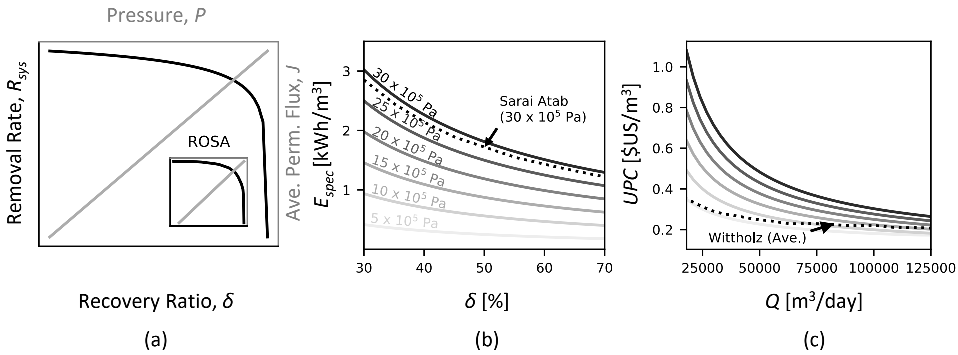


Figure S12-1 Verification of the BWRO evaluation method: (a) general performance for the removal rate and average permeate flux as compared to ROSA's expected general relations [311]; (b) specific energy performance of the BWRO evaluation method based on the recovery ratio and applied pressure and compared to Sarai Atab et al. results which operated at 30E5 Pa [30]; and (c) cost performance of the BWRO evaluation method based on the product flowrate and applied pressure as compared to the average cost curve presented by Wittholz et al. [312]

S12

S13 Electrodialysis evaluation method

S13.1 Electrodialysis technology parameters

Table S13-1 Technology parameters used for the ED evaluation.

ED technology parameters				
General	*Min*	*Max*	**Impact factors**	
Driving force: V_{cp}	0.05V	0.20V	Capital: UPC coefficient b	6,772.04
Variable A: δ	50%	80%	Capital: UPC coefficient m	-0.22
Variable B: N_{cp}	500	250,000	CO_2 conversion factor	0.41 kg/m³
			O&M: UPC coefficient b	2.41
General performance			O&M: UPC coefficient m	-0.26
Availability	90%		O&M: Share general	50%
Technology life-time	20 years			
			Technology-specific parameters	
Feed limits	*Min*	*Max*	Channel length	0.43 m
Bicarbonate	- mg/L	- mg/L	Channel thickness	0.1 m
Calcium	- mg/L	- mg/L	Membrane diffusivity	2.00E-12 m²/s
Chloride	- mg/L	- mg/L	Membrane height	1.30E-4 m
Flowrate	- m³/hour	- m³/hour	No. cell-pairs	500
Iron	0 mg/L	35,000 mg/L	Permselectivity (AEM)	0.969
Magnesium	- mg/L	- mg/L	Permselectivity (CEM)	0.975
Pressure	100 kPa	200 kPa	Resistance (AEM)	1.77E-4 Ω m²
Salinity	0 mg/L	16,000 mg/L	Resistance (CEM)	1.89E-4 Ω m²
Temperature	0°C	45°C	Shadow effect (x)	1.471
TOC	0 mg/L	35,000 mg/L	Shadow effect (y)	1.212
			Spacer height	1.55E-4 m
Test conditions			Void fraction	0.83%
Feed salinity	- mg/L		Water permeability (AEM)	1.75E-14 m³/Pa s m²
Flowrate	- m³/hour		Water permeability (CEM)	2.16E-14 m³/Pa s m²
Pressure	- Pa			
Product salinity	- mg/L			
Recovery ratio	- %			
TDS removal rate	- %			
Temperature	- °C			
TOC removal rate	- %			

S13.2 Technology evaluation method: Electrodialysis

The ED model used in the DESALT model is based on the model developed in Chapter 3. This was based on a semi-empirical approach which was to be the best model for a systems-level application. The ED evaluation method developed uses the applied cell-pair voltage (V_{cp}) as the primary driving force. This is because V_{cp} is what forces ions in the diluate channels to move through the alternately charged membranes into concentrate channels [319]. Additionally, two secondary variables were included: the recovery ratio (δ) and the number of cell-pairs (N_{cp}).

This evaluation method is based on two transfer processes: salt transport and water transport. Salt transport ($J_{total,x}$), also known as the total salt flux, is the sum of the transport methods for each subcell located at point x and is calculated based on Equation 3.8. The total water transport ($q_{total,x}$), also known as the total water flux, is also calculated as the sum of the transport methods for each subcell and is calculated based on Equation 3.9.

The mass balance for the bulk salt concentration is developed for both the diluate channel (Equation 3.4) and concentrate channel (Equation 3.5). The mass balance for the flowrate distributions is also developed for both the diluate channel (Equation 3.6) and the concentrate channel (Equation 3.7) Using the feed water conditions as the initial conditions, the system of ordinary differential equations are solved using a Python solver (ODIENT). The output of the derivation is the concentration and flowrate for both channels at the outlet.

The recovery ratio directly relates to the diluate flowrate (Q_{dil}) and the concentrate flowrate (Q_{conc}) as presented in Equation S13-1 and Equation S13-2, respectively. The recovery ratio is reverse calculated from Equation S13-1 and the removal rate of the system ($\mathcal{R}_{sys}$) is calculated based on Equation S13-3.

$$Q_{dil} = \delta Q_{feed} \quad \text{Equation S13-1}$$

$$Q_{conc} = (1 - \delta) Q_{feed} \quad \text{Equation S13-2}$$

$$\mathcal{R}_{sys} = \frac{c_{conc}}{c_{feed}} \quad \text{Equation S13-3}$$

The ED stack is viewed as an analogous DC circuit where the total cell voltage (V_{total}) is calculated based on Equation 3.14. This is done using the potential across each membrane in the cell-pair ($V_{cp,y}$: Equation S13-11) and the potential across the channel which is the product of the current density ($i_{x,y}$: Equation S13 13) and the total resistance ($R_{total,x}$: Equation 3.11). The total current (I_{total}) is then calculated based on Equation 3.13.

In this evaluation, the total energy (E_{total}) used is comprised of two components: the energy used in the ED process and the energy used to pump the water through the channels. Note that the energy for the electrode reactions is neglected. E_{total} is calculated based on a modified Equation 3.15 to include the pump efficiency as presented in Equation 3.14.

$$E_{total} = V_{total} I_{total} + \frac{\Delta P Q_{feed,sec}}{\varkappa_{pump}} \qquad \text{Equation S13-4}$$

To keep the cost calculation for ED consistent with BWRO, the capital costs ($\mathbb{C}_{Cap}$) are calculated based on Equation S12-10. Though Abdulbaki et al. provides relations and constants ($\mathcal{B}_{cap}$ and $\mathcal{M}_{cap}$) for multiple technologies, ED was not included in their results [114]. Therefore, constant values for ED were derived from the data presented in Wittholz et al. so that they could be applied in the same format as Abdulbaki et al. (see S12.2). The O&M costs are calculated based on the information presented in S13.11. Once the annual O&M costs are found, the adjusted UPC (UPC_{adj}) is determined through Equation S12-12.

The CO_2eq for ED is calculated using Equation S12-13 with a conversion factor of 0.41 kg of CO_2 per cubic meter of product water. This was determined through the values presented in Raluy et al. and extrapolated from the findings in Youssef et al. [222], [320].

S13.3 Salt flux across membrane

Since the conductive flux (J_{cond}) is the main salt transport mechanism in ED, it is calculated using Equation S8-1 [151]. Further the back-diffusion salt transport (J_{diff}^{IEM}) is calculated via Equation S8-2 and the salt concentrations (c_{chan}^{IEM}) are calculated using Equation S8-3 through Equation S8-6

S13.4 Dimensionless numbers

Dimensionless numbers are used to describe the properties and functioning's of the water flow through the channels. Beginning with the Reynolds number ($\mathbb{Re}$) which helps determine if the flow of water is laminar or turbulent. Note that this equation assumes that the thickness of the stack is much larger than the height / space between the membranes. This is based on the density (ρ), velocity (u), height of the channel (h), and the dynamic viscosity (v).

$$\mathbb{Re} = \frac{2\rho u h}{v} \qquad \text{Equation S13-5}$$

The viscosity is determined using the flowrate (Q) and the cell-pair dimensions (W & h) and number (N_{cp}) [167].

$$v = \frac{N_{cp} h W}{Q} \qquad \text{Equation S13-6}$$

The Schmidt number ($\mathbb{Sc}$) is the ratio of the viscosity to the density and diffusivity (D). The general relation is the relative thickness of the hydrodynamic layer and mass transfer boundary layer.

$$\mathbb{Sc} = \frac{v}{\rho D} \qquad \text{Equation S13-7}$$

These two dimensionless numbers are then used for calculated the Sherwood number ($\mathbb{Sh}$). It is the ratio of the convective mass transfer coefficient (k_m) and effective diameter (d_e) to rate of diffusive mass transport (D).

$$\mathbb{Sh} = \frac{k_m d_e}{D} = \frac{1}{4}\mathbb{Re}^{\frac{1}{2}}\mathbb{Sc}^{\frac{1}{3}} \qquad \text{Equation S13-8}$$

These dimensionless numbers are then used to determine k_m based on Equation S8-15.

S13.5 Water flux across membrane

Water transport over the membrane (q_{osm}^{IEM}) is calculated based on Equation S8-7. Additionally, water transport also occurs as a result of water being dragged by ions across the membrane (electroosmosis). The water flux due to electroosmosis (q_{eosm}) is calculated based on Equation S8-9.

S13.6 Osmotic pressure using Pitzer's correlation

The osmotic pressure (π_{chan}^{IEM}) is calculated based on Equation S8-8. The osmotic coefficients (φ) can be estimated by using Pitzer's correlation presented below.

$$\varphi - 1 = -A_1 \frac{\sqrt{m}}{1 + b'\sqrt{m}} + mB^{\varphi} + m^2 C^{\varphi} \qquad \text{Equation S13-9}$$

$$B^{\varphi} = \beta^{(0)} + \beta^{(1)} e^{-\alpha\sqrt{m}} \qquad \text{Equation S13-10}$$

A_1 is the Debye-Huckel constant (0.3915 at 25°C), b' is 1.2, m is the molarity of the electrolyte, and α is the fixed constant (2 $kg^{0.5}/mol^{0.5}$). Meanwhile, the nature of the electrolyte is represented in $\beta^{(0)}$, $\beta^{(1)}$, and C^{φ} which are 0.06743, 0.3301 and 0.00263, respectively [296].

S13.7 Electrical potential across the membrane pair

The electrical potential across each membrane pair ($V_{cp,y}$) is seen as the sum of potential across each membrane (V_y^{IEM}) [149].

$$V_{cp,y} = V_y^{AEM} + V_y^{CEM} \qquad \text{Equation S13-11}$$

The potentials are determined based on the activity coefficient of the solution, transport numbers of the counter-ions, and the concentrations [149].

$$V_y^{IEM} = \frac{(2\tau^{IEM} - 1)R_g T}{F} \log\left(\frac{\gamma_c c_{c,y}^{IEM}}{\gamma_d c_{d,y}^{IEM}}\right) \qquad \text{Equation S13-12}$$

S13.8 Current density

As stated in Campione et al., the relation between the current density ($i_{x,y}$) and the cell-pair voltage (V_{cp}) is crucial to the evaluation process [151]. The relation is stated to be that $i_{x,y}$ is equal to V_{cp} minus the non-ohmic voltage drop ($V_{drop,x}$ see Campione et al., Page 83) divided by the total resistance (R_{total}).

$$i_{x,y} = \frac{V_{cp} - V_{drop,x}}{R_{total}} \qquad \text{Equation S13-13}$$

S13.9 Total area resistance

The total area resistance is defined as the sum of the resistances across each channel and across each membrane (Equation 3.11) [151]. The resistance of the membrane (R_x^{IEM}) is calculated based on Equation S8-10. The resistance across each channel (R_{chan}) is calculated based on Equation S8-11. The resistance of the boundary layer (R_{bound}) is calculated based on Equation S8-12

S13.10 Islam's correlation

Islam's correlation (Equation S13-14) estimates the equivalent conductivity based on the molar concentration, electrolyte temperature and a series of constants as presented in Equation S13-15 through Equation S13-18 [173].

$$\Lambda_x = \left(\Lambda_o - \frac{B_1'(c)\sqrt{c}}{1 + B'(c)a\sqrt{c}}\right)\left(1 - \frac{B_2'(c)\sqrt{c}}{1 + B'(c)a\sqrt{c}}F'(c)\right) \qquad \text{Equation S13-14}$$

$$B'(c) = \frac{50.2910^8}{\sqrt{\varepsilon T}} \qquad \text{Equation S13-15}$$

$$B_1'(c) = \frac{82.50}{\eta\sqrt{\varepsilon T}} \qquad \text{Equation S13-16}$$

$$B_2'(c) = \frac{8.20410^5}{(\varepsilon T)^{2/3}} \qquad \text{Equation S13-17}$$

$$F'(c) = \frac{e^{0.2929B'\sqrt{a}} - 1}{0.2929B'a\sqrt{c}} \qquad \text{Equation S13-18}$$

In Islam's correlation the viscosity (Equation S13-19) and dielectric constant (Equation S13-20) depend on the salt concentration [321].

$$\eta = \eta_0\,(1 + 0.0061\,\sqrt{c} + 0.078\,c + 0.013\,c^2) \qquad \text{Equation S13-19}$$

$$\varepsilon = \varepsilon_0 - 15.2\,c + 3.64\,c^2 \qquad \text{Equation S13-20}$$

S13.11 Operation and maintenance costs

Since ED is a newer technology, there is less data available to accurately model its costs. As such, several approximations were applied to conform the available data to the evaluation process. Extreme caution should be taken when considering the ED cost results. The membrane replacement cost ($\mathbb{C}_{OM,mem}$) is determined by the number of cell-pairs (N_{cp}), cell-pair membrane area (A_{cp}), their expected lifetime (l_{mem}) vs. the plant life time (l), and the cost per membrane area ($\mathfrak{c}_{mem}$).

$$\mathbb{C}_{OM,mem} = N_{cp}\mathrm{A}_{cp}\frac{l_{mem}}{l}\mathfrak{c}_{mem} \qquad \text{Equation S13-21}$$

S13

The energy costs ($\mathbb{C}_{OM,elec}$) are calculated based on the local cost of electricity ($\mathfrak{c}_{energy}$) and the amount of energy consumed (E_{total}).

$$\mathbb{C}_{OM,elec} = \mathfrak{c}_{energy} E_{total}$$ Equation S13-22

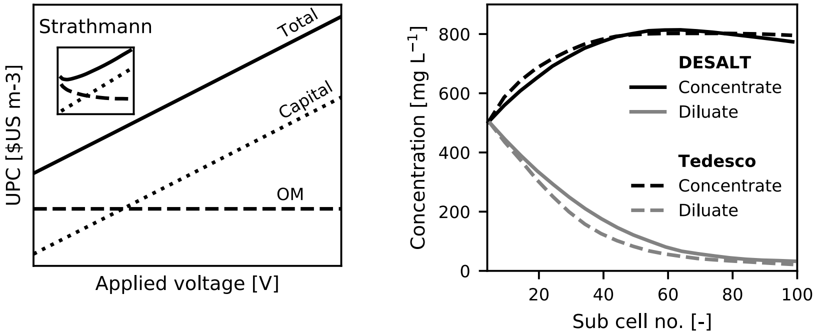
Due to the limited amount of information regarding how ED O&M costs are divided at various scales, the general relation found in Strathmann was used as a starting point [150]. A general relation for the O&M costs was determined based on the linear relation between the applied voltage and the O&M UPC. This relation was then applied to the estimated O&M costs calculated in Equation S12 10 where the general O&M conversion factor is viewed as the ratio between the cell voltage and the maximum applied cell voltage.

$$\mathbb{C}_{OM,gen} = Q_{dil,day} \mathfrak{c}_{OM,gen} \mathcal{B}_{OM} Q_{installed,day}{}^{\mathcal{M}_{OM}}$$ Equation S13-23

S13.12 Validation

Less information was available regarding the performance of ED. In terms of technical performance, the general relation for UPC and applied voltage presented in Strathmann were used [150]. It can be seen in Figure S13-1 a that the evaluation method behaves similarly to what was expected, however, there are some notable differences in the capital UPC. Strathmann found that the capital UPC increases at lower applied voltages. This is because the active area would need to increase to account for the lower performance at lower voltages. The ED evaluation method, however, does not show an increase at the lower applied voltage. This is because the capital cost is based on the capacity, which is related to the number of cell-pairs, not the applied voltage. Though effective at giving a general capital cost it is a reminder that with newer technologies, an accurate cost calculation is more difficult to achieve. Therefore, the results should be seen as indicators and not final values.

The accuracy of the ED evaluation method was tested using an ED model developed by Tedesco et al. [165], [169], [172]. As can be seen from Figure S13-1b, the concentration of salt in both the concentrate and diluate channels grow and decrease at different rates. However, the output from the channel is similar in both models. Since the DESALT model is primarily concerned with the inputs and outputs of the channel, the variation within the channel can be neglected.



(a) (b)

Figure S13-1 Verification of the ED evaluation method: (a) general cost performance relations resulting from the ED evaluation method and compared to the general relations found in Strathmann [150]; and (b) salt concentrations of the diluate and concentrate channels for both the ED evaluation method and the results from Tedesco [169]

S14 DESALT data points

Table S14-1 Overview of the output of the desalination model with quality constraints according to industrial requirements. The min, max, and average represent the ranges and averages of the values over a standard year. This is the same output used for the case study.

Output	Min	Max	Average	Description	Unit
CO_2eq	0.12	2.95	0.52	CO_2 equivalent	kg/m^3
E_{spec}	0.05	1.25	0.33	Total energy	kWh/m^3
Q_{brine}	219.20	5136.99	2076.01	Flowrate	m^3/day
$Q_{prod,day}$	34.25	3287.57	841.82	Flowrate	m^3/day
$c_{EC,brine}$	2051.42	4805.92	2821.86	Conductivity	mg/L
c_{EC}	0.03	2.56	0.96	Conductivity	mg/L
$c_{TOC,brine}$	47.69	94.83	61.15	Total Organic Carbon	mg/L
$CAPEX$	0.42	8.24	3.20	Capital costs	mil $US
$OPEX$	0.04	0.91	0.35	O&M costs	mil $US/year
TOC	5.99	47.69	17.43	Total Organic Carbon	mg/L
UPC	0.67	5.60	1.40	Unit production costs	$US/m^3

Table S14-2 Overview of the input required for the desalination model. The values represent the actual input used for the case study. The quality is constant. Operating parameters such as pressure and voltage are varied.

Input	Min	Max	Average	Description	Unit
$\mathbb{C}_{CO_2}$	3.58	3.58	3.58	CO_2 factor	g/m^3
N_{cp}	50,000	350,000	n/a	Cell-pairs	-
P_{app}	2.00	10.00	n/a	Pressure	bar
P_{feed}	1.00	1.00	1.00	Pressure	bar
Q_{feed}	547.95	5,479.45	4,054.80	Flowrate	m^3/day
T_{feed}	20.00	20.00	20.00	Temperature	°C
V_{total}	0.05	0.20	n/a	Voltage	V
c_{EC}	1,923.21	1,923.21	1,923.21	Conductivity	mg/L
c_{TOC}	47.69	47.69	47.69	Total Organic Carbon	mg/L
β_{bar}	0.00	0.00	0.00	Pressure conversion	bar/mg/L
β_{kPa}	0.06	0.06	0.06	Pressure conversion	kPa/mg/L
δ_{BWRO}	0.25	0.75	n/a	Recovery ratio	%
δ_{ED}	0.50	0.80	n/a	Recovery ratio	%
pH	7.70	7.70	7.70	pH	-

S15 WSN data points

Table S15-1 Overview of transport model input and output data for the case study. These inputs and outputs are determined based on the desalination output presented in S14.

	Min	Max	Average	Description	Unit
Input					
Demand	2192	5445	4638	Water demand	m^3/day
Drawdown	n/a	0.05	n/a	Drawdown allowance	m
Output					
Total distance	26.64	53.45	27.03	Pipeline length	km
Costs	0.17	0.28	0.19	Transport costs	$US/$m^3$
Energy use	0.03	0.39	0.12	Pumping energy	kWh/m^3
CO_2 emission	0.12	0.35	0.13	Construction and operation	kg CO_2-eq/m^3

S16 Additional simulation model results

Table S16-1 The range of values relative to the three indicators shown in the figures.

Source	Indicator	Min	Max	Average	Unit
Desalination	Cost	0.67	5.60	1.40	$US/m^3
	Energy	0.05	1.25	0.33	kWh/m^3
	CO_2	0.12	2.95	0.52	kg CO_2-eq/m^3
Transport	Cost	0.17	0.28	0.19	$US/m^3
	Energy	0.03	0.39	0.12	kWh/m^3
	CO_2	0.13	0.35	0.14	kg CO_2-eq/m^3

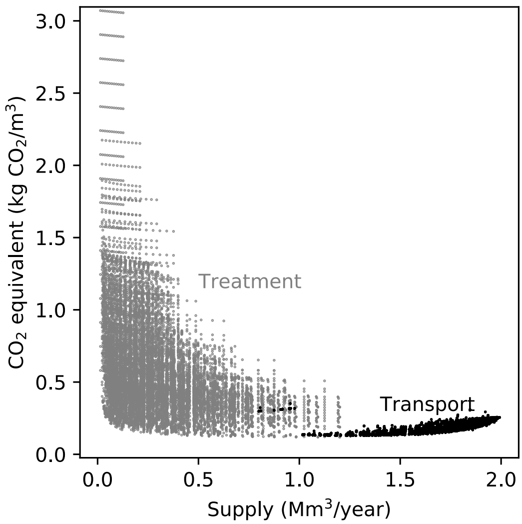


Figure S16-1 Volumetric CO_2-eq performance outputs from the simulation model portion of the DEA-IWRM framework as applied to the Dow case study and plotted against supply.

S17 Detailed treatment train operating conditions

Table S17-1 Desalination model parameters for the treatment trains appearing in the efficient DMU set. The combination is the specific desalination and transport percentage. Desalination parameters are read as follows: RO [pressure, recovery ratio], ED [voltage, cell-pairs, recovery ratio]. Note that the voltage for ED is for each cell-pair.

DMU	Combination	Treatment train
36	D47 T53	BWRO [2.00 bar / 58%] + ED [0.15 V / 150000 cp / 80%]
92	D42 T58	BWRO [2.00 bar / 58%] + ED [0.15 V / 150000 cp / 80%]
96	D47 T53	BWRO [2.00 bar / 58%] + ED [0.15 V / 250000 cp / 80%]
164	D44 T56	BWRO [2.00 bar / 58%] + BWRO [2.00 bar / 75%]
216	D38 T62	BWRO [2.00 bar / 58%] + ED [0.15 V / 150000 cp / 80%]
352	D38 T62	BWRO [2.00 bar / 75%] + ED [0.15 V / 250000 cp / 80%]
356	D38 T62	BWRO [2.00 bar / 58%] + ED [0.15 V / 250000 cp / 80%]
360	D34 T66	BWRO [2.00 bar / 58%] + ED [0.15 V / 150000 cp / 80%]
384	D33 T67	BWRO [2.00 bar / 42%] + ED [0.15 V / 150000 cp / 80%]
392	D36 T64	BWRO [2.00 bar / 75%] + BWRO [2.00 bar / 75%]
500	D38 T62	BWRO [2.00 bar / 75%] + ED [0.15 V / 350000 cp / 80%]
512	D38 T62	BWRO [2.00 bar / 58%] + ED [0.15 V / 350000 cp / 80%]
548	D30 T70	BWRO [2.00 bar / 42%] + ED [0.15 V / 150000 cp / 80%]
592	D30 T70	BWRO [2.00 bar / 58%] + ED [0.15 V / 150000 cp / 80%]
632	D33 T67	BWRO [2.00 bar / 75%] + ED [0.15 V / 250000 cp / 80%]
644	D31 T69	BWRO [2.00 bar / 75%] + BWRO [2.00 bar / 75%]
764	D28 T72	BWRO [2.00 bar / 75%] + ED [0.15 V / 150000 cp / 80%]
1036	D21 T79	BWRO [2.00 bar / 42%] + ED [0.15 V / 50000 cp / 80%]
1048	D26 T74	BWRO [2.00 bar / 75%] + BWRO [2.0 bar / 75%]
1248	D20 T80	BWRO [2.00 bar / 25%] + ED [0.15 V / 50000 cp / 80%]
1460	D22 T78	BWRO [2.00 bar / 75%] + ED [0.15 V / 150000 cp / 80%]
1512	D18 T82	BWRO [2.00 bar / 42%] + ED [0.15 V / 50000 cp / 80%]
1604	D21 T79	BWRO [2.00 bar / 58%] + ED [0.15 V / 150000 cp / 80%]
1724	D17 T83	BWRO [2.00 bar / 58%] + ED [0.15 V / 50000 cp / 80%]
1916	D16 T84	BWRO [2.00 bar / 25%] + ED [0.15 V / 50000 cp / 80%]
2856	D13 T87	BWRO [2.00 bar / 58%] + ED [0.15 V / 50000 cp / 80%]
4784	D11 T89	BWRO [2.00 bar / 75%] + ED [0.20 V / 50000 cp / 80%]
6808	D6 T94	BWRO [2.00 bar / 75%] + ED [0.15 V / 50000 cp / 80%]
12920	D1 T99	BWRO [2.00 bar / 25%] + BWRO [2.00 bar / 58%]
12921	D1 T99	BWRO [2.00 bar / 25%] + BWRO [4.67 bar / 58%]
12922	D1 T99	BWRO [2.00 bar / 25%] + BWRO [7.33 bar / 58%]
12923	D1 T99	BWRO [2.00 bar / 25%] + BWRO [10.0 bar / 58%]
12924	D1 T99	BWRO [4.67 bar / 25%] + BWRO [2.00 bar / 58%]
12925	D1 T99	BWRO [4.67 bar / 25%] + BWRO [4.67 bar / 58%]
12926	D1 T99	BWRO [4.67 bar / 25%] + BWRO [7.33 bar / 58%]
12927	D1 T99	BWRO [4.67 bar / 25%] + BWRO [10.0 bar / 58%]
12928	D1 T99	BWRO [7.33 bar / 25%] + BWRO [2.00 bar / 58%]
12929	D1 T99	BWRO [7.33 bar / 25%] + BWRO [4.67 bar / 58%]
12930	D1 T99	BWRO [7.33 bar / 25%] + BWRO [7.33 bar / 58%]
12931	D1 T99	BWRO [7.33 bar / 25%] + BWRO [10.0 bar / 58%]
12932	D1 T99	BWRO [10.0 bar / 25%] + BWRO [2.00 bar / 58%]
12933	D1 T99	BWRO [10.0 bar / 25%] + BWRO [4.67 bar / 58%]
12934	D1 T99	BWRO [10.0 bar / 25%] + BWRO [7.33 bar / 58%]
12935	D1 T99	BWRO [10.0 bar / 25%] + BWRO [10.0 bar / 58%]

S18 Compiled results of all DEA models

Table S18-1 Results of the different DEA models applied to the efficient DMU set determined by the basic efficiency

DMU	Comb.	Treatment Train	Basin	Weight constraints				Cross-efficiency		Super-eff.
				Bal.	Cost	Energy	Envi	Aggr.	Benev.	
36	D47 T53	BWRO + ED	•				•	0.917	0.915	1.006
92	D42 T58	BWRO + ED	•	•			•	0.939	0.936	1.002
96	D47 T53	BWRO + ED	•					0.916	0.914	1.000
164	D44 T56	BWRO + BWRO	•	•		•	•	0.931	0.925	1.001
216	D38 T62	BWRO + ED	•				•	0.934	0.931	1.000
352	D38 T62	BWRO + ED	•				•	0.945	0.941	1.002
356	D38 T62	BWRO + ED	•				•	0.930	0.928	1.004
360	D34 T66	BWRO + ED	•				•	0.931	0.928	1.012
384	D33 T67	BWRO + ED	•	•				0.937	0.931	1.001
392	D36 T64	BWRO + BWRO	•				•	0.926	0.920	1.000
500	D38 T62	BWRO + ED	•				•	0.930	0.926	1.000
512	D38 T62	BWRO + ED	•					0.911	0.909	1.000
548	D30 T70	BWRO + ED	•	•				0.939	0.935	1.003
592	D30 T70	BWRO + ED	•				•	0.949	0.943	1.002
632	D33 T67	BWRO + ED	•				•	0.938	0.932	1.002
644	D31 T69	BWRO + BWRO	•				•	0.944	0.938	1.001
764	D28 T72	BWRO + ED	•				•	0.947	0.939	1.003
1036	D21 T79	BWRO + ED	•	•				0.950	0.943	1.005
1048	D26 T74	BWRO + BWRO	•					0.948	0.941	1.000
1248	D20 T80	BWRO + ED	•	•				0.923	0.917	1.005
1460	D22 T78	BWRO + ED	•				•	0.950	0.942	1.003
1512	D18 T82	BWRO + ED	•	•				0.950	0.942	1.001
1604	D21 T79	BWRO + ED	•	•				0.953	0.946	1.001
1724	D17 T83	BWRO + ED	•					0.956	0.947	1.004
1916	D16 T84	BWRO + ED	•				•	0.929	0.922	1.000
2856	D13 T87	BWRO + ED	•	•				0.951	0.943	1.000
4784	D11 T89	BWRO + ED	•				•	0.945	0.936	1.000
6808	D6 T94	BWRO + ED	•				•	0.945	0.935	1.002
12920	D1 T99	BWRO + BWRO	•				•	0.950	0.940	1.004
12921	D1 T99	BWRO + BWRO	•	•	•		•	0.946	0.937	1.000
12922	D1 T99	BWRO + BWRO	•		•			0.943	0.933	1.000
12923	D1 T99	BWRO + BWRO	•		•			0.939	0.930	1.000
12924	D1 T99	BWRO + BWRO	•		•			0.936	0.926	1.000
12925	D1 T99	BWRO + BWRO	•		•			0.932	0.923	1.000
12926	D1 T99	BWRO + BWRO	•		•			0.929	0.920	1.000
12927	D1 T99	BWRO + BWRO	•		•			0.925	0.916	1.000
12928	D1 T99	BWRO + BWRO	•		•			0.922	0.913	1.000
12929	D1 T99	BWRO + BWRO	•					0.919	0.910	1.000
12930	D1 T99	BWRO + BWRO	•					0.916	0.907	1.000
12931	D1 T99	BWRO + BWRO	•					0.912	0.904	1.000
12932	D1 T99	BWRO + BWRO	•					0.909	0.900	1.000
12933	D1 T99	BWRO + BWRO	•					0.906	0.897	1.000
12934	D1 T99	BWRO + BWRO	•					0.903	0.894	1.000
12935	D1 T99	BWRO + BWRO	•					0.900	0.891	1.000

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- *Modelling of desalination technologies for industrial water (re)use.* Aquatech. 8 November 2017, Amsterdam, The Netherlands
- *Modelling of desalination technologies*. Ministry of Infrastructure and Water Management, 2 Juli 2018, The Hague, The Netherlands

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Dr. ir. Peter Vermeulen

A prayer to Titivillus, the demon of typos

Oh Titivillus, stay thy hand,

and make this at my own command.

If they should an error see,

I pray they will blame you, not me.

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