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SUSTAINABILITY ASSESMENT OF DESALINATION AND RESOURCE RECOVERY FROM BRINES

RODOULA KTORI

Sustainability Assessment of Desalination and Resource Recovery from Brines

Rodoula Ktori

Sustainability Assessment of Desalination and Resource Recovery from Brines

Dissertation

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Keywords: Sustainability assessment; Desalination; Brine treatment; Resource recovery; Multi-criteria decision making; Value-sensitive design; Life-cycle assessment

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To all the supergirls.

Contents

SUMMARY

Desalination plays a vital role in addressing water scarcity, but its high energy consumption and brine, a saline waste stream, disposal pose significant environmental and economic challenges. Seawater is a rich source of valuable and scarce materials that are lost when brine is discharged, making resource recovery a promising approach to improve sustainability. Integrating multiple technologies to recover water and valuable materials improves technological performance, but it introduces technical, economic, and societal complexities.

While desalination with resource recovery offers an alternative source of water, salts, and chemicals, its sustainability depends on local conditions and necessitates a holistic evaluation. Assessing these systems is particularly complex when water, a primary good, is among the recovered products. This research aims to refine assessment methodologies and explore trade-offs in integrated desalination and brine treatment. It adopts an exploratory, mixed-methods approach, beginning with a systematic literature review and the development of a sustainability assessment framework that prioritizes stakeholder participation.

In **Chapter 2,** the current sustainability assessment frameworks in desalination, water treatment, and resource recovery were reviewed and analysed. The literature review identified critical shortcomings in current sustainability assessments for seawater desalination and brine treatment systems. These assessments notably neglect social aspects and stakeholder involvement. To address these deficiencies, we proposed a new Sustainability Assessment (SA) framework that integrates participatory multi-criteria analysis and value-sensitive design into the decision-making process.

An open-source software tool in Python was developed in **Chapter 3** to simulate the desalination and mineral recovery processes, providing data that will inform later assessments. The outputs from this software directly support the analyses presented in Chapters 4–7, illustrating its integral role in this thesis and its potential for broader applicability.

The value-sensitive design (VSD) approach was applied in **Chapter 4** to design and evaluate integrated seawater desalination and brine treatment, ensuring that technical scenarios align with societal values. Four configurations were assessed for trade-offs between resource recovery, energy consumption, and environmental impact. While maximizing water and salt recovery improves resource security, it increases energy use and CO_2 emissions. The study highlights the need for region-specific solutions and demonstrates how VSD fosters stakeholder dialogue, supporting

sustainable and socially acceptable designs. These scenarios serve as the basis for analysis in subsequent chapters.

In **Chapter 5,** the economic performance of desalination systems focused on resource recovery was assessed using the levelized cost indicator. Allocation factors were used to fairly distribute costs and income from recovered products. A comparison of traditional Non-allocation and novel cost calculation methods revealed that the Non-allocation method overestimates production costs, resulting in inflated product prices. The Economic allocation approach, by redistributing costs to higher-value products, assigns a minimal percentage to water costs, unlike the heavy loading seen with Non-allocation.

Chapter 6 investigates the environmental performance of integrated desalination and brine treatment systems for resource recovery using Life Cycle Assessment (LCA). The study highlights how key methodological choices—like functional unit and treatment of waste heat—substantially affect results. Overall, resource recovery systems demonstrated superior performance compared to conventional production systems of the same product basket, highlighting the need for integrated practices.

Finally, the effect of interdependence among decision criteria in the multi-criteria decision-making process for sustainability assessment was evaluated in **Chapter 7**. By combining the Best-Worst Model and the Decision-Making Trial and Evaluation Laboratory technique, we proposed a novel weighting method that accounts for interdependencies. Applied to desalination and brine treatment, results showed that while numerical impacts are moderate, capturing interdependencies improves conceptual understanding—particularly in single-stakeholder settings.

In **Chapter 8**, a summary of the main findings of this thesis is provided, along with the limitations of this work and an outlook for future research directions based on these findings.

SAMENVATTING

Ontzilting speelt een cruciale rol in het aanpakken van waterschaarste, maar het hoge energieverbruik en de lozing van pekel, een zoute reststroom, brengen aanzienlijke milieutechnische en economische uitdagingen met zich mee. Zeewater is een rijke bron van waardevolle en schaarse materialen die verloren gaan wanneer pekel wordt geloosd, waardoor grondstoffenwinning uit pekel een veelbelovende benadering is om de duurzaamheid van ontzilting te verbeteren. De integratie van meerdere technologieën om water en waardevolle materialen terug te winnen, verhoogt de technologische prestaties, maar brengt technische, economische en maatschappelijke complexiteit met zich mee.

Hoewel ontzilting met grondstoffenwinning een alternatief biedt voor de levering van water, zouten en chemicaliën, hangt de duurzaamheid af van lokale omstandigheden en vereist deze een holistische evaluatie. De beoordeling van dergelijke systemen is bijzonder complex wanneer water, een primaire levensbehoefte, tot de teruggewonnen producten behoort. Dit onderzoek heeft tot doel beoordelingsmethodologieën te verfijnen en afwegingen te onderzoeken binnen geïntegreerde systemen voor ontzilting en pekelbehandeling. Hiervoor werd een verkennende aanpak met gemengde methoden gevolgd, te beginnen met een systematische literatuurstudie en de ontwikkeling van een duurzaamheidsbeoordelingskader waarin participatie van belanghebbenden centraal staat.

In **Hoofdstuk 2** werden bestaande duurzaamheidsbeoordelingskaders voor ontzilting, waterzuivering en grondstoffenwinning onderzocht en geanalyseerd. De literatuurstudie bracht belangrijke tekortkomingen van de beoordelingskaders aan het licht, waaronder het negeren van sociale aspecten en de betrokkenheid van belanghebbenden. Om deze tekortkomingen te verhelpen, is een nieuw beoordelingskader voorgesteld dat participatieve multicriteria-analyse en waardegevoelig ontwerp (Value-Sensitive Design, VSD) integreert in het besluitvormingsproces.

In **Hoofdstuk 3** werd een open-source softwaretool in Python ontwikkeld om ontziltings- en mineraalterugwinningsprocessen te simuleren. De gegevens uit deze tool ondersteunen de analyses in Hoofdstukken 4–7, wat het centrale belang ervan in dit proefschrift en het potentieel voor bredere toepassingen onderstreept.

De waardegevoelige ontwerpaanpak (VSD) werd in **Hoofdstuk 4** toegepast voor het ontwerp en de evaluatie van geïntegreerde systemen voor zeewaterontzilting en pekelbehandeling, zodat technische scenario's afgestemd zijn op maatschappelijke waarden. Vier configuraties werden geëvalueerd op basis van afwegingen tussen grondstoffenwinning, energieverbruik en milieueffecten. Maximale terugwinning van water en zouten verhoogt de grondstoffenveiligheid,

maar leidt ook tot meer energieverbruik en CO_2-uitstoot. De studie benadrukt de noodzaak van regio-specifieke oplossingen en toont aan hoe VSD de dialoog met belanghebbenden bevordert en leidt tot sociaal aanvaardbare en duurzame ontwerpen. Deze scenario's vormen de basis voor de analyses in de volgende hoofdstukken.

In **Hoofdstuk 5** werd de economische prestatie van ontziltingssystemen gericht op grondstoffenwinning beoordeeld aan de hand van de levelized cost-indicator. Er werden allocatiefactoren gebruikt om kosten en opbrengsten eerlijk te verdelen over de teruggewonnen producten. Vergelijking van traditionele en nieuwe kostenberekeningsmethoden toonde aan dat de Non-allocatie-methode de productiekosten overschat, wat leidt tot opgeblazen prijzen. De Economische-allocatie-methode herverdeelt de kosten naar producten met hogere waarde en kent daardoor een minimaal deel toe aan water, in tegenstelling tot de hoge kosten bij de Non-allocatie.

Hoofdstuk 6 onderzoekt de milieuprestaties van geïntegreerde ontziltings- en pekelbehandelingssystemen voor grondstoffenwinning met behulp van levenscyclusanalyse (LCA). De studie benadrukt dat methodologische keuzes – zoals de functionele eenheid en de verwerking van restwarmte – grote invloed hebben op de resultaten. Over het algemeen presteren systemen met grondstoffenwinning beter dan conventionele productiesystemen met een vergelijkbare productmand, wat het belang van geïntegreerde benaderingen onderstreept.

Tot slot werd in **Hoofdstuk 7** de invloed van onderlinge afhankelijkheid tussen beoordelingscriteria onderzocht in het multicriteria-besluitvormingsproces voor duurzaamheidsbeoordeling. Door de Best-Worst Method te combineren met de Decision-Making Trial and Evaluation Laboratory (DEMATEL)-techniek, ontwikkelden we een nieuwe wegingmethode die rekening houdt met onderlinge afhankelijkheden. Toegepast op ontzilting en pekelbehandeling toonde de studie aan dat hoewel de numerieke impact gematigd is, het meenemen van onderlinge afhankelijkheden bijdraagt aan een beter conceptueel begrip – vooral in contexten met een enkele belanghebbende.

In **Hoofdstuk 8** worden de belangrijkste bevindingen van dit proefschrift samengevat, worden de beperkingen van het onderzoek besproken, en worden aanbevelingen gedaan voor toekomstig onderzoek.

ΠΕΡΙΛΗΨΗ

Η αφαλάτωση διαδραματίζει καθοριστικό ρόλο στην αντιμετώπιση της λειψυδρίας, ωστόσο η υψηλή ενεργειακή της κατανάλωση και η απόρριψη της άλμης φέρει σημαντικές περιβαλλοντικές και οικονομικές προκλήσεις. Το θαλασσινό νερό αποτελεί πλούσια πηγή πολύτιμων και σπάνιων υλικών, τα οποία χάνονται όταν η άλμη απορρίπτεται, καθιστώντας την ανάκτηση πόρων μια ελπιδοφόρα προσέγγιση για τη βελτίωση της βιωσιμότητας. Η ενσωμάτωση πολλαπλών τεχνολογιών για την ανάκτηση νερού και πολύτιμων υλικών ενισχύει την τεχνολογική απόδοση, ωστόσο εισάγει τεχνικές, οικονομικές και κοινωνικές πολυπλοκότητες.

Αν και η αφαλάτωση με ανάκτηση πόρων προσφέρει μια εναλλακτική πηγή νερού, αλάτων και χημικών, η βιωσιμότητά της εξαρτάται από τις τοπικές συνθήκες και απαιτεί ολιστική αξιολόγηση. Η εκτίμηση αυτών των συστημάτων είναι ιδιαίτερα πολύπλοκη όταν το νερό, ένα βασικό αγαθό, συγκαταλέγεται στα ανακτώμενα προϊόντα. Η παρούσα έρευνα στοχεύει στη βελτίωση των μεθοδολογιών αξιολόγησης των ενσωματωμένων συστημάτων αφαλάτωσης και επεξεργασίας της άλμης. Ακολουθείται μια διερευνητική, μικτή μεθοδολογική προσέγγιση, ξεκινώντας από μια συστηματική βιβλιογραφική ανασκόπηση και έπειτα, στην ανάπτυξη ενός πλαισίου αξιολόγησης βιωσιμότητας, το οποίο δίνει προτεραιότητα στη συμμετοχή των ενδιαφερομένων.

Στο **Κεφάλαιο 2**, αναλύθηκαν τα υφιστάμενα πλαίσια αξιολόγησης βιωσιμότητας στην αφαλάτωση, την επεξεργασία νερού και την ανάκτηση πόρων. Η βιβλιογραφική ανασκόπηση ανέδειξε σημαντικά κενά στις τρέχουσες προσεγγίσεις, ειδικά, την ενσωμάτωση κοινωνικών πτυχών και τη συμμετοχή των ενδιαφερομένων. Για την αντιμετώπιση αυτών των αδυναμιών, προτείνεται ένα νέο πλαίσιο αξιολόγησης βιωσιμότητας που ενσωματώνει συμμετοχική ανάλυση πολλαπών κριτηρίων και σχεδιασμό ευαίσθητο στις αξίες (VSD) στη διαδικασία λήψης αποφάσεων.

Στο **Κεφάλαιο 3**, αναπτύχθηκε ένα λογισμικό ανοιχτού κώδικα σε Python για τη μοντελοποίηση της αφαλάτωσης και της ανάκτησης υλικών, παρέχοντας δεδομένα για τις αξιολογήσεις των επόμενων κεφαλαίων. Τα δεδομένα που προκύπτουν από το λογισμικό υποστηρίζουν άμεσα τις αναλύσεις των **Κεφαλαίων 4–7**, επιβεβαιώνοντας τον κεντρικό του ρόλο στη διατριβή και τη δυναμική του για ευρύτερη εφαρμογή.

Η προσέγγιση σχεδιασμού ευαίσθητου στις αξίες (VSD) εφαρμόστηκε στο **Κεφάλαιο 4** για τον σχεδιασμό και την αξιολόγηση ολοκληρωμένων συστημάτων αφαλάτωσης και επεξεργασίας άλμης, διασφαλίζοντας ότι τα τεχνικά σενάρια ανταποκρίνονται σε κοινωνικές αξίες. Τέσσερα σενάρια αξιολογήθηκαν ως προς τους συμβιβασμούς ανάμεσα στην ανάκτηση πόρων, την ενεργειακή κατανάλωση και τις περιβαλλοντικές επιπτώσεις. Η μέγιστη ανάκτηση νερού και

αλάτων ενώ ενισχύει την ασφάλεια πόρων, ταυτόχρονα αυξάνει την ενεργειακή χρήση και τις εκπομπές CO_2. Η μελέτη τονίζει την ανάγκη για λύσεις προσαρμοσμένες σε περιφερειακές συνθήκες και αναδεικνύει πώς το VSD ενισχύει τον διάλογο με τους ενδιαφερομένους, προωθώντας κοινωνικά αποδεκτά και βιώσιμα σχέδια. Αυτά τα σενάρια αποτελούν τη βάση για τις αναλύσεις των επόμενων κεφαλαίων.

Στο **Κεφάλαιο 5**, αξιολογήθηκε η οικονομική απόδοση συστημάτων αφαλάτωσης με έμφαση στην ανάκτηση πόρων, χρησιμοποιώντας τον δείκτη levelized cost. Χρησιμοποιήθηκαν συντελεστές κατανομής για το δίκαιο επιμερισμό κόστους και εσόδων από τα ανακτώμενα προϊόντα. Η σύγκριση παραδοσιακών και νέων μεθόδων υπολογισμού κόστους έδειξε ότι η μέθοδος Μη Κατανομής υπερεκτιμά το κόστος παραγωγής, οδηγώντας σε φουσκωμένες τιμές προϊόντων. Η μέθοδος Οικονομικής Κατανομής, με ανακατανομή του κόστους προς τα προϊόντα υψηλότερης αξίας, αποδίδει ελάχιστο ποσοστό στο κόστος νερού.

Στο **Κεφάλαιο 6**, διερευνήθηκε η περιβαλλοντική απόδοση ολοκληρωμένων συστημάτων αφαλάτωσης και επεξεργασίας άλμης για ανάκτηση πόρων μέσω ανάλυσης κύκλου ζωής (LCA). Η μελέτη ανέδειξε πώς οι μεθοδολογικές επιλογές, όπως η επιλογή της λειτουργικής μονάδας και η ενσωμάτωση της απορριπτόμενης θερμότητας, επηρεάζουν σημαντικά τα αποτελέσματα. Συνολικά, τα συστήματα ανάκτησης πόρων εμφάνισαν ανώτερη απόδοση σε σύγκριση με τα συμβατικά συστήματα παραγωγής των ίδιων προϊόντων, υπογραμμίζοντας την ανάγκη για ολοκληρωμένες πρακτικές.

Τέλος, στο **Κεφάλαιο 7** αξιολογήθηκε η επίδραση της αλληλεξάρτησης μεταξύ κριτηρίων στη διαδικασία λήψης αποφάσεων με πολυκριτηριακή ανάλυση για την αξιολόγηση βιωσιμότητας. Μέσω του συνδυασμού των μεθόδων Best-Worst και DEMATEL, προτάθηκε μια νέα μέθοδος στάθμισης που λαμβάνει υπόψη τις αλληλεξαρτήσεις. Εφαρμοσμένη στην αφαλάτωση και την επεξεργασία άλμης, η μελέτη έδειξε ότι παρότι οι ποσοτικές επιπτώσεις είναι ελάχιστες, η ενσωμάτωση των αλληλεξαρτήσεων ενισχύει την κατανόηση, ιδιαίτερα σε περιπτώσεις με έναν μόνο εμπλεκόμενο φορέα.

Στο **Κεφάλαιο 8**, συνοψίζονται τα κύρια ευρήματα της διατριβής, καταγράφονται οι περιορισμοί του έργου και παρουσιάζονται προτάσεις για μελλοντική έρευνα.

1

Introduction

1

1.1. Words with meaning

A decade ago, terms like "carbon footprint", "climate change," or "sustainability" were limited to academic circles. Today, they are part of our casual conversations. Last summer, while visiting a Greek island, I found myself in a discussion with an older man about climate change. The phrase that stuck with me was *"αυτή η καραμέλα της κλιματική αλλαγής"*, meaning "this new trend: climate change". He did not really understand the term and the consequences of this phenomenon, and to be honest, he didn't really agree with the term. But he knew those words, and he had formed an opinion.

And sustainability – what does sustainability truly mean? Sustainability is a vague term that means different things to different people. It's something abstract—you can't see it, and you can't measure it…or can you? It's one of those words that can mean anything you want. Someone said, *"Sustainability is like football: everyone talks about it, and everyone has the perfect solution"*. But perhaps that's exactly the point—sustainability is not a one-size-fits-all concept. It's deeply related to ethics, culture, and context. There is no single sustainable solution for everyone.

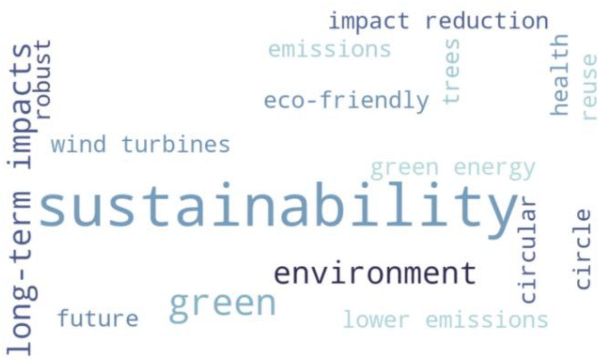

Figure 1. 1. Key themes in public perspectives on sustainability[1].

But if you still don't know what sustainability is. The most common definition is by the United Nations Brundtland Commission [1], which defines sustainability as:

> *"Meeting the needs of the present without compromising the ability of future generations to meet their own needs."*

So, is sustainability just a trend, or is it a lifeline for our future?

[1]Figure 1. 1 is based on insights gathered by the author through informal discussions with a diverse group, including colleagues, friends, and family members. The themes reflect general perceptions and ideas shared during these conversations.

1.2. Resource recovery: beyond waste

Resource recovery plays a key role in advancing sustainable development by transforming waste into valuable resources. Instead of simply discarding waste, resource recovery treats it as raw material that can produce valuable products, helping to reduce waste generation and promote resource efficiency. Resource recovery is not a new concept either. Ancient civilizations, including Romans, recycled metals such as gold, silver, and copper from waste materials. In modern times, the European Union formalized resource recovery strategies by introducing the waste hierarchy in 1975 [2].

But why is resource recovery critical for sustainability? One of the answers is resource depletion. As natural resources become increasingly scarce, the need to maximize resource efficiency and extract value from waste grows more urgent. Besides that, conventional mineral extraction, when poorly managed, can lead to severe environmental and social impacts, hindering progress toward Sustainable Development Goals (SDGs) [3]. Resource recovery, on the other hand, not only reduces the demand for raw materials but also aligns with the principles of a circular economy, which aims to secure essential resources while minimizing environmental harm [4].

Worldwide, numerous policy initiatives are being implemented aimed toward the transition to a circular economy [5]. For example, the European Investment Bank invested €3.83 billion from 2019-2023 to co-finance 132 circular economy projects in a variety of sectors, underscoring the commitment to sustainable practices [6]. Investments like these are a driving force for advancing resource recovery and fostering sustainable industry practices.

Despite advancements, resource recovery still faces significant non-technical challenges that require careful consideration of the broader socio-technical context [7]. Key barriers include market competitiveness, the need for dedicated markets for recovered resources, and the development of supportive policy and legal frameworks [8]. Importantly, neither resource recovery nor the circular economy is inherently sustainable; their success depends on how they are implemented and whether they truly minimize environmental impact and resource consumption. These limitations emphasize that while resource recovery holds great promise, effective adoption depends on creating both economic and regulatory environments that support sustainable resource use.

1.3. Water as a resource

Water is one of the most valuable resources. Beyond human consumption, water is an essential resource for agriculture, industry, electricity generation and urban and recreational activities [9,10]. Unlike other resources, water has no substitute. However, freshwater availability is declining due to climate change, pollution, and overuse, necessitating a shift toward more sustainable water management. Just as resource recovery redefines waste as a source of valuable materials, water recovery and reuse are key to a circular economy [11] and align with Sustainable Development Goal 6 [12]. With natural freshwater sources under increasing pressure, alternative water sources such as seawater and wastewater are becoming essential to meeting global demand.

1.4. Seawater desalination: more than just water

The rising demand for water driven by population growth and economic development, coupled with decreasing natural water resources due to climate change and pollution, is invoking water scarcity worldwide [13]. In 2023, rivers experienced their driest year in over three decades, leading to severe water shortages in many regions [14]. Currently, 3.6 billion people—40% of the global population—face water shortages, a figure projected to exceed 5 billion by 2050 [14]. These trends make it clear that natural water sources like rainfall and river runoff are increasingly insufficient, especially in water-stressed areas. Water scarcity is not a problem for the future but for now. Alternative sources such as seawater and wastewater must be considered to meet demand. Desalination of seawater has gained much attention as a "solution" to the water scarcity problem [13].

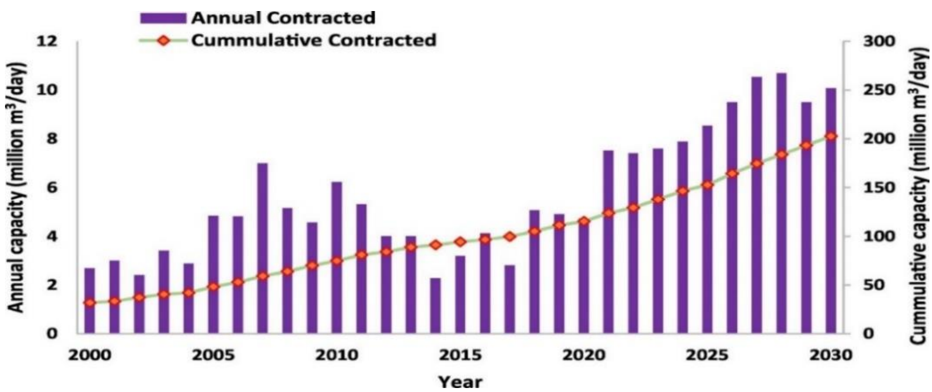

Figure 1. 2. Desalination capacity forecast plot over 30 years [49].

Desalination is a process that removes salts from seawater to produce water that meets the quality (salinity) requirements of different human uses [15]. Desalination technologies have been developed over the past 60 years, where the first large commercial scale started around 1965 and a worldwide capacity of only about 8000 m^3/day in 1970 [16]. Today, desalination capacity has expanded to about 109 million m^3/day [17], with seawater desalination accounting for over half of this capacity worldwide [18]. Besides water production, brine, which is water with high salinity (higher than seawater), is also produced. Based on the current technological status, for every 1m^3 of desalinated water, approx. 2.5 m^3 of brine is also produced, and usually, it is disposed of back into the environment (recovery ratio range from 40-55%) [19].

Despite its benefits, desalination is a highly energy-intensive process, and it comes with some economic [20] and environmental costs [21]. The price of desalinated water from large plants ranges between \$0.45 and \$6/m^3 [16], which is significantly higher than conventional water resources [20,22]. The significant installation and operation costs of desalination facilities directly affect the cost of produced water [20]. So, who covers these costs to keep desalinated water—a fundamental common-pool good—affordable? Public funding has made desalinated water more affordable for some users, such as farmers, who contribute to the common good by producing food and supporting societal needs. However, this raises questions about the balance of public subsidies: how can they equitably support essential users like farmers while ensuring that the broader societal costs and benefits are fairly distributed [23]?

Environmental concerns also arise with desalination. High salt levels in desalination brine can harm plants in the surrounding environment, slowing their growth or even leading to their death. There are also concerns about metals from corroded equipment and chemicals added during desalination, which can leak into the brine. Studies show that brine with high chemical levels can damage marine ecosystems and cause toxic substances to build up in organisms like seaweed and mussels, raising important environmental concerns about desalination's impact on ocean life [21].

Seawater contains large amounts of valuable and rare materials [15] that end up in the brine [24]. The economic value of these materials in desalination brine is estimated at around €6 per m^3 [25]. Despite this, brine is generally considered waste, and it is disposed of through methods such as deep well injection or evaporation ponds [19]. Simple calculations show that for every 1m^3 of desalinated water, valued at around €1, approximately €15 worth of valuable materials is *"lost"*, highlighting both economic and environmental opportunities in brine treatment and recovery.

An example of this potential is the chemical industry's demand for salt, which exceeds 11.5 million tons annually, suggesting a strong opportunity for salt recovery from brine to support resource-efficient processes [26]. Thus, while traditionally, the role of desalination is to provide water in water scarcity regions, the economic costs and the environmental impacts related mainly to brine discharge are shifting research and future investments towards brine minimization and resource recovery. With significant technological advancements over recent decades (see literature review from [27]), desalination offers a promising example of the transition to resource recovery systems.

1.5. Designing for water and resource recovery

Zero Liquid Discharge (ZLD) and Minimal Liquid Discharge (MLD) systems, which aim to recover nearly all water (100% and 95%, respectively) and significantly reduce brine disposal, were initially developed to increase water recovery and limit environmental discharge [28]. Traditionally, these systems focused primarily on extracting water and mixed salts from brine. However, recent technological advancements have shifted the emphasis towards resource recovery (from brine) and circularity, expanding the focus beyond water alone.

Recent research has increasingly explored methods for recovering specific salts and metals from brine, including magnesium, calcium, sodium, and other valuable elements [15,29–31]. However, no single technology can efficiently recover all of these valuable materials, making it necessary to integrate multiple technologies. Although combining different methods improves the range of recoverable products, it also adds complexity to system design and operation [32].

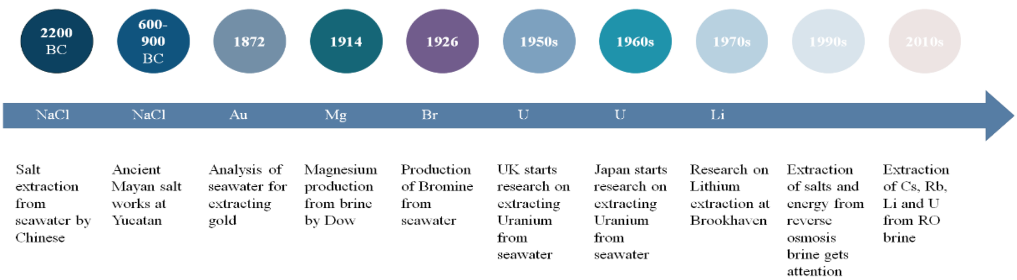

Figure 1. 3. Timeline representing the development of resource recovery from seawater and brine (adjusted from [15]).

To develop reliable and efficient resource recovery configurations, it is crucial to carefully select and combine various technologies, optimizing for high water recovery, minimized energy use, and effective byproduct management [31,33]. However, there is no guide available for selecting the right processes. Effective integrated systems should be tailored to meet both local market demand and community needs, ensuring that solutions are not only technically effective but also economically viable and socially relevant.

1.6. Balancing the scale: challenges in sustainability

Economic: Integrating resource recovery (and ZLD systems) in desalination plants is recommended in literature as an approach to lower desalinated water costs [20]. But is this true in practice? While those systems promise reduced waste and resource recovery, they come with high operational and capital costs [34], which present significant barriers to full-scale implementation [35]. In fact, integrating energy- and chemical-intensive processes into desalination may further increase the cost of water, which remains the primary product of these systems. This raises important questions: Will water remain affordable in regions where those desalination systems are implemented? And, will recovered products from these systems be competitive in the market, or will high production costs make them unviable? Such challenges highlight the economic dilemma of desalination aiming at resource recovery, balancing the potential for resource recovery against the risk of increased water prices and the uncertain marketability of recovered resources.

Environmental: While resource recovery systems can reduce brine disposal from desalination, this doesn't necessarily equate to a reduced overall environmental impact. Desalination for resource recovery is highly energy-intensive [35], often requiring substantial amounts of energy and chemicals to treat brine and recover valuable byproducts. As a result, the environmental impacts associated with energy consumption can increase, especially in regions reliant on non-renewable energy sources.

To fairly evaluate the environmental benefits of these integrated systems, it is important to compare their impacts with those of conventional production methods for the same recovered materials. In line with approaches seen in wastewater treatment and solid waste management, a fair environmental assessment should allocate a portion of the upstream environmental burden from desalination processes to the downstream recovered products, treating waste streams as co-products [36]. Effective management of solid residuals, such as mixed salts without market value, is another environmental challenge that could simply shift the environmental burden to other waste streams.

Social: Resource recovery in desalination introduces complex social implications, particularly in balancing benefits and costs across different groups. When costs are imposed on one group while benefits are enjoyed by another, policies may be seen as inequitable or 'unsustainable' [23]. Key concerns also emerge around ownership, management, and benefit distribution. Public trust, often affected by concerns over environmental impacts, privatization, and the quality of recovered products, plays a crucial role in the acceptance of these systems [37].

Additionally, the relevance of recovered products to local needs presents another challenge. For example, in energy-scarce regions, the high energy demands of resource recovery could create tension if the products recovered are less essential than the energy consumed, potentially undermining public (and relevant stakeholders) trust. Community concerns and needs, combined with stakeholder knowledge, should help build a clear, shared understanding of resource recovery systems. Transparent operations, effective communication, and active stakeholder engagement are essential in building public support and aligning resource recovery efforts with local values [4,38].

Transitioning from a linear to a circular economy through resource recovery in desalination changes how we assess the sustainability of these systems. Are current assessment tools effective in capturing the full range of economic, environmental, and social implications for resource recovery systems? Developing refined tools will be essential to evaluate and guide sustainable resource recovery in desalination accurately.

1.7. Breaking barriers: connecting technological development and society

Although technological development is inherently embedded in society, in practice, the two are often treated as separate domains, particularly in technical fields such as desalination and resource recovery. This functional disconnect can limit the relevance and effectiveness of innovations, as development processes frequently proceed without meaningful input from social scientists, policymakers, or affected communities [39].

Effective sustainability solutions rely on collaboration across diverse stakeholder groups, which can significantly influence how well these projects work in real-life [40,41]. Stakeholders bring essential insights—often beyond technical knowledge—that are critical for accurately defining problems, assessing the feasibility, and evaluating their sustainability.

Yet, in many technical fields, like desalination, they often isolate technological development from societal considerations, creating a disconnect that can limit the relevance and effectiveness of solutions. This gap—the *“elephant in the room”*— acts as an invisible barrier,

Figure 1. 4. Sustainability as the 'elephant in the room' amid stakeholders focused on their own priorities.

as technological innovations may not fully align with the real problem, societal priorities and sustainability goals.

To develop resource recovery systems that truly advance sustainability, stakeholders must be involved in design, assessment and implementation, ensuring that these systems reflect public priorities and local needs [4]. Bridging this gap, it is essential to co-produce knowledge by integrating perspectives from multiple disciplines and stakeholder groups. This collaborative approach can foster *"win-win"* solutions that are both technically viable and socially accepted. Stakeholder participation promotes transparency and trust, creating a shared understanding of goals and challenges [42]. However, achieving such integration requires specific methodologies and tools that enable stakeholders to contribute effectively to the development and assessment of sustainability solutions [40].

1.8. Knowledge gap

Sustainability assessment (SA) has evolved substantially over the past decades, with integrated frameworks developed across sectors such as wastewater, bioenergy, biorefineries, manufacturing [43–47]. These frameworks have contributed important advancements, such as the inclusion of multiple sustainability dimensions and increased stakeholder engagement, and have helped guide sustainable decision-making in emerging industrial contexts. However, such frameworks are typically designed for industrial, market-driven systems, where the primary goals are production efficiency, environmental mitigation, and economic optimization.

In contrast, desalination and drinking water systems operate as public services, with a focus on providing secure and equitable water. They are embedded in governance structures and shaped by societal values, regulatory constraints, and public perception. In this context, resource recovery cannot be assessed solely through technical or economic metrics; it must account for societal values, local constraints, and political acceptability.

Frameworks developed for other sectors (e.g. biorefinery design), while advanced in integrating sustainability principles, are not directly transferable to water systems. Thus, a context-specific assessment framework is required—one that accounts for the particular societal role of water systems and the unique challenges of integrating new recovery technologies into existing infrastructures. A framework that extends previous work and is tailored to the distinct context of desalination and resource recovery is therefore needed. A detailed literature review of SA approaches in desalination and wastewater-based resource recovery is presented in **Chapter 2**.

Beyond the framework level, commonly used methodologies, such as life cycle assessment, economic evaluation, and multi-criteria decision analysis, require adjustments for the complexities of circular resource recovery systems. For instance, environmental assessments often overlook critical decisions, such as allocation or boundary choices. Economic analyses often rely on cost metrics unsuited to multi-output systems, and decision-making methods fail to account for interdependencies among sustainability criteria. These challenges form the basis for the research questions and methodologies developed in this thesis.

1.9. Research approach and thesis outline

This research responds to these gaps by developing a comprehensive framework and methodologies for assessing the sustainability of desalination systems integrated with resource recovery. This includes evaluating technical, economic, and environmental performance, integrating stakeholder values, and exploring innovative economic assessment methods and decision-making strategies to guide the design and optimization of desalination systems that meet regional needs and resource recovery goals. To address these objectives, this research explores the following key research questions (RQ):

- *RQ1 - How can SA methodology be tailored to ensure comprehensive evaluation and stakeholder participation in multi-objective systems of integrated desalination and brine management?*
- *RQ2 - What are the benefits and drawbacks of different technical configurations in integrated resource recovery desalination vis-à-vis identified values, and how do they apply to different societal contexts?*
- *RQ3 - How do different cost allocation methods influence the levelized cost of products in multi-product resource recovery systems, and what are the implications for economic feasibility assessments?*
- *RQ4 - How do key methodological decisions such as functional unit, allocation and energy source influence the results and decisions within the context of an integrated desalination and brine treatment systems?*
- *RQ5 - What are the environmental benefits and disadvantages of integrated desalination and brine treatment systems compared with both conventional seawater desalination and salt production systems?*
- *RQ6 - How do interdependencies among criteria impact decision outcomes in sustainability assessments?*

This thesis adopts a prescriptive decision-analysis approach, aiming to support decision-makers in selecting sustainable and context-appropriate desalination and resource recovery systems. Prescriptive approaches focus on recommending actions based on structured evaluation and analysis, typically incorporating expert knowledge and stakeholders' values. This differs from descriptive approaches, which explore how decisions are made in practice, often influenced by cognitive biases, emotions, and heuristics, and normative approaches, which define how decisions should be made in theory under ideal conditions using formal logic and mathematical models. The use of multi-criteria decision-analysis methods and stakeholder-oriented frameworks in this research aligns with this prescriptive focus, as it seeks to guide and structure decisions in complex, multi-objective settings [48].

1.9.1. Thesis outline

Chapter 2 reviews current sustainability assessment frameworks in desalination, water treatment, and resource recovery, analyses available tools, and identifies research gaps. A participatory framework that integrates value-sensitive design elements with a multi-criteria approach for sustainability assessment is proposed. This chapter addresses RQ 1.

Chapter 3 focuses on developing an open-source software tool designed to simulate desalination and mineral recovery processes. This tool combines technical process models with economic and environmental analyses, providing data that will inform later assessments. Unlike the subsequent chapters, **Chapter 3** is methodology-oriented and does not directly address specific research questions. Instead, it provides the conceptual and technical foundations that support the analyses conducted in the rest of the thesis.

In **Chapter 4**, a value-sensitive design approach is applied to design and evaluate integrated desalination and brine treatment systems. The goal is to understand the benefits and drawbacks of different technical configurations in integrated resource recovery desalination vis-à-vis identified values. The scenarios developed here will be used in the following chapters, creating a cohesive, iterative evaluation process. This chapter addresses RQ 2.

Chapter 5 delves into the economic assessment of desalination systems focused on resource recovery. It aims to investigate how different cost calculation methods influence the levelized cost of products in these systems. Traditional and novel cost calculation methods are compared to determine their impact on the economic feasibility of resource recovery. This chapter addresses RQ 3.

Chapter 6 delves into the assessment of the environmental performance of integrated desalination and brine treatment systems. The aim is to first understand the effect of key methodological decisions needed to make for resource recovery assessments on the results. Then, the environmental benefits and disadvantages of integrated desalination and brine treatment systems are analysed and compared with those of conventional seawater desalination and salt production systems. This chapter addresses RQ 4&5.

In **Chapter 7**, a desalination case study is used to evaluate how the interdependence among decision criteria affects the multi-criteria decision-making process for sustainability assessment. In real-world applications, sustainability criteria often influence one another; however, traditional multi-criteria decision-making methods typically assume these criteria are independent, which can lead to an incomplete or oversimplified analysis. This chapter examines methods that account for these cross-criteria influences, offering a more realistic and comprehensive assessment of sustainability. This chapter addresses RQ 6.

In **Chapter 8**, a summary of the main findings of this thesis is provided, along with the limitations of this work and an outlook for future research directions based on these findings.

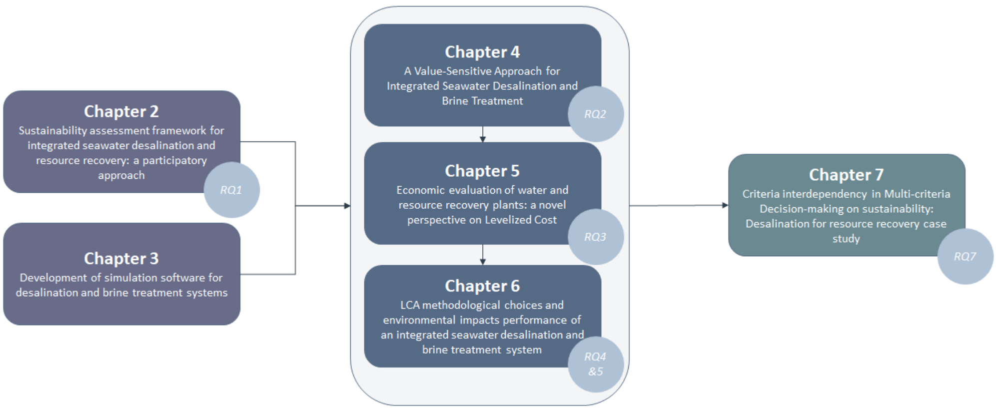

Figure 1. 5. Structure overview of this thesis. RQ: Research question.

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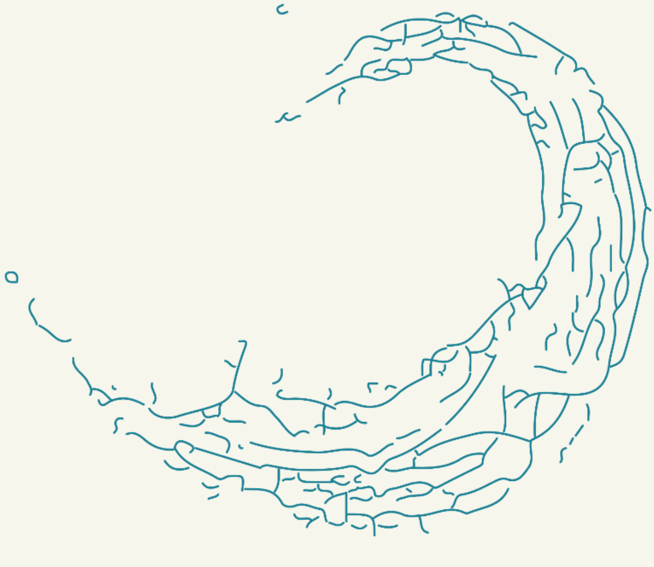
2

Sustainability assessment framework for integrated seawater desalination and resource recovery: a participatory approach



ABSTRACT

Valuable and rare materials in seawater brine are often discarded during desalination. However, there is an increasing focus on recovering these resources, due to the economic and environmental opportunities they can bring. Despite this shift, current Sustainability Assessments (SA) in desalination overlook the brine handling and social dimensions, and brine treatment assessments remain centered on techno-economic dimensions. This work proposes a comprehensive framework for the SA of integrated desalination and resource recovery options, focusing on recovering valuable materials from brine. The framework not only evaluates pre-defined systems but also supports the identification of system features of interest, such as products to assess and technologies to include, as well as the transparent selection of indicators, considering specific contexts. To develop this framework, a review of the literature on SA in desalination and brine treatment systems was conducted. Looking at the identified gaps, we synthesized the findings and key messages and proposed the integration of Multi-Criteria Analysis and Value-Sensitive Design in the decision-making process. This allows stakeholders to be involved and incorporates their values at different stages of the assessment, making it distinct from traditional SA methods. This framework offers structured guidance to stakeholders on how to carry out qualitative and quantitative assessments while ensuring transparency in the assessment process.

Keywords: *Sustainability assessment framework, Stakeholders' participation, Value-sensitive design, Desalination, Brine treatment*

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2.1. Introduction

Seawater desalination is one of the most crucial water treatment technologies for addressing water scarcity in water-stressed regions. This is an energy-intensive process, and besides water production, there is a residual stream called brine. Brine is often discharged into the ocean or back to the environment with various methods, such as deep well injection and evaporation ponds [1]. Seawater contains large amounts of valuable and rare materials [2] that end up in the brine [3], presenting economic and environmental opportunities from their recovery through brine treatment [4,5]. Recent studies have focused on developing technologies to recover materials such as magnesium, calcium, and sodium [2,6,7], as well as metals from seawater brine [8]. These efforts aim to go beyond water production, demonstrating a more substantial commitment to resource recovery and circular economy principles.

No single technology can efficiently recover all the valuable materials from seawater brine, necessitating integrated approaches tailored to specific products and conditions, with attention to the market potential of individual products [3]. For instance, the technological feasibility of such an integrated seawater desalination and brine treatment was shown in a pilot project in Lampedusa, Italy, with five unit operations integrated for the recovery of water and five high-quality products [7]. This integration can improve the technological and economic performance of desalination systems but also introduces complexities, making comprehensive sustainability assessments (SA) essential to evaluate the impacts beyond technical and economic performance [9].

Sustainability assessment has become a rapidly developing area that supports the evaluation of emerging processes, such as the integration of desalination and brine treatment technologies, beyond traditional techno-economic analysis (TEA) [10]. Early sustainability assessments of desalination processes focused on techno-economic indicators (evaluating technical feasibility and economic performance, such as capital and operational costs, and return on investment) and brine disposal while neglecting environmental and social aspects [11,12]. Although environmental impact assessments using methodologies like Life Cycle Assessment (LCA), which assesses environmental impacts across a system's life cycle, have been reported, their integration with techno-economic and socio-economic analyses remains limited, hindering comprehensive sustainability evaluation [13–16]. On the other hand, in techno-economic studies, economic sustainability focuses on business economics, while environmental is often limited to GHG emissions [17]. The environmental assessments and LCAs need to be combined with techno-economic [18] and socio-economic analysis to reduce uncertainties and incorporate a broader range of parameters [19–21]. There is no sustained progress in one pillar (dimension) without progress in all [22].

Despite advancements in SA frameworks for desalination processes over the past decade, incorporating more comprehensive three-dimensional assessment [20,23,24], there remains a notable gap in consideration of brine and resource recovery within existing frameworks. Previous studies focusing on the assessment of water and salt recovery from brine have often overlooked the social aspect, with environmental assessments primarily focused on emissions from energy consumption [17,25,26] and environmental impacts from brine disposal into the marine environment [27]. Existing studies have typically centered on either desalination or zero liquid discharge (ZLD) systems, failing to provide a comprehensive evaluation of integrated desalination and brine management approaches. Moving towards brine minimization and resource recovery systems, the existing frameworks need to be updated. To address the gap, we formulate the following question:

How can SA methodology be tailored to ensure comprehensive evaluation and stakeholder participation in multi-objective systems of integrated desalination and brine management?

To answer the research question, this work aims to develop a methodological approach to assess the sustainability performance of extended treatment chains aiming to achieve resource recovery in the desalination industry. While seawater desalination is used as a primary example, the principles and steps outlined in our framework can be applied to various water sources, making it a robust tool for sustainability assessment across diverse desalination processes.

This work is organized as follows: Section 2.2 provides the theoretical foundation for developing the assessment framework. Section 2.3 presents the methodology for the literature review and the development of the assessment framework. Section 2.4 presents an extensive literature analysis of assessment frameworks for desalination and brine treatment systems (Section 2.4.2.1) a review of the available assessment indicators (Section 2.4.2.2), and a literature analysis of assessment frameworks and decision-support tools on resource recovery from other sources (Section 2.4.2.3). Drawing on the theoretical background of SA, key insights, and research gap, an assessment framework is developed and presented in Section 2.4.3. Finally, Section 2.5 discusses the impact and limitations of this study and future work. The developed indicator database is provided in Supplementary Information I.

2.2. Theoretical background on sustainability assessment and multi-criteria decision making

Sustainability assessment guides decision-making towards sustainability [28], encompassing both negative impacts and positive contributions across various dimensions. [29] defined SA as a method that provides decision-makers with "*an evaluation of global to local integrated nature–society systems in short and long term perspectives in order to assist them to determine which actions should or should not be taken in an attempt to make society sustainable*". SAs are critical tools used to evaluate the sustainability of various systems and processes, typically applied to compare the sustainability of two or more systems, whether they be technologies, processes, or entire organizations. The eligibility for SA usually depends on the availability of relevant data and the defined indicators that measure sustainability aspects such as environmental impact, economic viability, and social equity [30]. SA has also the role of improving the decision-making process by:

- Integrating sustainability dimensions and considering their interdependencies.
- Including intragenerational and intergenerational considerations.
- Supporting constructive interaction among stakeholders
- Accounting for uncertainties [30,31]
- Managing trade-offs, prioritization, comparability, and compensation between sustainability categories [32].

Traditional sustainability assessments relied on reductionist methods [30], using one measurable indicator, one dimension, a single scale of analysis, one objective, and a one-time horizon [30,33]. However, there is now a move towards more indicator-based assessments, which offer a more comprehensive understanding of sustainability. Indicator-based SA, such as multi-criteria decision analysis (MCDA[1]), is the most commonly used because "*They can translate physical and social science knowledge into manageable units of information that can facilitate the decision-making process*" [34,35].

MCDA is a methodology used to evaluate and prioritize different options based on multiple criteria [36], considering multiple sustainability dimensions, stakeholders' values, and uncertainties [31]. MCDA frameworks vary from simple to sophisticated methods, including horizontal or soft MCDA, which aims to structure knowledge for decision support, requiring very little information, and vertical or hard MCDA, which uses mathematical programming techniques for ranking alternatives, requiring extensive information [36,37]. The key elements

[1] *To ensure clarity and consistency, this thesis distinguishes between related terms commonly used in the literature. The term Multi-Criteria Decision Analysis (MCDA) is used to describe the overall analytical framework adopted in this work, which emphasizes a participatory, value-sensitive approach to sustainability assessment involving multiple, often conflicting criteria and stakeholder perspectives. In contrast, Multi-Criteria Decision Making (MCDM) refers specifically to the structured application of decision-support methods (e.g., BWM, PROMETHEE) used for ranking or prioritizing alternatives in more deterministic contexts. While these terms are often used interchangeably, they are differentiated here to reflect their roles within the thesis.*

identified in traditional MCDA are scope definition (including selection of alternatives), criteria selection, and interpretation methods (assigning weights, aggregating scores and ranking alternatives) [32,38]. For more detailed methodological insights, readers can refer to works by [32,34,39].

The technical dimension is often included indirectly in the evaluation of well-developed technologies, but directly for emerging technologies to assess the performance and feasibility of the process [32,40] since the operational performance is uncertain [32]. Technical aspects significantly influence economic, environmental, and social dimensions [40,41]. Thus, SA must integrate economic, environmental, social, and technological issues and their interactions and consider the consequences of present actions into the future and drivers of change [30,42]. This integrated approach is particularly valuable in desalination and brine treatment projects aiming at resource recovery, where technologies are relatively new, and cost, environmental impact, and resource recovery potential need to be balanced.

Moving towards interdisciplinary and trans-disciplinary approaches underscores the necessity of integrating methods, concepts, and theories from various disciplines and effectively engaging stakeholders [39]. Stakeholder participation is crucial for aligning resource recovery innovations with their socio-technical context, democratizing decision-making, and ensuring the relevance of sustainability assessments [43,44]. Stakeholder participation goes beyond merely incorporating expert opinions in the weighting process of decision-making studies, empowering stakeholders and providing them with the opportunity to understand the problem and influence the decision [44].

Value-sensitive design (VSD) is a participatory approach that proactively incorporates societal values [45] into technological designs by investigating stakeholder values and identifying desirable technical features [46,47]. In particular, VSD incorporates social aspects into emerging technologies consciously [48], which are often developed in processes that are blind to the context and the stakeholders' realities [10]. This inclusive design process allows stakeholders to co-design technologies that align with their values, perceptions, and expectations [43]. It is a valuable methodology for ensuring stakeholder participation and comprehensive evaluation in addressing multi-objective systems.

While VSD has been utilized in various contexts, such as ICT and robotics projects [49], the design of biorefineries [50], wind turbines and wind parks [51], and digital platforms [52], its application in the water and wastewater sectors remains limited. Only an approach based on VSD has been used to proactively integrate societal values in the design of technologies for resource recovery and gain first insights into its societal implications in the context of small islands [53].

2.3. Methodology: developing the conceptual framework

To develop an assessment framework and answer the research question, a literature review was conducted as a “preparation”. The key results were gathered and analysed. The findings and key messages from the literature review were composed to develop the proposed framework (synthesis phase) according to the methodology in **Figure 2.1**.

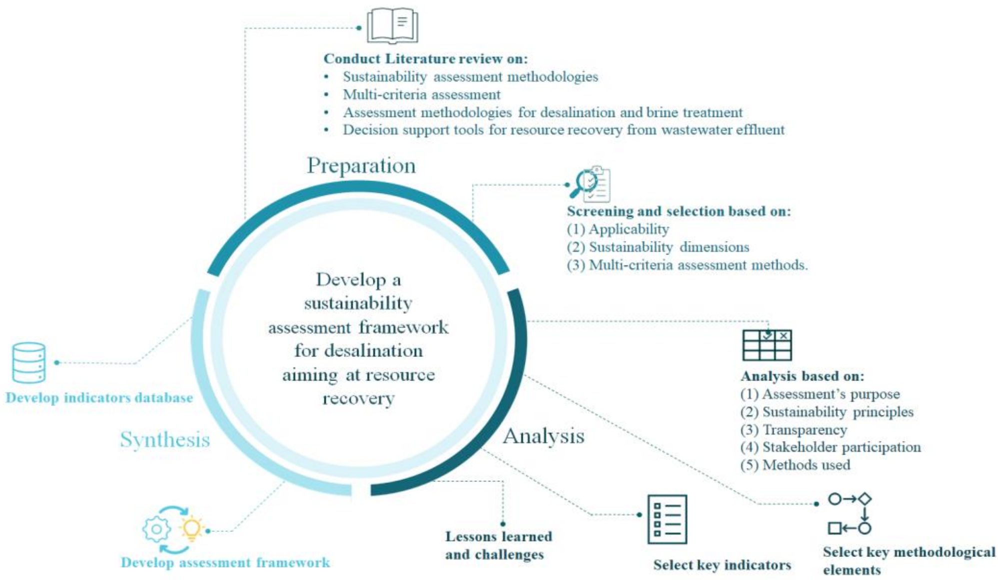

Figure 2.1. Scheme of research methodology to develop sustainability assessment framework.

2.3.1. Preparation phase

The review was conducted through various steps, as described in **Figure 2.1**, and with a focus on:

1) Sustainability assessment methodologies,
2) Multi-criteria assessment for sustainability assessment,
3) The available assessment methodologies for desalination and brine treatment systems.
4) The available assessment methodologies for resource recovery from wastewater effluent

The literature search was conducted using Scopus and Google Scholar databases, focusing on recent publications in English. Keywords such as “MCDA for SA”, “sustainability assessment of desalination and brine treatment”, “environmental assessment of desalination and brine”, and “techno-economic assessment of desalination and brine treatment” were utilized. Additionally, terms like “sustainability assessment of ZLD”, “sustainability assessment of

Minimum Liquid Discharge", and "techno-economic assessment of ZLD" were included to capture relevant studies. Grey literature was excluded to maintain a focus on peer-reviewed sources, ensuring scientific rigor and reliability. The review process does not delve into the discussion of specific desalination and brine treatment technologies.

After the initial screening, studies were selected and analysed based on their relevance to (1) applicability to the context of desalination, brine management, and resource recovery, (2) alignment with sustainability assessment dimensions, and (3) multi-criteria assessment methods. Snowballing techniques, including backward and forward citation tracing, were also employed to ensure comprehensive coverage.

The literature review has been expanded to encompass fields beyond desalination, such as those of resource recovery from sources other than seawater, using snowballing. Given that resource recovery in desalination is still emerging and the assessment of such systems is in its developmental stages, insights and experiences gained from more established fields could prove very useful in developing an assessment framework for desalination.

A review of indicators for evaluating desalination, brine treatment systems, or water treatment systems was conducted. This included dimensions and indicators from the previous steps, as well as studies on LCA, environmental impact assessment (EIA), energy assessment, techno-economic, and social life cycle assessment studies. The review also covered multi-criteria or sustainability assessment tools for wastewater, urban water systems, and the water industry, in general. The search was extended to specific articles or topics identified in the reviewed literature. The relevant indicators were collected using the same criteria of relevance.

2.3.2. Analysis phase

After the preparation phase, the most relevant studies were selected for analysis based on the above criteria of relevance. Firstly, the key elements regarding the methodological approach for SA and MCDA were scrutinized. The importance, which means how vital each step is, and the order, indicating the sequence in which these elements should be followed, were evaluated. The studies were qualitatively assessed in terms of sustainability principles, transparency, and consideration of sustainability dimensions. Then, they were analysed based on the assessment's purpose and the methods or combinations of methods used. Transparency in this phase means openly sharing procedural steps, providing required data, and clearly explaining decisions, such as the selection of indicators. This allows others to replicate the study, verify its findings, and hold the process accountable. Finally, stakeholder participation was evaluated by analysing which stakeholders were considered relevant, their knowledge background, how they were selected, and how and in which phases they were engaged.

2.3.3. Synthesis

In this phase, we synthesize the findings and key messages from the literature review into a framework for multi-criteria SA of desalination for resource recovery. As a result, the proposed framework was developed, drawing inspiration from sustainability science and building on the key elements of multi-criteria sustainability methodologies [54–60], the review of current assessment frameworks for desalination and brine treatment, and research gaps. Additionally, elements identified as promising for a non-reductionist approach to SA in desalination and resource recovery were combined into a framework (see **Figure 2.2**) that thus draws from value-sensitive design (VSD) and MCDA (as an SA approach). This work integrates VSD elements into different steps of the proposed framework. Specifically, key characteristics of VSD, such as stakeholders' values and value tensions, will be used in the selection of the assessment indicators and design of alternative scenarios and contribute to the system's assessment and design. By incorporating values into the assessment process, we can ensure that the selected criteria and indicators are relevant and meaningful to the stakeholders involved and that the assessment addresses the real concerns and ambitions of those affected by the decisions. The order of the key elements that compose the framework was adjusted to enhance transparency in the selection of indicators and alternatives and address social challenges to overcome the weak points of the existing methodology.

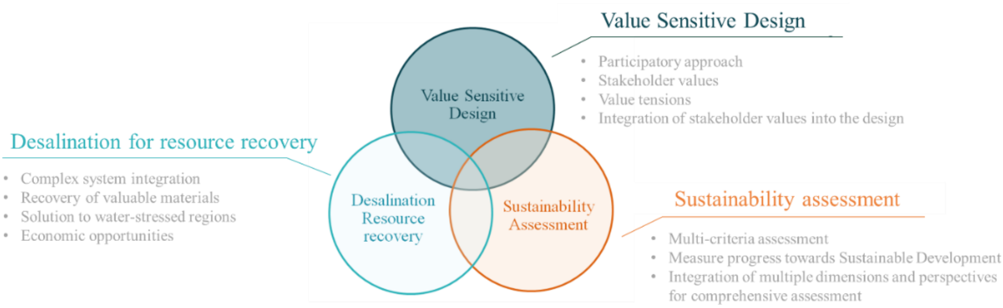

Figure 2.2. The intersectionality of Value Sensitive Design, Sustainability assessment and Desalination aiming at resource recovery.

Transparency is one of the key elements of an objective SA framework and can ensure credibility [39]. [61] emphasized the need to enhance methodological transparency by providing insights into the selection of alternatives, dimensions, and indicators. The proposed framework addresses this issue by explicitly outlining the procedures for selecting assessment indicators, which are then disclosed as part of the presented results. Additionally, VSD's participatory approach enhances transparency in indicator selection and scenario design, which is particularly valuable given the frequent lack of detailed explanations for selected indicators or alternative scenarios in the literature.

Finally, within the synthesis phase, a database with 208 performance indicators has been developed (see Supplementary Information I) for a comprehensive assessment of desalination and brine treatment systems. The developed database gives an overview of the most used indicators in the field, and it can help users select the most applicable performance indicators. The indicators are categorized into technical, economic, environmental, and social, focusing solely on a plant's planning and operation phase. It includes both qualitative (e.g., reliability) and quantitative (e.g., water recovery) indicators, along with the tools or methodologies in which they are utilized.

Please refer to Supplementary Information III (see Section A) for a more detailed explanation of concepts like value and value tension, along with examples. The supplementary information includes comprehensive definitions of the terminology used in this work.

2.4. Results and discussion

2.4.1. Preparation: Sustainability assessment trends and indicator utilization in the desalination field

The research interest in sustainability assessment for the desalination field has grown over recent years (see **Figure 2.3**), driven by global capacity expansion, cost reduction, environmental concerns around desalination and significant technological developments in brine valorisation. However, despite this growing interest, the number of publications specifically addressing sustainability assessment for brine treatment remains notably low, indicating a field ready for further exploration and research. On the contrary, there has been a significant increase in scientific publications focusing on the environmental impacts of desalination or brine treatment, particularly over the last decade. This trend underscores the growing recognition of environmental concerns associated with desalination processes, likely influenced by advancements in brine management technology and heightened awareness of brine disposal issues.

A detailed review of the literature reveals a marked imbalance in the application of sustainability indicators: while technical (91%) and economic (100%) indicators are extensively employed,, environmental (61%) and social (48%) indicators fell behind. This imbalance raises questions about the comprehensiveness of current assessment methodologies in the field and underscores the need for a more balanced approach that incorporates economic, technical, environmental and social indicators into the assessment process.

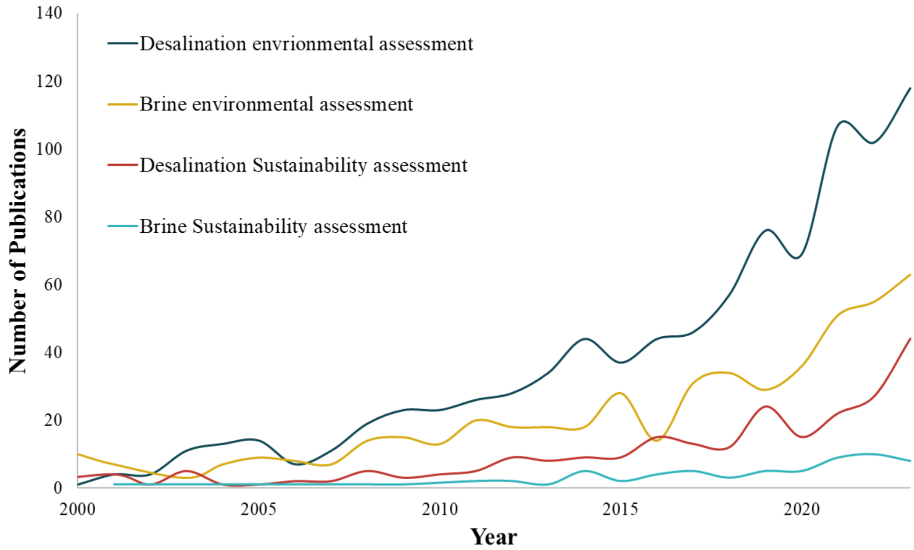

Figure 2.3. The number of publications related to sustainability assessment for desalination and brine management from 2000 to 2023. Data was obtained from SCOPUS Database using the following keywords: "sustainability assessment AND brine ", "sustainability assessment AND desalination", "brine AND environmental assessment", and "desalination AND environmental assessment".

Currently, only 35% of the studies employ the three sustainability dimensions (economic, environmental, and social), indicating a significant opportunity for methodological enhancement. Incorporating social and environmental indicators enhances the overall understanding of the impacts and benefits associated with desalination and brine treatment projects, enabling stakeholders to make more informed decisions. Details of the empirical analysis that informed these adaptations are available in Supplementary Information II.

The dominance of technical and economic indicators in desalination assessments may be due to the lack of standardized methodologies and the complexity of social and environmental impacts [23,62]. Unlike technical and economic dimensions, social and environmental indicators are still challenging to quantify consistently in desalination and brine treatment domains. Additionally, the limited availability and accessibility of relevant data [63] contribute to their limited use, as they require extensive data collection and active stakeholder engagement.

2.4.2. Analysis

2.4.2.1. Review of current assessment frameworks/methodologies for desalination and brine treatment

This section reviews the assessment approaches used in examining the sustainability of desalination systems and later brine treatment systems. Early sustainability assessments of desalination processes focused on techno-economic indicators and brine disposal while neglecting environmental and social aspects [11,12]. Over the last decade, more comprehensive SA frameworks for desalination processes have emerged, as summarised in **Table 2. 1** and illustrated in **Figure 2.3**.

Many SA methodologies have historically involved only a small group of experts in the identification and weighting of indicators, lacking robust stakeholder participation. For instance, [63] developed a multi-criteria decision-making model that considers environmental, technical, and economic indicators, but overlooked social indicators. Similarly, [62] and [20] proposed methodologies to evaluate desalination processes, addressing economic, environmental, and social issues but limiting stakeholder engagement to data collection and weight determination. [64] proposed a multi-criteria decision-making tool for the optimum selection of seawater desalination technology using technical, economic, environmental, and social criteria, involving experts only in weighting via survey. Limited stakeholder engagement can result in biased outcomes and reduce the assessment's applicability. The process of assigning weightings to different indicators lacks uniformity across studies, leading to inconsistent results. [24] proposed a methodology for the SA of desalination processes under hybrid information, focusing on improving weighting and sustainability ranking through integrated techniques. However, the selection of indicators and their weightings often lacked transparency, and stakeholder involvement, which could result in biased outcomes. This variability underscores the need for standardized approaches to ensure comparability and reliability across different studies.

Recent contributions have continued to advance the field. [41] emphasized the importance of stakeholder interactions, expert input, and case-specific contextual effects in the assessment and final decision-making. Similarly, [9] provided a well-described case study and indicator selection. However, stakeholders (experts) are involved only in the ranking process.

Until this stage of the review, brine has received limited attention, mainly as a waste stream. The above studies have not considered brine valorisation or the impact of brine disposal methods. Recent research has explored the value of recovered products from ZLD systems. However, the assessment of those systems has primarily focused on TEA [65–69]. In particular, [70] evaluated ZLD systems based on economic, technical, and administrative indicators, but environmental and social criteria were not considered in the assessment, focusing instead on integrating essential tools with decision-making tools, and experts were involved only in the weighting procedure.

Although not targeting sustainability assessment per se, [4] developed a transparent methodology for brine valorization, estimating the value that can be captured by treating the brine with a novel brine treatment system.

[17] proposed a methodological approach for identifying suitable treatment chains based on technical, economic, and environmental analysis. The technical analysis includes only the energy requirements, and the environmental study is limited to the CO_2 emissions due to the energy consumption (operational CO_2 emissions). In addition, [71] performed a TEA of brine treatment to identify the most feasible and less energy-intensive system. The analysis is oriented toward salt production, not water production, and introduces a novel parameter, the levelized cost of the NaCl crystals.

[72] performed a TEA of a seawater ZLD system, focusing on freshwater, mixed solid salt, and high-purity NaCl production. [26] studied the economic feasibility of a novel treatment chain, highlighting the added value of recovering multiple high-quality products from seawater desalination brine. Their economic assessment used two main indicators: the levelized cost of the individual products and the brine treatment-specific cost. However, the environmental and social aspects and the impact of technical aspects on the environment were not included in the analysis.

While some efforts have incorporated environmental indicators [17,25,26,73], comprehensive sustainability assessments of ZLD systems remain scarce. A first attempt to integrate social aspects into the analysis/evaluation of desalination and brine management systems was proposed by [74] through social LCA.

Few studies attempted to evaluate integrated desalination and brine treatment systems with technical and economic criteria. For instance, [75] presented a TEA of an integrated Reverse osmosis (RO), electrodialysis and crystallizer to treat seawater, aiming at salt production. The added value of salt production is included in the analysis. [25] evaluated the desalination system RO integrated with brine treatment technologies (brine concentrator, brine Crystallizer), using technical, economic, and environmental (only CO_2 emissions) criteria. The performance of the system was analysed with respect to both water and salt.

Table 2. 1. Summary of literature findings on Sustainability Assessment frameworks in the desalination and brine treatment field.

Study Reference	Methodology and MCDA method	Dimensions considered	Context	Stakeholder participation and social relevance	Main limitations
[11]	Techno-economic analysis	Technical, economic and environmental	Desalination	Stakeholders considered as data sources	Limited consideration of social aspects
[12]	Multi-criteria decision-making with AHP	Technical, economic and Environmental	Desalination	Experts involved in the weighting procedure	Lack of social dimensions, stakeholder participation
[62]	Multi-criteria decision-making with AHP	Economic, environmental, social	Desalination	Stakeholders involved in the weighting procedure	Poor stakeholder participation
[20]	Multi-criteria decision-making with AHP, Swing	Techno-economic, environmental, social	Desalination	A diverse group of stakeholders involved in the data collection and weighting procedure	Poor stakeholder participation
[24]	Multi-criteria decision-making with AHP and TOPSIS	Techno-economic, environmental, social	Desalination	No diverse group of stakeholders, Stakeholders involved in the weighting procedure	Limited transparency in indicator selection
[63]	Multi-criteria decision-making with fuzzy-AHP and TOPSIS	Environmental, technical, economic	Desalination	A small group of experts involved in indicator identification and weighting procedure	Lack of social dimension
[41]	System-level decision support tool	Technical, economic, environmental	Desalination	Experts involved in indicator selection	Expand the model to address brine management
[9]	Multi-criteria decision-making with fuzzy model	Environmental, economic, social	Desalination	Experts involved in the ranking procedure	Limited stakeholder involvement
[64]	Multi-criteria decision-making	Technical, economic, environmental, social	Desalination	Experts involved in the weighting procedure	Limitations in applying MCDA-based solutions, Lack of data

[76]	Multi-criteria decision-making with AHP	Economic, environmental, social	Desalination	Experts involved in the weighting procedure	Lack of data, Recommendation for the introduction of more metrics highlighted
[17]	Techno-economic assessment	Technical, economic, environmental	Brine treatment	No stakeholder participation	Lack of social dimension and stakeholder participation, the technical assessment includes only the energy requirements.
[77]	Techno-economic assessment	Technical, economic	Brine treatment and resource recovery	Experts involved in the design	Lack of environmental and social dimensions, lack of stakeholder participation
[69]	Cost assessment	Economic	Brine treatment	NA	Only economic dimension, lack of stakeholder participation
[75]	Techno-economic assessment	Technical, economic	Brine treatment and resource recovery	NA	Lack of environmental and social dimensions, lack of stakeholder participation
[70]	Multi-criteria decision-making with AHP and grey relational analysis (GRA)	Technical, economic, administrative (social)	Brine treatment	NA	Lack of environmental dimensions, lack of stakeholder participation
[65]	Techno-economic assessment	Technical, economic, social	Brine treatment and resource recovery	NA	Lack of environmental dimensions, lack of stakeholder participation
[66]	Techno-economic assessment	Technical, economic	Brine treatment	NA	Lack of environmental and social dimensions,

					lack of stakeholder participation
[71]	Techno-economic assessment	Technical, economic	Brine treatment and resource recovery	NA	Lack of environmental and social dimensions, lack of stakeholder participation
[26]	Techno-economic assessment	Technical, economic	Brine treatment and resource recovery	NA	Lack of environmental and social dimensions, lack of stakeholder participation

AHP: Analytic Hierarchy Process, TOPSIS: Technique for Order Preference by Similarity to an Ideal Solution.

2.4.2.2. Review of assessment indicators

This section examines the key findings from the review of sustainability assessment indicators commonly used in desalination and brine treatment systems, focusing on their suitability, challenges, and insights from the literature.

The **technical dimension** aims to evaluate the technical performance of a system. A good understanding of the process is essential [23], particularly when integrating multiple technologies. Even with high Technology Readiness Level (TRL) technologies, performance evaluation offers insights into the improvements/optimization of the system. In reported studies, the technical aspect is often combined with the economic and typically limited to the energy requirements of the technologies, overlooking more specialized technical indicators. This may be due to the assumption that the systems are already optimized. However, the technological dimension encompasses more than energy usage, including system efficiency and technology integration. However, limitations exist, as some indicators are overestimated with respect to others because of the availability of data [76].

Regarding the energy-related indicators (in the technical dimension), the energy consumption of the process or the specific energy consumption are two of the most used indicators found in the literature. Indicators to evaluate the integration of the desalination or brine treatment systems with renewable energy systems are rarely considered, though the technical feasibility of using renewable energy sources to cover the energy requirements of the desalination sector. On the other hand, the direct impact of energy use is measured extensively with environmental indicators such as GHG intensity.

The **economic dimension** aims to evaluate the economic performance of the studied systems. All the reviewed studies include economic indicators in their analysis, which underlines that the economic aspect has historically dominated decision-making [23]. Various indicators with similar outcomes have been used in the economic analysis of desalination or brine treatment systems, such as levelized cost, unit cost, treatment cost, and production cost. Levelized cost is defined as the sum of annual operational costs and capital investment, divided by the production capacity [78]. It represents the break-even price of the main product, taking into account revenues from by-products [17]. Unit cost is defined as it reflects the cost per unit of desalinated water, encompassing capital, operation, maintenance, and fuel costs [11,25,65,79]. The normalization to production capacity, used in both levelized cost and unit cost calculations, ensures that comparisons are based on standardized units of output, allowing for clearer assessments of economic efficiency and scalability across various water production methods [78].

Treatment cost, utilized by [80] and [81], considers capital costs, energy costs, and operating costs. [24] and [66] employed production cost, however, its specific definition and the formula were not provided. The main difference is that levelized cost includes revenues from by-products, while unit cost, treatment cost, and product cost do not. Unit cost and treatment costs primarily focus on energy expenses (fuel costs). Further exploration into the economic value of seawater desalination brine effluent was conducted by [82], considering the potential value of the main compounds that can be recovered from the brine. Recently, the economic impact of brine treatment has been calculated as brine treatment-specific cost [17] for ZLD/MLD systems. However, the costs of brine disposal are usually excluded from the analysis.

The **environmental dimension** aims to evaluate the effects of desalination and brine treatment processes on the environment. It is well known that the main environmental impacts of desalination are associated with high energy consumption and brine disposal. Only 61% of the reported studies used environmental indicators, with 36% assessing CO_2 emissions from the operation, such as CO_2 emissions/m^3 of desalinated water [62] or CO_2 emissions/m^3 of brine [17]. The carbon footprint can be considered one of the simplest ways to measure the environmental impact of a process, and it can give an excellent first insight.

Regarding brine, limited efforts have been made, with 60% of the sustainability assessments for desalination processes, including the brine disposal in the analysis [76], often without detailed analysis. Notably, brine disposal or minimization is typically not included in the environmental assessment of ZLD or MLD systems. The main indicators found in the literature are the pollution potential from brine disposal [62,76], eco-toxicity [14,20,83,84], and increased salinity and temperature [20,23].

The use of chemicals is directly related to environmental impacts in the desalination sector; however, it is not considered in the reviewed works. While [85] referred to chemical consumption in the economic assessment, it was not included in their subsequent work where the proposed framework was implemented [62]. Similarly, [81] estimated the cost of chemicals in the economic assessment of the system but not in the environmental assessment.

The **social dimension** aims to evaluate the effect on the local community and the employees [23]. Only 48% of the reported studies used social indicators, with 45% assessing impacts on the local economy and communities [20,23,25]. These studies considered indicators such as the level of aesthetic acceptability, noise levels, provision of employment opportunities, safety levels, quality of life, and effectiveness and equity of employment. [65] recommended the indicator of willingness to pay. Water quality was used in 25% of the studies to assess social-technical aspects [76]. [70] included the operational complexity of the processes as a social indicator, reflecting the need for skilled labour. Similarly, [24] emphasized the importance of specific expertise, and [25] highlighted the significance of high-skilled employees and specialized knowledge. [86] stressed the importance of practical and real-world factors in the assessment by considering the industry's past experiences, local public stakeholders, investors, and media values.

Acknowledging the social dimension's challenges, particularly in data availability, uncertainty, and survey bias, is crucial [32]. The data collection for social indicators can be challenging, especially for indicators like political risks/impacts and benthic seabed damages [20]. These challenges are exacerbated when collecting data from multiple individuals within an organization without direct collaboration with S-LCA practitioners [74]. Such complexities often lead to the reliance on assumptions when evaluating social impacts [87], introducing an element of uncertainty into assessments and questioning their comprehensiveness. To address the issue of data availability and improve the robustness of assessments, researchers should explore new data collection methods, such as community surveys, and actively involve stakeholders, including local communities and industry experts. This involvement can enhance the accuracy of impact assessments and bridge the gap between available data and a comprehensive evaluation of social and environmental impacts.

In summary, the review underscores the need for a more balanced and holistic approach to sustainability assessments in this field. A paradigm shift from a predominantly technical and economic focus to a more inclusive assessment of social and environmental aspects is warranted. Moreover, addressing the data availability issue and tackling uncertainty will enhance the robustness of assessments, contributing to a comprehensive understanding of system sustainability. **Table 2. 2** gives a summary of the most frequently used indicators in the literature. Their definition and mathematical description are given in Supplementary Information III (see Section B). Notably, brine disposal is not commonly considered in sustainability assessments, which encompass economic factors, such as disposal costs, as well as environmental and social impacts.

Table 2. 2. Summary of the most frequently used indicators in the literature.

Dimension	Indicator	Frequency	Method/Concept
Technical	Specific energy consumption	56%	MCDA, TEA, SA, EIA, Energy assessment
	Water recovery	44%	MCDA, TEA, SA, EIA, Energy assessment
	Energy consumption	33%	MCDA, TEA, SA, EIA, LCA
	Water quality	28%	MCDA, TEA, SA
Economic	OPEX	85%	MCDA, TEA, SA, Cost assessment, EIA, Energy assessment
	CAPEX	69%	MCDA, TEA, SA, Cost assessment, 3E assessment
	Freshwater produced cost	31%	MCDA, TEA, SA, 4E assessment, EIA, Energy assessment
	Unit cost	28%	MCDA, TEA, SA
Environmental	GHG emissions	62%	MCDA, TEA, SA, LCA, EIA
	GHG intensity	38%	MCDA, TEA, SA, 3E assessment, 4E assessment, LCA, EIA, Economic assessment
	Global warming	31%	LCA
	Ecotoxicity	31%	LCA, EIA
Social	Health and sanitation;	28%	SA
	Acceptability	23%	Decision support tool
	Education and training	13%	SA
	Public safety	13%	SA

EIA: environmental impact assessment, LCA: life cycle assessment, MCDA: multi-criteria decision analysis, SA: sustainability assessment, TEA:techno-economic assessment.

2.4.2.3. Review of decision-support tools for resource recovery systems from wastewater effluent and waste

In addition to reviewing sustainability assessments on desalination and brine treatment studies, decision-support tools for resource recovery systems from wastewater effluent and waste have been incorporated to inform the development of an assessment framework for desalination. The analysis focuses on stakeholder participation and methodological strengths and weaknesses.

While stakeholders' participation emerges as a fundamental aspect across many studies, its implementation varies. For instance, [60] and [88] acknowledged the importance of stakeholder engagement in the development and application of sustainability assessments and decision-support tools, but lacked actual stakeholder involvement, raising questions about the validity and applicability of their findings. Conversely, [89] and [90] emphasized the system thinking approach and stakeholder participation in the assessment, advocating for transparent and inclusive approaches. [91] advocated for a context-specific approach that enables the involvement of stakeholders in diverse ways throughout the stages of the assessment process to strengthen assessment credibility.

Stakeholder participation also varies across the methodological stages and among the studies. For example, [92] stressed the necessity of understanding the decision context and engaging stakeholders. They found that preliminary interviews can offer insights into current drivers and challenges and help identify key stakeholders. Similarly, [93] and [92] proposed comprehensive assessment tools that involve stakeholders in indicator selection. [92] selected the indicators and criteria based on the insights from the preliminary interviews, while [93] involved stakeholders through workshops, interviews and webinars for indicator selection. Similarly, [94], defined indicators based on experts' input and [91] based on specific context relevance. Conversely, [60] defined the criteria and the indicators based on their frequency of use in previous studies.

It has also been noticed that stakeholder participation in the design of alternative scenarios (treatment chains) for evaluation varies. In particular, [94] designed alternative scenarios based on necessity and viability, while [89] incorporated concepts from the circular economy and industrial symbiosis and actively engaged stakeholders in scenario communication. Similarly, [91] developed alternative scenarios based on experts' knowledge through interviews and workshops. However, almost none of the above studies used and explained a robust methodology for the design of the alternative scenarios. Only [94] explicitly discussed the improvement of a methodology for the scenario development by exploring existing regulations, guidelines and standards for wastewater treatment and water reuse in the understudied region. Conversely, [95] and [60] use an existing knowledge database to design alternative scenarios without any feedback from relevant stakeholders, mentioning that the validity of the results depends on the information provided by the user since there is no feedback loop.

Reviews by [91], [96], and [97] highlighted the ongoing need for further research and improvement in decision-support tools for resource recovery plants. Specifically, [98] emphasized the importance of understanding practitioner interaction with those tools, while [97] stressed the importance of close collaboration with stakeholders in the MCDA for better problem structuring and transparent inclusion of public values and concerns.

2.4.2.4. Key insights

The review indicates that the domain of research is relatively new, leaving room for improvements and enhancements. A key question arises: Why are existing SA methodologies underutilized in the desalination literature? Researchers often develop methodologies based on fundamental principles rather than utilizing existing frameworks, seeking greater transparency. These new approaches often focus solely on weighting and ranking methodologies, overlooking other critical steps. Without clear methodological choices, such as indicator selection and multi-criteria decision-making (MCDM) methods, results interpretation may be misleading [42]. Furthermore, the review exposes a common misuse of the term 'sustainability' in analyses, suggesting a need for greater adherence to sustainability principles. While sustainability is a popular term, its misuse can compromise the integrity of studies, undermining their credibility.

The MCDA approach is favored for sustainability assessment also in the desalination field due to its ability to address the multidimensional nature of sustainability challenges. While certain studies have made progress in proposing frameworks or methodologies (e.g. [20,24,62]), there remains a general lack of comprehensive stakeholder engagement. Relevant stakeholders’ involvement in decision-making processes is often limited to the final stages in a less integrated way. This narrow engagement can lead to biased outcomes and reduce the applicability of the assessment. Furthermore, potential biases in data collection methods, such as surveys and interviews, can affect the validity of the assessments. Although social indicators provide valuable insights, they alone are not sufficient to address the complex challenges posed by desalination and resource recovery systems. The consideration of all sustainability dimensions (economic, environmental, social and/or technical) must be complemented by meaningful stakeholder participation to align resource recovery innovations with policies, markets, and societal concerns.

The reviewed studies mostly involved experts in the desalination field, neglecting the input of stakeholders with diverse backgrounds, including local community members. Additionally, data availability and quality pose challenges in obtaining reliable data, particularly for social indicators, which complicate comprehensive sustainability assessments. Culture, values, and drivers for change are rarely considered, except in works by [41] and [9], which emphasized the significance of case-specific contextual effects in sustainability assessments, underscoring the need to consider local conditions and stakeholder insights. Conversely, studies on resource recovery from other sources (see Section 2.4.2.3) have demonstrated various approaches to involve stakeholders throughout the assessment process, promoting transparency and inclusivity. These studies emphasized the importance of understanding decision contexts, engaging stakeholders in indicator selection, and considering contextual relevance to enhance the credibility of the assessment.

This lack of stakeholder involvement and consideration of contextual factors highlights the need for improvements in existing works and an approach that addresses these limitations. In this regard, the implementation of VSD in the desalination field and resource recovery from seawater can significantly contribute to overcoming these shortcomings and enhancing the overall sustainability assessment process.

Based on the key insights and best practices for engaging stakeholders from the literature review, below is a list of key criteria that an SA needs to include:

- Comprehensiveness: Provide a holistic approach by integrating environmental, social, economic, and technical dimensions.
- Transparency: Provide explicit information on stakeholder participation, data collection and methodological choices, such as selecting indicators and alternative options at every stage of the process. This ensures that all decisions are open to scrutiny and accountability.
- Stakeholder participation: Promote continuous engagement and open communication with stakeholders representing diverse perspectives and interests, ensuring their inclusion in its development to provide relevant and democratic solutions. Clearly define the criteria for stakeholder selection and methods of engagement. Use participatory tools such as surveys, workshops, and focus groups to gather diverse perspectives. Identify and mitigate potential biases early by involving a diverse group of stakeholders and using reflective frameworks
- Transdisciplinary: Integrate methodologies and knowledge from different disciplines for knowledge co-production and social learning.

2.4.3. Synthesis: A proposed framework to assess integrated desalination and brine treatment systems

Building upon the theoretical background outlined in Section 2.2 and insights from the literature reviews in Sections 2.4.2.2 and 2.4.2.3, an assessment framework was developed. The framework consists of six steps: 1) Problem definition, 2) Assessment indicators definition, 3) Design of alternative scenarios, 4) Data acquisition, 5) Assessment indicators quantification, and 6) Performance analysis. **Figure 2.4** illustrates the proposed framework in a block flow diagram, incorporating the stakeholder engagement gradient to denote the degree of participation at each step. This framework provides various levels of investigation by considering insights from experts and literature. The following sub-sections give a detailed description of the individual steps

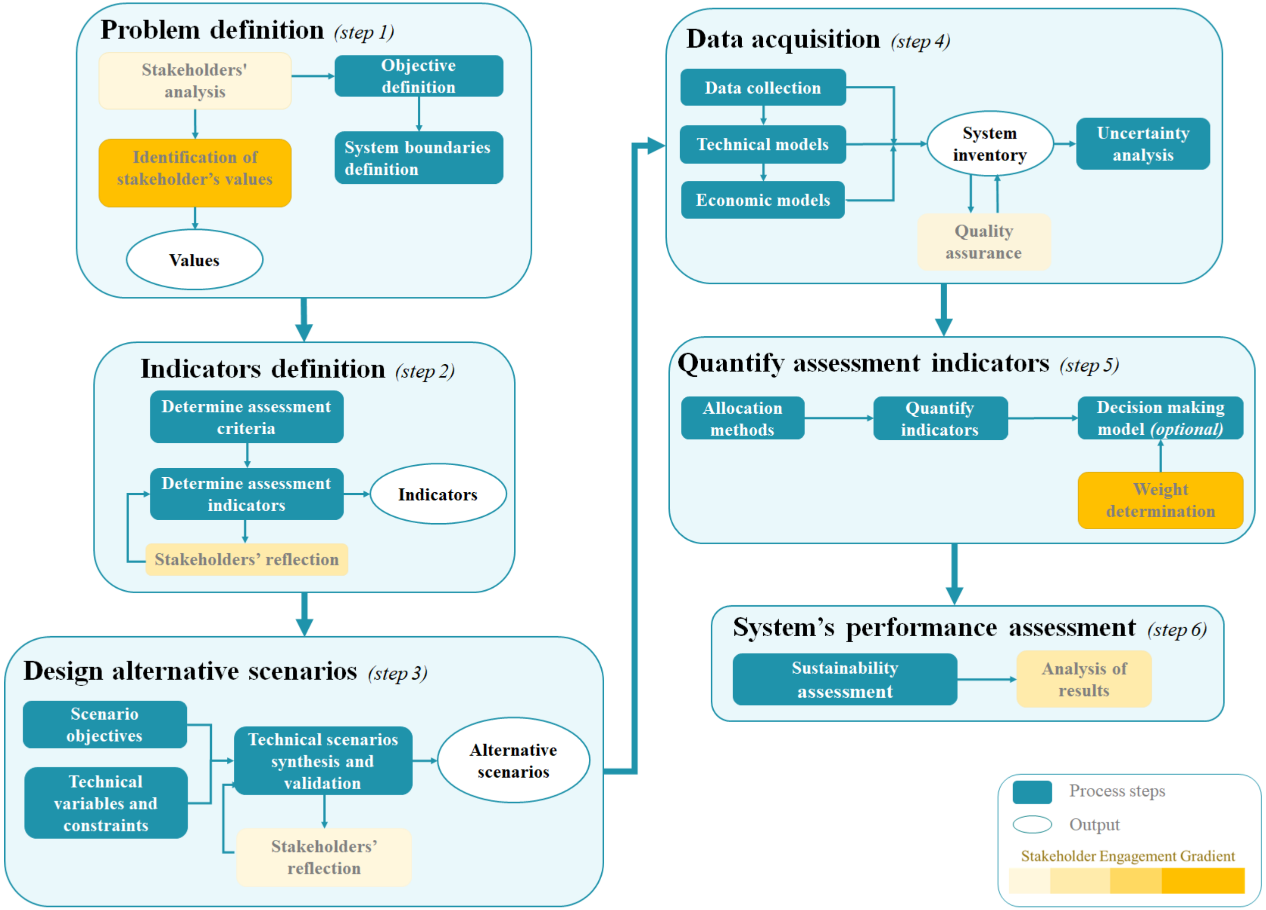

Figure 2.4. Schematic representation of the proposed framework for a VSD-informed sustainability assessment of desalination and brine management. The Stakeholder Engagement Gradient illustrates varying degrees of stakeholder involvement across different steps, ranging from light gold-yellow indicating low involvement to dark gold-yellow indicating high involvement.

2.4.3.1. Problem definition

The proposed framework is developed to be applicable to different case studies; thus, it is essential to describe and understand the case study in the early stage of the assessment. For this, the framework proposes establishing stakeholder engagement followed by a participatory definition of the problem statement.

Stakeholder analysis and engagement: The involvement of a diverse range of stakeholders, including researchers, policymakers, engineers, and affected communities, is crucial. Grouping these stakeholders by their interests and potential impact ensures that all relevant perspectives are integrated into the assessment process [99,100]. Note that not only technical experts or stakeholders that benefit from the integrated system should be considered in the analysis, but also stakeholders that might be indirectly affected or even lose from it need to be part of the group [101]. For example, in an integrated seawater desalination and resource recovery project, stakeholders might include local communities affected by brine disposal, companies involved in resource recovery like the salt industry and technology developers/suppliers, and environmental organizations overseeing the environmental impacts. A list of potential stakeholder groups is given in Supplementary Information III (see Section C), while [100] discusses in detail the stakeholder identification and analysis techniques.

Active involvement: Once the stakeholder analysis is conducted, the next step is to actively involve stakeholders in the assessment process. While the proposed participatory approach aims to involve stakeholders at various stages of the assessment process, the level of participation of each stakeholder can vary. Factors such as power, capacity, interest, and the ability to engage must be considered when determining their participation (see example in Supplementary Information III, Section C). The level of participation ranges from informing them to collaborating with them to initiate the process. The most intense participation occurs when local stakeholders initiate the process, perform the analyses, and are involved in the decision-making processes. They also have ownership of the data inputs and final products. There is no optimal level of participation. The degree of participation depends on the specific study [101]. It is important to ensure that all stakeholders, regardless of their interests or potential gains or losses, are given equal consideration in the participatory process, promoting democratization, ownership, and transparency. Participation should start early and continue throughout the stakeholder analysis to enhance process effectiveness.

Each step clarifies when and how stakeholders should be involved and at what level of engagement, ensuring a transparent and collaborative process. For example, in the problem definition step, stakeholder participation and engagement are particularly crucial, as early involvement generates interest and ensures that community needs and values are accurately reflected. The level of participation should be high, requiring substantial input and feedback from stakeholders, while the degree of engagement should involve a wide variety of stakeholders to gather diverse perspectives. This early and continuous involvement ensures that the assessment is grounded in a comprehensive understanding of the stakeholders' concerns and objectives.

Addressing biases: Identifying and addressing potential biases early in the assessment process is crucial. Involving a diverse group of stakeholders will not only provide multiple perspectives but also reduce individual bias. Critical Systems Heuristics offers a reflective framework and tools, such as *"boundary questions"* to explore system biases [102].

Transparency: is a critical aspect at all participatory stages, from the selection and invitation of stakeholders to the development of engagement activities and the analysis of outcomes. Transparency in stakeholder engagement means openly communicating the criteria for stakeholder selection, the methods of engagement, and how stakeholder inputs are integrated into the assessment. This ensures that decisions regarding stakeholder participation are made openly, addressing questions of who is included and on what grounds, taking into account the motivations and intentions of both stakeholders and practitioners/ facilitators [101]. Participatory tools, including surveys, workshops, focus groups, brainstorming, group facilitation, SWOT (Strengths, Weaknesses, Opportunities, Threats) analysis, and mind mapping or a combination of tools facilitate stakeholder engagement [44,101].

Problem statement definition: Described and analysed the problem statement and information, such as location, available energy sources, market availability, and constraints. Furthermore, to identify and analyse the main sustainability issues considering the socio-technical context around the case study, a thorough review of relevant literature, policy documents, and stakeholder inputs should be conducted [58]. This process can involve evaluating the environmental, economic, and social impacts and exploring potential trade-offs between different sustainability dimensions. It is crucial to transparently communicate any simplifications made during this process to ensure the study's robustness and clarity.

Additionally, understanding the current challenges and drivers is an essential opportunity to engage with key stakeholders. Including social-cultural aspects in the description of the case study will not only add value to the assessment [103] but also help in the design of alternative scenarios (see Section 2.4.3.3). This can be achieved by conducting workshops, interviews, or surveys with stakeholders (local communities, experts, researchers) to gather insights on the socio-cultural context, values, and preferences that should be considered during the assessment process. The identification of stakeholders' values is a critical step in the proposed framework, and it has to be carried out in the early stage of the assessment.

System boundaries and objectives: Define the objectives of the assessment and set system boundaries. The system boundary outlines the scope of the system being assessed, specifying what is included and excluded in the analysis. For instance, in a sustainability assessment of an integrated seawater desalination and brine treatment plant, the system boundary might include the intake of seawater, the desalination process itself, brine treatment processes for resource recovery, the output of fresh water and other recovered materials, and the disposal of brine. This represents a cradle-to-gate system boundary, focusing on the operation phase of the system and excluding equipment manufacturing and downstream activities like the distribution of desalinated water to consumers. Recognizing biases related to system boundaries and key assumptions is inherent, as these are defined by the practitioners/ facilitators and can influence the assessment outcomes. For example, excluding the distribution network might overlook significant environmental impacts from transportation and emissions. Transparency about biases and their implications is essential for managing their impact.

Decision-making tools: The proposed framework can be applied either for soft decision-making tools, which focus on decision support and require minimal information, or hard decision-making tools, which utilize mathematical programming techniques and require extensive information. However, the choice between soft and hard decision-making tools needs to be determined in this step. The choice between soft and hard MCDA depends on several factors, such as the objective, the complexity of the problem, the availability of data, and resource availability [37] (see example in Supplementary Information III, Section C).

To sum up, the following questions need to be answered:

- Who are the stakeholders, and what is their level of participation?
- What is the goal of the assessment?
- What are stakeholders' values?
- What are the current drivers and challenges?
- What is the approach of the decision-making tool (soft or hard) and the level of comprehensiveness?
- What are the system boundaries (geographical, time) of the assessment?

For a visual representation of the problem definition process, tools, and considerations, refer to **Figure C.1** (see Supplementary Information III, Section C).

2.4.3.2. Indicators definition

This section describes how sustainability issues and the identified values from the previous step (see problem definition) are translated into performance indicators. The connection between the identified values and the selected indicators ensures that the assessment is relevant and focused on the case study. This work proposes the definition of the performance indicators before the development of alternative scenarios and data acquisition. This is essential to ensure a consistent and transparent approach, minimizing the potential influence of participants' interests on the assessment process. By selecting indicators at this stage, the methodology remains robust and unbiased throughout its execution. After designing alternative scenarios, the indicators can always be updated to ensure their relevance and representativeness.

The indicators can be selected on the basis of a literature review (see the developed database in Supplementary Information I). This database serves as a solid foundation, offering a comprehensive list of indicators categorized by their relevance and application in desalination and brine treatment studies. For instance, in a case study focusing on the technical performance of resource recovery, users can refer to technical indicators such as water recovery efficiency and specific energy consumption for a product from the database. While this database is a starting point, it is crucial to remain open to other performance indicators from the literature and adjust them individually to each case study, the identified values, and the objective of the assessment. The goal is not to lead directly to common indicators but to offer guidance on overall indicator system design and analysis [42].

A large number of indicators would increase the complexity of the assessment. For this reason, a clear-cut approach is needed for selecting the individual indicators [55], and some of them are excluded. The most relevant indicators are selected to comprehensively assess the systems and provide valuable insights, following guidelines. A theory-driven approach is used, and data is only one of the many aspects considered [30]. In particular, the selection of performance indicators is primarily based on four critical criteria:

1) Relevance to stakeholders' values: Indicators should directly reflect stakeholders' values and address the problem statement and the systems under study (applicability and practicability).
2) Measurability and data availability: The selected indicators should be measurable, and data should be readily available to quantify them.
3) Comprehensiveness: The indicators should collectively provide a comprehensive view of the system's performance.
4) Transparency: Indicator selection and measurement should be transparent and easily understandable [57,58]. This means providing stakeholders with detailed information about how indicators were chosen, how they align with stakeholder values, and the process for evaluating their relevance.

Note that the selected indicators should not allow compensation. This means that a gain in one aspect (e.g., economic benefits) should not be used to justify a loss in another (e.g., environmental degradation). Furthermore, a well-balanced set of indicators might better represent the diverse value orientations of the stakeholders [34]. In a participatory approach, as in our study, effective communication with the stakeholders and guiding decision-makers is essential. To enhance communication and evaluate the result better, the indicators have to be understandable, straightforward (using clear and plain language), and present information objectively [42]. Although “user friendliness” is one of the main advantages of reductionism [30], for this framework, we can accept partial reductionism for the benefit of effective communication.

Finally, it’s essential to share both the selected indicators and the followed procedure with relevant stakeholders to ensure transparency and collaboration in the final selection of the indicators. The level of participation should be substantial, with stakeholders providing critical feedback and recommendations on the selection process, and the degree of engagement should be high, involving a variety of stakeholders to gather diverse opinions. For instance, during workshops or surveys, stakeholders could identify alternative indicators or suggest modifications to existing ones that better align with their concerns. This feedback could lead to adjustments in the selection of indicators to ensure they reflect the stakeholders’ values more accurately. Below is an example of a primary selection of indicators based on given values.

For a practical example, the relationship between values, objectives, and indicators is that values determine the objective employed to evaluate alternative scenarios, while the indicators are the parameters that measure the performance of those scenarios in alignment with the objective. Consider evaluating a resource recovery configuration (integrated seawater desalination and brine treatment system) in terms of water and energy security. Specifically, the value of water security might be evaluated by measuring the system’s water production quantity, which reflects how effectively the system recovers water from seawater. This enables an assessment of the overall resource recovery from seawater and ensures a comprehensive evaluation of water security. This contribution/impact is assigned to the technical dimension. Similarly, 'energy security' can be assessed by monitoring both electrical and thermal energy consumption, alongside the integration of renewable energy sources. By quantifying these indicators, we can assess the overall impact of the configuration on water and energy security, ensuring that the system aligns with stakeholder values and objectives.

2.4.3.3. Design of alternative scenarios

The review of existing assessment studies in the literature reveals a lack of robust reasoning behind the selection of alternatives or the design of alternative scenarios (systems) [32] (see also [17,104]). Choosing what alternatives to include can become very challenging and complicated, especially when technologies are integrated into a system. While conventional MCDA methodologies begin by selecting alternatives after or within the scope definition. [32,105], in this work, the design of alternative scenarios comes after the definition of the indicators. This adjustment is made to ensure transparency in the assessment process and prevent stakeholders' interests or preferences from influencing indicator selection. By selecting indicators without prior knowledge of the alternatives, we ensure that stakeholders' interests or preferences do not affect the choice of indicators. This approach allows for a more objective and unbiased assessment, as the selected indicators are independent of the specific scenarios and are solely based on their relevance to the sustainability dimensions and identified values. Consequently, the evaluation of alternatives remains consistent and fair, focusing on their actual contribution to sustainability objectives rather than being influenced by any predetermined preferences or expectations.

The development of technical scenarios is based on the identified values from Step 1 (see Section 2.4.3.1) and active participation in the identification of solutions. These technical scenarios present various ways of combining technologies to achieve the objectives(s) while considering stakeholders' values. They aim to gain valuable insights into important variables around the technology and how different technical configurations address specific societal aspects. Transparency in this phase involves clearly documenting the process and rationale behind the selection of any technical alternatives (process configuration). This includes being aware of potential biases for specific technologies or products Clearly documenting these choices helps ensure unbiased evaluation and builds stakeholder trust.

For a practical example, in a recent review of resource recovery from brines and other wastewater [43], energy and GHG emissions, cost and affordability impacts, and societal perceptions on the ownership of water and recovered resources were discussed as prominent issues that can bring forth tensions around resource recovery from desalination brines. These issues are distinct from the identified values in the sense that they represent the broader concerns and challenges related to the sustainability of the case study. While their analysis was not specific for a given geographical context or case study, it allows us to derive general objectives in response to sustainability and societal concerns around resource recovery innovations for seawater desalination:

- Minimize energy use and GHG emissions: ensuring that resource recovery processes are energy-efficient and have a low carbon footprint.

- Minimize additional costs to existing water supply services: ensuring that the resource recovery does not significantly increase the cost of water for consumers.
- Maximize the recovery of resources, especially water and scarce or critical resources: focusing on extracting valuable materials from brine, such as minerals and high-quality water.

However, it is impossible to satisfy all objectives at once. Thus, technical scenarios can serve to evaluate and bring trade-offs to discussion. Considering the objectives and the associated challenges mentioned above, three principles for developing scenarios are:

- Water recovery focus: Prioritizing the recovery of fresh water from brine.
- Resource recovery focus: Emphasizing the extraction of valuable minerals and other resources.
- Minimum liquid discharge: Aiming to minimize the volume of brine discharge and not resource recovery.

These principles are proposed as a starting point for developing detailed scenarios for specific case studies, structured around three main technical scenario variables: 1) process and technology, 2) product and by-products, and 3) raw materials and utilities [106]. Additionally, insights and lessons learned from the literature and technology experts are used to design the technical scenarios.

Stakeholders should be engaged in providing feedback on the design of the technical scenarios to ensure the incorporation of diverse perspectives and technical knowledge and to avoid biases. The level of participation should be moderate, with stakeholders offering critical insights and recommendations. The degree of engagement should be low, involving a small, focused group of stakeholders with technical expertise to refine the scenarios and ensure they align with the broader sustainability objectives.

2.4.3.4. Data acquisition

One of the most critical steps in the assessment frameworks is data acquisition because it is directly related to the accuracy, reliability, and quality of the results. The effectiveness of the assessment framework depends on securing access to accurate and high-quality data from different sources [55,107]. From the literature review, it was found that one of the main limitations of previous works is the availability of data [76,108]. For these reasons, when reliable data from stakeholders are not available, the use of technical models consisting mainly of mass and energy balances is recommended as an alternative.

For instance, a GitHub repository offers technical process and economic models for integrated seawater desalination and brine treatment technologies for resource recovery (https://github.com/rodoulak/Desalination-and-Brine-Treatment-Simulation-.git). These models provide a valuable resource for generating data when direct stakeholder inputs are limited. They offer pre-built models for simulating various desalination and brine treatment scenarios, which can be tailored to fit the specific parameters and indicators identified in Section 2.4.3.2.

In general, more complex models can provide more data, but the complexity does not necessarily correlate with usefulness or accuracy [109]. The selection of the methods, models, tools, or algorithms depends on the assessment's objective. In light of the challenges associated with data availability, particularly in early-stage assessments, the use of technical and economic models emerges as a valuable approach to ensure the availability of sufficient and high-quality data for quantifying technical, economic, and environmental indicators.

It is important to note that the framework does not rely on specific tools like LCA. Instead, it suggests using simpler methods for data generation. Surveys, interviews, and literature reviews are required to determine the social indicators [110]. These methods play a crucial role in the data collection process, providing valuable information and ensuring consideration of different perspectives. High-quality survey and workshop methodologies are essential for robust data collection.

It is important to recognize that biases can arise in data acquisition due to assumptions made during data collection and model selection. For example, excluding certain data sources or relying on specific models can introduce bias, impacting the results. To manage these biases, use a broad range of data sources to balance perspectives and clearly document and communicate all assumptions made.

The participation of stakeholders is important to ensure the availability of high-quality data and manage bias. Engaging stakeholders actively in this step not only enhances data reliability but also fosters transparency, trust, and collaboration among stakeholders, and their feedback helps identify and correct biases in the data. Transparency in this phase means clearly documenting the sources of data, the methods of collection, and any assumptions made during this process. Stakeholders play a dual role in providing and validating data. In particular, stakeholders have a dual role in this process: they provide data and validate it. Their involvement in giving data—through sources such as local knowledge, expert insights, and empirical evidence—ensures the inclusion of diverse perspectives and real-world relevance. Additionally, stakeholders help to validate the data by reviewing and confirming its accuracy and applicability. Stakeholders should receive both performance data during stakeholder engagement and the final results of the analysis [111].

In case of data gaps, methods like mean substitution or correlation results can be applied. However, it is necessary to assess the suitable method that can produce reliable results [55]. After the data collection, uncertainty analysis has to be done to increase the reliability, accuracy, and validity of the data. The various sources of data or some of the input data to the model can affect the uncertainty of the model [107]. Thus, it is vital to analyse and quantify the uncertainty of the data [112]. This can be done through various methods, such as sensitivity analysis or Monte Carlo simulation [109]. The choice of method depends on the specific assessment and the data being analysed. The next step is the integration of the technical, economic, and environmental models. The number of models to be combined should be decided carefully. The higher the number of coupled models and tools, the higher the complexity of the integrated model [107].

Overall, engaging stakeholders in the data acquisition process not only provides access to crucial information but also helps to build trust and increase transparency. Stakeholder participation helps to validate the data, address data gaps, and improve the overall quality of the assessment results. Note that the degree of participation (number of stakeholders involved) is low.

2.4.3.5. Performance analysis: Quantify assessment indicators and alternative scenarios analysis

In this step, the interpretation of the results is carried out to provide decision-makers with a comprehensive evaluation of the alternative scenarios and required information for decision-making. The approach in this step must be adjusted based on the nature of the MCDA being employed (soft or hard), see problem definition (Section 2.4.3.1) and Supplementary Information III (Section C). Particularly in hard MCDA, once the selected indicators are determined using the data acquired in Step 4 (Section 2.4.3.4), their values must be scaled into dimensionless values (normalized) for analysis and comparison. This is necessary because the various performance indicators have different physical dimensions (units) [113]. Additionally, the performance analysis in hard MCDA includes more steps, such as selecting the MCDA method for weight determination, aggregation, alternatives ranking, and sensitivity analysis. Conversely, in soft MCDA, normalization is not necessary. The performance analysis in soft MCDA focuses on interpreting the results without the need to scale the indicator values to provide structured knowledge and support decision-making.

Nowadays, it is well-accepted that there is no “best” MCDM method [114]. Instead, the selection of suitable methods for ranking and weighting depends on the characteristics of the problem, such as the data, the scope of the study, and the number of indicators [55,114]. Determining weights aims to assign relative importance to indicators, reflecting their significance in decision-making. Weighting dimensions and indicators have been a critical issue in the sustainability literature [115]. In general, MCDM methods have been classified as (i) utility function (AHP, Multi-Attribute Utility Theory (MAUT), Simple Additive Weighting (SAW)), (ii) outranking relation (ELECTRE, PROMETHEE) and (iii) sets of decision rules [31]. [116] and [38] give an overview of MCDM methods, their description, strengths, and weaknesses. Note that for strong sustainability, only outranking methods can be selected due to the limited or abolished compensation among/within sustainability dimensions. This means that improvements in one dimension (e.g., economic) cannot offset or *"compensate"* for declines in another (e.g., environmental). In contrast, methods such as MAUT and AHP are more aligned with a weak sustainability perspective, with criteria trade-offs as the norm [31,117]. Detailed definitions of strong and weak sustainability are provided in Supplementary Information III (see Section A).

In the field of desalination, AHP emerged as the most frequently utilized method in the reviewed studies to handle complexity, uncertainty and consistency, followed by Technique for Order Preference by Similarity to an Ideal Solution (TOPSIS) (see **Table 2. 1**). However, it was observed that many studies did not provide explicit justification for selecting a particular MCDM method. There were exceptions, such as the work by [62] that briefly explained the rationale for choosing and [63], who explained that fuzzy-AHP and TOPSIS were selected to address uncertainty and sensible attributes with simplified programming methods. More recently, the Best-Worst method (BMW), developed by [118], has been extensively applied in other fields [116,119,120] but has not yet been explored in the context of desalination.

Stakeholder groups often have varying preferences when evaluating options. Traditional methods of evaluation aggregate these preferences into a single weight or index. However, aggregation can be problematic when dealing with a large number of stakeholders, conflicting opinions or extreme opinions. In such cases, the average weight may not represent everyone's opinion, leading to a loss of valuable information. This can ultimately reduce the effectiveness of the decision-making process [97,121]. In sustainability assessment studies, it can be more beneficial to focus on understanding the decision-making process and differences in stakeholders' opinions rather than arriving at a final ranking for alternatives. While there may not be a definitive answer to sustainability performance, a participatory approach that involves stakeholders can help them learn and better understand the situation.

Transparency in performance analysis involves documenting and communicating every methodological choice, rationale, and assumption made during this phase. This includes explaining why certain methods are chosen, how weights are determined, and how indicators are normalized or not. This transparency is further ensured by presenting analysis results and interpretations to stakeholders, as mentioned in data acquisition. This approach allows stakeholders to understand the decision-making process, fostering accountability and trust in the assessment outcomes.

Stakeholder involvement is crucial in decision-making for informed choices that reflect community needs and values. The active participation of diverse stakeholders ensures a comprehensive evaluation that considers diverse perspectives, values, and stakeholder needs.

2.5. Impact, limitations, and future work

A critical review of the state of SA for desalination and brine treatment systems found that there is no existing sustainability framework for integrated systems in the literature. To address this gap, this study proposed an SA framework integrating methods from various fields, including VSD, to assess the sustainability performance of integrated desalination and brine treatment systems for resource recovery.

Incorporating VSD helped consider social challenges and enhance existing methodologies. By incorporating stakeholders' values and value tensions into the assessment process, we encourage a context-specific selection of indicators that resonates with the preferences and priorities of those affected by the decisions. This integration allows for a more inclusive and participatory approach, democratizing the decision-making process and promoting transparency and credibility.

The developed indicator database (see Supplementary Information I) is a valuable resource for selecting performance indicators tailored to desalination and brine treatment case studies. It significantly contributes to the research community by providing a structured, accessible repository of indicators, enhancing SAs through transparent and adaptable selection. Offering a wide range of technical, economic, environmental, and social indicators, the database supports comprehensive and relevant evaluations, advancing the field of SA. The proposed methodology can guide the user in identifying improved opportunities through the development and evaluation of alternative technical scenarios where social and stakeholders' values are incorporated. This broadened step is missing in existing frameworks in the literature. Overall, the integration of key elements from VSD and other fields enabled the development of a robust SA framework, filling the research gap with a comprehensive and transparent assessment methodology that considers the interconnections between economic, environmental, social, and technical aspects. It involves stakeholders throughout the assessment process and incorporates their values, ensuring relevance to their concerns and ambitions.

The developed sustainability assessment framework is designed to be applicable to a range of users. Potential users include researchers conducting academic studies on desalination and resource recovery, government agencies involved in policy-making and regulation of water treatment technologies, plant owners or operators looking to enhance the sustainability of their operations, and investors or consultants evaluating future developments in the desalination sector.

The framework can be applied beyond seawater desalination to various technological domains. By adapting indicators to suit specific contexts, it offers a consistent and robust assessment methodology across different fields, such as wastewater treatment, renewable energy systems, and industrial resource recovery. This systematic approach facilitates informed decision-making and promotes sustainable practices.

Bias in SA is unavoidable, stemming from the decision-makers' choices regarding system boundaries and assumptions. To manage bias, this framework recommends several strategies: (1) explicitly identify and document potential biases from the start, (2) involve a diverse range of stakeholders to balance perspectives, (3) ensure transparency in all methodological choices, (4) use reflective tools like Critical Systems Heuristics to examine and refine assumptions, and (5) regularly update the assessment based on feedback and new insights. These steps aim to enhance the robustness and credibility of assessments.

While this study recognizes the significance of stakeholder involvement and proposes a participatory approach, it is crucial not only to engage stakeholders in an existing project or process but also to include them in its development. However, effective stakeholder engagement throughout the assessment requires substantial time, resources, and coordination. Stakeholders' availability, influenced by their existing tasks and commitments, can limit their engagement. To address this, it is essential to communicate the benefits of the assessment framework [92].

Moreover, reducing conflicts and building trust among stakeholders is vital for moving towards a shared vision [44]. Educating stakeholders, including researchers and decision-makers, about the benefits of collaboration can facilitate meaningful engagement. Future research should focus on developing effective strategies and methodologies to enhance participation. Finally, exploring case studies and real-world applications of the framework in different contexts can provide valuable insights into the practical implementation of stakeholder engagement and the associated benefits and limitations.

Future work should implement the proposed framework, including mathematical models for formulating, calculating, and analysing sustainability performance and integrating different analytical tools to develop a multi-sectoral system without increasing the complexity.

2.6. Conclusions

The literature review identified critical shortcomings in current sustainability assessments for seawater desalination and brine treatment systems. These assessments notably lack a comprehensive approach and neglect social aspects and stakeholder involvement. To address these deficiencies, we proposed a novel Sustainability Assessment (SA) framework that integrates participatory multi-criteria analysis and value-sensitive design into the decision-making process. This approach advances SA by recognizing the importance of incorporating social dimensions through stakeholders' values, enhancing the framework's robustness, and aligning decision-making with stakeholders' concerns and ambitions.

The proposed framework offers a comprehensive tool for evaluating the sustainability of integrated seawater desalination and resource recovery systems. By incorporating detailed stakeholder analysis and practical examples, it guides users/decision-makers in identifying improved opportunities through the development and evaluation of alternative technical scenarios, considering social and stakeholders' values, a vital step missing in current literature. Additionally, the developed indicator database, readily available for researchers and practitioners, serves as a starting point for selecting indicators to support the implementation of the proposed framework.

The proposed SA framework offers a comprehensive and transparent assessment methodology ready to be employed in real-world situations. Future work should include implementing the proposed framework in real-world situations to prove its effectiveness and address the limitations and improvements that need to be made.

2.7. Supplementary information

2.7.1. Supplementary information I

See Excel file.

2.7.2. Supplementary information II

See Excel file.

2.7.3. Supplementary information III

See documentation.

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3

Development of simulation software for desalination and brine treatment systems

ABSTRACT

Desalination plays a crucial role in addressing the growing challenges of water scarcity. In recent years, the integration of desalination and brine treatment technologies has been increasingly studied, aiming to develop sustainable solutions for resource recovery from seawater. However, designing treatment trains and optimizing these processes for maximum efficiency, sustainability, and cost-effectiveness are complex tasks that require data, sophisticated analysis and decision-making strategies. This chapter presents the development of a novel software tool designed to address these challenges by providing an integrated modelling framework for the simulation and evaluation of desalination and mineral recovery processes. The software combines technical process modelling with comprehensive economic and environmental assessments, enabling a holistic understanding of system performance. Its key functionalities include the simulation of diverse process configurations, evaluation of energy consumption and greenhouse gas emissions, and estimation of the economic viability of resource recovery strategies. These capabilities facilitate the analysis of trade-offs among critical performance metrics such as production efficiency, environmental sustainability, and operational costs. Additionally, the software developed in this chapter is a source of data for ***Chapters 4-7****. This chapter outlines the software's architecture, functionalities, and validation, establishing its role as a decision-support tool for researchers, engineers, and policymakers in advancing sustainable water management practices.*

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3.1. Introduction

Traditionally, simulation models were developed to evaluate the influence of certain parameters on the characteristics of the recovered products and the performance of the technology in terms of energy, chemicals, and water consumption. However, in the desalination field, open-access simulation tools are notably lacking. While commercial software programs, like WAVE from Dupont, exist for membranes, and numerous publications discuss techno-economic models for desalination [1] and brine treatment technologies [2–7], there is a noticeable absence of open-access simulation tools in the literature. The WaterTAP platform [8] offers an open-source library for modelling water treatment technologies like reverse osmosis and electrodialysis. While it provides valuable simulation capabilities, it mainly focuses on desalination technologies and lacks extensive brine treatment.

With the shift towards circular systems and integrated desalination and brine treatment technologies for resource recovery, there is a need for a unified tool. Our software addresses this need by integrating a diverse range of technologies—reverse osmosis, nanofiltration, multi-effect distillation, chemical precipitation, eutectic freeze crystallization, electrodialysis, and thermal crystallization—into a comprehensive platform. This platform not only models these processes but also provides detailed techno-economic and environmental analyses.

The software provides a variety of examples to help modellers design and evaluate different technical configurations. An open-access simulation tool is crucial for enhancing the credibility, repeatability, and comparability of desalination studies, and for supporting informed design and decision-making. By offering transparent and accessible models, our software aims to advance research and practice in desalination and resource recovery.

This chapter is structured as a technical description of the software developed to address key challenges in desalination and resource recovery. Unlike the other chapter in this thesis, it does not include a results and discussion section. Instead, the focus is on presenting the design, functionalities, and application examples of the software, which is used as a modelling tool throughout this thesis. The intent is to provide a detailed explanation of the software's capabilities and its role in supporting subsequent chapters, where it supplies critical data for process optimization, sustainability analysis, and strategic decision-making.

3.2. Usage

Each simulation model serves as a standalone tool for analysing the performance of a specific desalination or brine treatment technology. Before running the simulation, ensure that you have provided the necessary input parameters, such as feed flow rates, salinity levels, membrane properties, heat sources, and operating conditions.

The simulation results, including salt concentration profiles, ion fluxes, energy consumption, chemical consumption, and operational costs, will be generated based on the specified inputs and displayed in the console output or saved to output files for further analysis.

However, simulation models of more than one technology can be combined to simulate and evaluate the performance of a treatment chain (desalination and brine treatment system). In this case, the output flow rates and stream concentrate are the input data for the next technology.

Additionally, two example files are provided to demonstrate the usage of the simulation suite (see Example Folder, Example 1 and Example 2). These examples simulate and evaluate two different treatment chains, showcasing the integration of multiple technologies. The provided examples are not intended as experimental validations but serve as illustrative case studies to demonstrate the potential configurations and analyses achievable using the software. The economic evaluation of the treatment chain is given in Example 1 and in the Economic Tutorial.

Furthermore, a comparison file is included, where the results of the two examples are compared in terms of various parameters. Users can extend this comparison by adding more indicators as needed.

For more details on input/output parameters and assumptions, see the Tutorial File. The Desalsim software tool is accessible as a Python package https://pypi.org/project/desalsim/.

3.3. Documentation

Extensive documentation, installation steps, tutorials and examples are available in GitHub environment (Tutorials and documents in Tutorial File). Additionally, you can find tests for every process unit and the economic model in the tests folder that verify that the code is running properly.

Besides the GitHub environment, you can find tutorials and documents on the Desalsim webpage.

3.4. Mathematical description of the technical model

For each process unit of the scenarios' treatment trains, a process model has been developed in Python. The models have been validated with experimental data (pilot scale). **Table 3. 1** shows the feed seawater composition used in the present study.

Table 3. 1. Feed seawater composition.

	Na^+	Cl^-	K^+	Mg^{2+}	Ca^{2+}	SO_4^{2-}	HCO_3^-
Conc. (mg/l)	11900	21800	400	1400	400	3200	-

For all units, the necessary electricity for pumping is determined by taking into account the volumetric flows of inputs (including chemicals and cooling water), outputs, and in-between streams. This calculation considers factors such as viscosity, pressure drop, and pump efficiency (assumed to be 0.8). Equation 68 provides an illustrative example of this calculation.

3.4.1. Nanofiltration (NF) and Reverse Osmosis (RO) models

NF is a pressure-driven membrane process that is used to concentrate and separate solutes. In this work, NF aims to separate monovalent and multivalent ions from seawater or brine feed solutions. A process model was developed to simulate the NF process. The process model is built based on the [9] report, as it is described in **Table 3. 2**. The model calculates the flow rates and the ion concentration of the permeate and concentrate streams. Mass balances are employed for the evaluation of the concentration and flow rate on the concentrate and permeate sides. Additionally, the required energy is calculated based on the osmotic pressure.

Assumptions on NF model:

1. Rejection factors (from experimental data)
2. Water recovery ratio (from experimental data)
3. Pressure drop

Note that the same model is used for RO units with different assumptions for rejection factors and water recovery ratio.

Table 3. 2. Equations for NF process unit [9].

Equations	
$C_{permeate,i} = (1 - R_i) \cdot C_{feed,i}$	1
$Q_{permeate} = WR \cdot Q_{feed}$	2
$Q_{concentrate} = Q_{feed} - Q_{permeate}$	3
$C_{concentrate,i} = \frac{(Q_{feed} \cdot C_{feed,i}) - (Q_{permeate} \cdot C_{permeate,i})}{Q_{concentrate}}$	4
$Q_{feed\_pass\ I} = Q_{sea\ water} + Q_{concentrate\_pass\ II}$	5
$C_{feed,i\_pass\ I} = \frac{(Q_{sea\ water} \cdot C_{sea\ water,i}) + (Q_{concentrate\_pass\ II} \cdot C_{concentrate,i\_pass\ II})}{Q_{feed\_pass\ I}}$	6

$$Q_{feed\_pass\ II} = Q_{permeate\_pass\ I} \quad 7$$

$$C_{feed,i\_pass\ II} = C_{permeate,i\_pass\ I} \quad 8$$

$$\pi = \sum C_i \cdot R \cdot T \quad 9$$

$$P_{applied} = \frac{\pi_{concentrate} + \pi_{feed}}{2} - \pi_{permeate} + dP \quad 10$$

$$P_{pump} = P_{applied} \cdot Q_{permeate} \quad 11$$

$$E = \frac{P_{pump}}{Q_{sea\ water}} \quad 12$$

3

Nomenclature

Symbol	Quantity	Unit
C_i	Ion concentration in the stream	g/L
R_i	Rejection rate of ion *i* by the membrane	%
E	Electrical energy consumption	kW
P	Pressure	bar
Q	Flow rate	Kg/h
R	Gas constant	L·atm/(mol·K)
T	Temperature	K
WR	Water recovery	%
dP	Pressure drop	bar
Greek symbols		
π	Osmotic pressure	bar
Subscripts and superscripts		
concentrate	Concentrate stream	
feed	Feed stream	
i	For compound *i*	
I	First pass (stage)	
II	Second pass (stage)	
Permeate	Permeate stream	

3.4.2. Multi-effect distillation (MED) model

MED is a thermal based process that is used to desalinate water. In this work, MED aims to recover high quality water and concentrate further the brine stream. The model is build based on [9] report (see Section 3.2.2.), as it is described in **Table 3. *3***. The model calculates the distillate and brine flow rates, brine stream ion concentration and the energy requirements (electrical and thermal).

Assumptions on MED model:

1. The product is salt free
2. Concentration factor
3. Cooling water temperature
4. Final effect temperature

5. Number of effects
6. Pressure drop

Table 3. 3. Equations for MED process unit [9].

Equations	
$B_n = \frac{X_f}{X_n - X_f} \cdot M_d\,,$	13
$M_f = M_d + B_n,$	14
$\Delta T_1 = \frac{\Delta T_t}{U_1 \cdot \sum_{i=1}^{n} \frac{1}{U_i}},$	15
$\Delta T_t = T_S - T_n,$	16
$U_{i+1} = 0.95 \cdot U_i\,,$	17
$\Delta T_i = \Delta T_1 \frac{U_1}{U_i}\,, \qquad i = 1,2,3, \dots, n-1, n$	18
$T_1 = T_s - \Delta T_1,$	19
$T_i = T_{i-1} - \Delta T_i\,, \qquad i = 2,3, \dots, n-1, n$	20
$\lambda_{v_i} = 2499.5698 - 2.204864 \cdot (T_i - \Delta T_{loss}) - 2.304 \cdot (T_i - \Delta T_{loss})^2,$ $i = 1, 2, \dots, n-1, n$	21
$D_1 = \frac{M_d}{\sum_{i=1}^{n} \frac{\lambda_{v_1}}{\lambda_{v_i}}},$	22
$D_i = D_1 \cdot \frac{\lambda_{v_1}}{\lambda_{v_i}}\,, \qquad i = 2,3, \dots, n-1, n$	23
$B_1 = M_f - D_1,$	24
$X_1 = X_f \cdot \frac{M_f}{B_1},$	25
$X_i = X_{i-1} \cdot \frac{B_{i-1}}{B_i}, i = 2,3, \dots, n-1, n$	26
$A_1 = \frac{D_1 \cdot \lambda_{v_1}}{U_1 \cdot (T_s - T_1)},$	27
$A_i = \frac{D_i \cdot \lambda_{v_i}}{U_i \cdot (\Delta T_i - \Delta T_{loss})}, \qquad i = 2,3, \dots, n-1, n$	28
$\Delta T_i^{new} = \Delta T_i^{old} \cdot \frac{A_i}{A_m},$	29
$M_s = D_1 \frac{\lambda_{v_1}}{\lambda_s},$	30
$Q_c = D_n \cdot \lambda_{v_n}\,,$	31
$Q_1 = M_s \cdot \lambda_s\,,$	32
$A_c = \frac{Q_c}{U_c \cdot (LMTD)_C},$	33
$(LMTD)_C = \frac{T_f - T_{cw}}{ln \frac{T_n - \Delta T_{loss} - T_{cw}}{T_n - \Delta T_{loss} - T_f}}$	34
$\mathrm{SA} = \frac{\sum_{i=1}^{n} A_i + A_c}{M_d}$	35
$M_{cw} = \frac{D_n \cdot \lambda_{v_n}}{C_p \cdot (T_f - T_{cw})} - M_f$	36

Nomenclature

Symbol	Quantity	Unit
A_c	Condenser heat transfer area	m^2
A_i	Heat transfer area	m^2
A_m	Mean average of the Heat transfer areas for all effects	m^2
B_n	brine flow rate of leaving effect n	Kg/s
C_p	specific Heat capacity of water	J/kgC
D_i	Distillate flow produces for each effect	Kg/s
$LMTD_c$	Logarithmic mean temperature difference in the condenser	ºC
M_d	Total distillate flow rate	Kg/s
M_f	Total feed flow rate	Kg/s
M_s	Total steam flow rate	Kg/s
Q_c	Condenser thermal load	W
SA	Specific heat transfer area	m^2/kg
T	Temperature of the motive steam	ºC
U	Overall heat transfer coefficients	W/(m^2 C)
X_f	Salt concentration in the feed stream	g/L
X_n	Salt concentration in the brine stream effect n	g/L
Greek symbols		
ΔT_i	temperature drop in the i effect	ºC
ΔT_i^{new}	New Temperature drops profile	ºC
ΔT_{loss}	Thermodynamic loss in each effect.	ºC
ΔT_t	Total temperature drop across all effects	ºC
λ_{v_i}	Latent heat of i effect	kJ/kg
λ_s	Latent heat of the motive steam	kJ/kg
Subscripts and superscripts		
b	Brine	
c	Condenser	
cw	Cooling water	
d	Distillate	
f	Feed entering into the first effect	
i	Ion	
loss	Thermodynamic loss	
n	Last effect index	
s	Steam	
t	Total	

3.4.3. Thermal crystallizer (TCr) model

- Thermal crystallizer is a thermal-based process that is used to crystallize salts. In this work, the thermal crystallizer is simulated as an evaporative crystallizer, enables the complete salt concentration up to saturation and promotes NaCl crystallization. The model is built based on [9] report (see Section 3.2.6.) as it is described in

Table 3. 4. The model calculates the distillate and salt flow rates, the ion concentration and the energy requirements (electrical and thermal).

Assumptions on TCr model:

- Salt moisture
- Latent heat of vaporization
- Cooling water temperature
- Power consumption for filtration unit
- Pressure drop

Table 3. 4. Equations for TCr process unit [9].

Equations	
$M_{NaCl} = \frac{M_{in} \cdot C_{in,Na}}{d_{in} \cdot 1000} \cdot \frac{MW_{NaCl}}{MW_{Na}}$	37
$M_{salt} = \frac{\frac{M_i \cdot C_{i,t}}{d_{in} \cdot 1000}}{(1 - \frac{\text{SaltMoisture}}{100})}$	38
$M_d = M_i - M_{salt}$	39
$Q = LHV_v \cdot M_d + M_i \cdot Cp_{in} \cdot (T_{op} - T_{in})$	40
$T_{st} = \frac{Q}{UA} + T_{op}$	41
$M_{st} = Q/LHV_s$	42
$M_{cw} = \frac{M_{st} \cdot LHV_v}{Cp_{cw} \cdot (T_{cw,o} - T_{cw,in})}$	43

Nomenclature

Symbol	Quantity	Unit
$C_{i,t}$	Ion concentration	g/L
Cp_{cw}	Specific Heat capacity of water	KJ/kgC
Cp_{in}	Specific Heat capacity of feed	KJ/kgC
d_{in}	Density of feed	Kg/L
LHV	Latent heat	kJ/kg
M_{NaCl}	Inlet NaCl mass flow rate	Kg/h
M_{in}	Inlet volumetric flow rate	L/h
M_d	Distillate mass flow rate	Kg/h
M_{salt}	Salt stream mass flow rate	Kg/h
M_{st}	Steam mass flow	Kg/h
MW	Molecular weight	g/mol
Q	Heat required	kJ/h
SaltMoisture	Moisture in salt stream	%
T	Temperature	ºC

3

UA	Heat transfer constant	W/ºC
Subscripts and superscripts		
i	Ion	
in	input	
t	total	
d	distillate	
v	vapor	
salt	Salt stream	
st	Steam	
cw	Cooling water	
o	Output	
op	Operating	

3.4.4. Multiple Feed Plug Flow Reactor (MF-PFR) model

MF-PFR is an innovative a plug flow reactor that is used to precipitate salts. In this work, MF-PFR aims to precipitate Mg and Ca with the addition of chemicals. The model is build based on [9] report (see Section 3.2.3.) and [2] as it is described in **Table 3. 5**. The model calculates the effluent and salt flow rates, the quantity of alkaline reactant, the ion concentration of the effluent, and the electricity requirements of the unit.

Assumptions on MF-PFR:

- Concentration of alkaline reactant
- Concentration of acid solution
- Power consumption for filtration unit
- 1st and 2nd step conversion factors
- Pressure drop

Table 3. 5. Equations for MF-PFR process unit [9].

Equations	
$Q_{Mg^{2+}}^{feed} = Q_{brine}^{feed} \cdot C_{Mg^{2+}}^{IN}$	44
$Q_{NaOH}^{1°\,step} = \dfrac{Q_{brine}^{feed} \cdot C_{Mg^{2+}}^{IN} \cdot \left(\dfrac{Conversion_{1°\,step}}{100}\right) \cdot 2}{C_{NaOH}^{1°\,step}}$	45
$Q_{tot}^{OUT,1°step} = Q_{brine}^{feed} + Q_{NaOH}^{1°\,step}$	46
$\dot{M}_{Mg(OH)_2}^{OUT,1°\,step} = \dfrac{Q_{tot}^{feed} \cdot C_{Mg^{2+}}^{IN} \cdot \left(\dfrac{Conversion_{1°\,step}}{100}\right) \cdot MW_{Mg(OH)_2}}{1000}$	47
$\text{magma density}_{Mg(OH)_2} = \dfrac{\dot{M}_{Mg(OH)_2}^{OUT,1°\,step} \cdot 1000}{Q_{tot}^{OUT}}$	48
$pH_{1°\,step} = 14 + Log_{10}(2 \cdot \sqrt[3]{\dfrac{Kps_{Mg(OH)_2}}{4}})$	49

$$C_{Mg^{2+}}^{OUT,1°step} = \frac{Q_{Mg^{2+}}^{feed} \cdot \left(1 - \frac{Conversion_{1°\,step}}{100}\right)}{Q_{tot}^{OUT}} \quad (50)$$

$$C_{Na^{+}}^{OUT,1°\,step} = \frac{(Q_{brine}^{feed} \cdot C_{Na^{+}}^{IN}) + (Q_{NaOH}^{1°\,step} \cdot C_{NaOH}^{1°\,step})}{Q_{tot}^{OUT}} \quad (51)$$

$$C_{i}^{OUT,1°\,step} = \frac{Q_{brine}^{feed} \cdot C_{i}^{IN}}{Q_{tot}^{OUT}} \quad (52)$$

$$Q_{Ca^{2+}}^{feed,2°\,step} = Q_{tot}^{Out,\;1°\,step} \cdot C_{Ca^{2+}}^{OUT,1°step} \quad (53)$$

$$Q_{NaOH_{stoich.}}^{2°\,step} = \frac{Q_{tot}^{Out\,,1°\,step} \cdot C_{Ca^{2+}}^{OUT,1°\,step} \cdot \left(1 - \frac{Conversion_{2°\,step}}{100}\right) \cdot 2}{C_{NaOH}^{2°\,step}} \quad (54)$$

$$Q_{NaOH_{added}}^{2°\,step} = \frac{(C_{OH}^{stoich.} - C_{OH}^{pH=13}) \cdot (Q_{tot}^{OUT\,,1°\,step} + Q_{NaOH_{stoich.}}^{2°\,step})}{C_{OH}^{pH=13} - C_{NaOH}^{2°\,step}} \quad (55)$$

$$Q_{tot}^{OUT,2°\,step} = Q_{tot}^{OUT,1°\,step} + Q_{NaOH_{stoich.}}^{2°\,step} + Q_{NaOH_{added}}^{2°\,step} \quad (56)$$

$$\dot{M}_{Ca(OH)_2}^{2°\,step} = \frac{Q_{tot}^{OUT,1°\,step} \cdot C_{Ca^{2+}}^{OUT,1°step} \cdot \left(\frac{Conversion_{2°\,step}}{100}\right) \cdot MW_{Ca(OH)_2}}{1000} \quad (57)$$

$$\dot{M}_{Mg(OH)_2}^{2°\,step} = \frac{Q_{tot}^{OUT,1°\,step} \cdot C_{Mg^{2+}}^{OUT,1°\,step} \cdot PM_{Mg(OH)_2}}{1000} \quad (58)$$

$$C_{Na^{+}}^{OUT,2°\,step} = \frac{(Q_{tot}^{OUT,1°\,step} \cdot C_{Na^{+}}^{OUT,1°\,step}) + (Q_{NaOH_{stoich.}}^{2°\,step} + Q_{NaOH_{added}}^{2°\,step}) \cdot C_{NaOH}^{2°\,step}}{Q_{tot}^{OUT,2°\,step}} \quad (59)$$

$$C_{Ca^{2+}}^{OUT,2°\,step} = \frac{Q_{Ca^{2+}}^{feed,2°\,step} \cdot \left(1 - \frac{Conversion_{2°\,step}}{100}\right)}{Q_{tot}^{OUT,2°\,step}} \quad (60)$$

$$C_{i}^{OUT,2°\,step} = \frac{Q_{tot}^{OUT,1°\,step} \cdot C_{i}^{OUT,1°\,step}}{Q_{tot}^{OUT,2°\,step}} \quad (61)$$

$$magma\ density_{2°\,step} = \frac{(\dot{M}_{Mg(OH)_2}^{OUT,2°\,step} + \dot{M}_{Ca(OH)_2}^{OUT,2°\,step}) \cdot 1000}{Q_{tot}^{OUT,2°\,step}} \quad (62)$$

$$pH_{2°\,step} = 14 + Log_{10}(0.1) \quad (63)$$

$$C_{OH,i}^{OUT,2°\,step} = 10^{-pH}/10^{-pH_{2o\,step}} \quad (64)$$

$$C_{OH,o}^{OUT,2°\,step} = 10^{-14}/10^{-7} \quad (65)$$

$$Q_{HCl_{added}}^{2°\,step} = \frac{(Q_{tot}^{OUT,2°\,step} \cdot C_{OH,i}^{OUT,2°\,step}) - (Q_{tot}^{OUT,2°\,step} \cdot C_{OH,o}^{OUT,2°\,step})}{C_{OH,o}^{OUT,2°\,step} + C_{HCl}} \quad (66)$$

$$Q_{tot}^{OUT,2°\,step} = Q_{tot}^{OUT,2°\,step} + Q_{HCl_{added}}^{2°\,step} \quad (67)$$

$$Energy_{pumping}^{1°\,step} = \frac{(Q_{total}^{feed,1°\,step} \cdot \Delta P^{feed,1°\,step}) + (Q_{total}^{NaOH,1°\,step} \cdot \Delta P^{NaOH,1°\,step})}{\eta_{pump}} \cdot 10^{-3} \quad (68)$$

$$Energy_{pumping}^{2°\,step} = \frac{(Q_{total}^{OUT,1°\,step} \cdot \Delta P^{feed,2°\,step}) + (Q_{total}^{NaOH,2°\,step} \cdot \Delta P^{NaOH,2°\,step})}{\eta_{pump}} \cdot 10^{-3} \quad (69)$$

Nomenclature

Symbol	Quantity	Unit
C_i^{IN}	Inlet concentration of compound i	mol/L
$C_i^{OUT,1° step}$	Outlet concentration of compound i in each step	mol/L
$Conversion_{step}$	Conversion rate of Magnesium/Calcium in each step	%
$Energy_{pumping}^{step}$	Energy required for pumping in each step	kWh
$K_{ps_{Mg(OH)_2}}$	Product solubility	
$\dot{M}_{Mg(OH)_2}^{OUT,\ step}$	Mass flow rate of magnesium hydroxide produced during each step	Kg/h
$\dot{M}_{Ca(OH)_2}^{OUT,step}$	Mass flow rate of calcium hydroxide produced during each step	Kg/h
$magma\ density_{Mg(OH)_2}$	magma density of Magnesium (the quantity of solids produced per volume of slurry)	Kg/L
pH_{step}	pH of the brine during the step of precipitation	-
$PM_{Mg(OH)_2}$	Molecular weight	g/mol
Q_{brine}^{feed}	Flow rate of the feed solution	L/h
$Q_{HCl_{added}}^{2° step}$	Added volumetric flow rate of HCl needed to reach pH=7	L/h
$Q_{Mg^{2+}}^{feed}$	Molar flow rate of Magnesium	mol/h
$Q_{NaOH_{added}}^{step}$	Added volumetric flow rate of sodium hydroxide needed to reach pH=13	L/h
$Q_{NaOH_{stoich.}}^{step}$	Stoichiometric volumetric flow rate of sodium hydroxide for each step	L/h
$Q_{tot}^{OUT,step}$	Total volumetric flow rate for each step	L/h
$Q_{total}^{NaOH,\ step}$	Total volumetric flow rate of sodium hydroxide for each step	L/h
$Q_{total}^{feed,1° step}$	total inlet outlet volumetric flow rate	L/h
Greek symbols		
ΔP	Pressure drop	bar
η_{pump}	Pump efficiency	-
Subscripts and superscripts		
i	Compound i	

3.4.5. Eutectic freeze crystallization (EFC) model

EFC is an alternative thermal based technology that is capable of separating aqueous solutions into pure water and pure solidified solutes, by cooling down the brine solution. In this work, EFC aims to recover sulphates, recover water in ice form and concentrate further the brine solution. The model is build based on [9] report (see Section 3.2.4.), as it is described in **Table 3. 6**. The crystal distribution, growth and nucleation were not considered in this work. Still, the detailed mathematical description can be found in [9]. The model calculates the effluent and salt flow rates, the ion concentration of the effluent, and the electricity requirements of the unit.

Assumptions on EFC:

- Eutectic conditions based on the ternary system (Na, Cl, SO_4), impurities (K, Ca) were neglected
- Cooling rate
- Power consumption for filtration unit
- Pressure drop

Table 3. 6. Equations for EFC process unit [9].

Equation	
$V_{liq,total} = 0.7 \cdot V_{reactor}$	70
$V_{mother\ liq} = V_{liq,total}$	71
$V_{water} = \frac{V_{mother\ liq}}{(1 + \frac{C_{C1} \cdot MW_{C1} \cdot d_{water})}{(1000 \cdot d_{C1})} + \cdots + \frac{C_{Ci} \cdot MW_{Ci} \cdot d_{water})}{(1000 \cdot d_{Ci})})}$	72
$V_{ci} = \frac{C_{C1} \cdot MW_{C1} \cdot V_{water} \cdot d_{water}}{1000 \cdot d_{Ci}}$	73
$M_{water} = V_{water} \cdot d_{water}$	74
$M_{ci} = V_{ci} \cdot d_{ci}$	75
$M_{mother\ liq} = M_{water} + M_{c1} + \cdots + M_{ci}$	76
$M_{liq,total} = M_{mother\ liq}$	77
$V_{total} = V_{liq,total} + V_{solids,total}$	78
$M_{total} = M_{liq,total} + M_{solids,total}$	79
$V_{ice} = V_{ice} + V_{ice,diff},$	80
$V_{ci,cr} = V_{ci,cr} + V_{ci,cr,diff},$	81
$V_{solids,total} = V_{ice} + V_{ci,cr},$	82
$V_{water} = \frac{M_{water}}{d_{water}},$	83
$V_{ci} = \frac{M_{ci}}{d_{ci}},$	84
$V_{mother\ liquor} = V_{water} + \sum_{i=1}^{N} V_{ci},$	85
$V_{liq,tot} = V_{mother\ liquor},$	86
$V_{tot} = V_{solids,total} + V_{liq,tot},$	87
$C_{ci} = \frac{M_{ci} \cdot 1000}{MW_{ci} \cdot M_{water}}$	88
$Qcryst_{ice} = \frac{M_{ice,reactions} \cdot \Delta H_{fus,ice}}{deltat}$	89
$Qcryst_{i,cr} = \frac{M_{ci,cr,r} \cdot \Delta H_{fusion,ci}}{deltat}$	90
$Q_{total} = Qcryst_{ice} + Qcryst_{i,cr} - r_{cooling}$	91
$\%Na_2SO_4 = \frac{M_{ci,cr}}{M_{liq,total}} \cdot 100$	92
$\%Water = \frac{M_{water}}{M_{liq,total}} \cdot 100$	93
$\%Ci = \frac{M_{ci}}{M_{liq,total}} \cdot 100$	94
$\%Ice = \frac{M_{ice}}{M_{liq,total}} \cdot 100$	95

$$Cp_{solution} = (0.9988 - 0.006494 \cdot \%Na_2SO_4 + 0.00003025 \cdot \%Na_2SO_4{}^2 - 0.0000001286 \cdot \%Na_2SO_4{}^3) \cdot 4.184 \cdot 1000 \quad (96)$$

$$T_{reactor} = \frac{Q_{total} \cdot deltat}{(M_{liq,total} \cdot Cp_{solution}) + (M_{ci,cr} \cdot Cp_{ci}) + (M_{ice} \cdot Cp_{ice})} + T_{reactor} \quad (97)$$

Nomenclature

Symbol	Quantity	Unit
C_{Ci}	Concentration	mol/kg
Cp	Heat capacity	J/(kgK)
d	Density	Kg/m^3
M	Mass of compound	kg
M_r	Mass of produced/consumed via reacting	kg
MW_{Ci}	Molecular weight of compound i	g/mol
$Qcryst_{ice}$	Heat flux to the system due to ice crystallization	J/s
$Qcryst_{i,cr}$	Heat flux to the system due to compound *i* crystallization crystallization	J/s
Q_{total}	Total heat flux to the system	J/s
$r_{cooling}$	Cooling rate	J/s
T	Temperature	K
V	Volume	m^3
$V_{reactor}$	Total reactor volume	m^3
V_{total}	Total volume	m^3
%	Weight percentage of compound in the liquid in the reactor	%
Greek symbols		
ΔH_{fus}	Enthalpy of fusion	J/kg
Subscripts and superscripts		
ci	Compound i	
cr	Crystals	
diff	Volume difference (increase/decrease)	
r	Reaction	
solution	Solution	
water	Water	
ice	Ice	
Mother	Mother liquid	
solid	Solids	

3.4.6. Electrodialysis with Bipolar membranes (EDBM) model

EDBM is a membrane-based technology that allows the production of acidic and alkaline solutions by applying an electric potential to the electrodes. In this work, EDBM aims to convert NaCl molecules of a brine solution to NaOH and HCl solutions. The model is build based on [9] report (see Section 3.2.5.) and described in **Table 3. 7**. The process is simulated as feed and bleed configuration as it is described in [10]. The model calculates the flow rate of the acid, base and salt solutions, their ion concentration, and the electricity requirements of the unit.

Assumptions on EDBM:

- Active area of the membrane across which ion permeation occurs
- Number of triplets
- Membrane characteristics (from experimental data)
- Ideal transport phenomena
- Recycling rate
- Pressure drop

Table 3. 7. Equations for EDBM process unit [9].

Equation	
$I_{ext} = A \cdot I_d$	98
$JA = \frac{3.6 \cdot I_{ext}}{F}$	99
$V_{ext} = EMF + \left(\frac{I_{ext} \cdot R_{int}}{A \cdot 10000}\right) N_{trip}$	100
$EMF = \left(\frac{R \cdot T}{z \cdot F}\left(\ln\left(\frac{C_{H^+}^{m,acid}}{C_{H^+}^{m,bp}}\right) + \ln\left(\frac{C_{OH^-}^{m,bp}}{C_{OH^-}^{m,base}}\right) + \ln\left(\frac{C_{Cl^-}^{m,salt}}{C_{Cl^-}^{m,acid}}\right) + \ln\left(\frac{C_{Na^+}^{m,base}}{C_{Na^+}^{m,salt}}\right)\right)\right) N_{trip}$	101
$P = V_{ext} \cdot I_{ext}$	102
$Q_{1\ triplet}^{IN,salt} = \frac{Q_{tot}^{salt}}{N_{trip}}$	103
$Q_{1\ triplet}^{IN,acid} = \frac{Q_{tot}^{acid}}{N_{trip}}$	104
$Q_{1\ triplet}^{IN,base} = \frac{Q_{tot}^{base}}{N_{trip}}$	105
$M_i^{IN,j} = Q_{1\ triplet}^{IN,j} \cdot C_i^{IN,j} \cdot PM_i \cdot 10^{-3}$	106
$M_{Cl^-}^{INN,salt} = (Q_{1\ triplet}^{IN,salt} \cdot C_{Cl^-}^{IN,salt} \cdot PM_{Cl^-} \cdot 10^{-3}) + \left(\frac{M_{H^+}^{IN,salt}}{PM_{H^+}} - \frac{M_{OH^-}^{IN,salt}}{PM_{OH^-}}\right) \cdot PM_{Cl^-} \quad if\ pH_{salt} < 7$ $M_{Cl^-}^{INN,salt} = (Q_{1\ triplet}^{IN,salt} \cdot C_{Cl^-}^{IN,salt} \cdot PM_{Cl^-} \cdot 10^{-3}) + \left(\frac{M_{OH^-}^{IN,salt}}{PM_{OH^-}} - \frac{M_{H^+}^{IN,salt}}{PM_{H^+}}\right) \cdot PM_{Cl^-} \quad if\ pH_{salt} > 7$	107
$M_{1\ triplet}^{IN,j} = Q_{1\ triplet}^{IN,j} \cdot density_{j\ sol.} \cdot 10^{-3}$	108
$M_{H_2O}^{IN,j} = M_{1\ triplet}^{IN,j} - \sum_{i=1}^{n} M_i^{IN,j}$	109
$K_w^{IN,j} = C_{H^+}^{IN,j} \cdot C_{OH^-}^{IN,j}$	110
$M_{H^+}^{OUT,acid} = M_{H^+}^{IN,acid} + JA \cdot PM_{H^+}$	111
$M_{Cl^-}^{OUT,acid} = M_{Cl^-}^{IN,acid} + JA \cdot PM_{Cl^-}$	112
$M_{OH^-}^{OUT,acid} = M_{OH^-}^{IN,acid}$	113

3

$$M_{Na^+}^{OUT,acid} = M_{Na^+}^{IN,acid} \quad (114)$$
$$M_{H_2O}^{OUT,acid} = M_{H_2O}^{IN,acid} - 0.5 \cdot JA \cdot PM_{H_2O} \quad (115)$$
$$M_{1\,triplet}^{OUT,acid} = \sum_{i=1}^{n} M_i^{IN,acid} \quad (116)$$
$$Q_{1\,triplet}^{OUT,acid} = \frac{Q_{1\,triplet}^{OUT,acid} \cdot 1000}{density_{acid}^{out}} \quad (117)$$
$$C_i^{OUT,acid} = \frac{M_i^{OUT,acid}}{Q_{1\,triplet}^{OUT,acid} \cdot PM_i \cdot 10^{-3}} \quad (118)$$
$$M_{Na^+}^{OUT,base} = M_{Na^+}^{IN,base} + JA \cdot PM_{Na^+} \quad (119)$$
$$M_{OH^-}^{OUT,base} = M_{OH^-}^{IN,base} + JA \cdot PM_{OH^-} \quad (120)$$
$$M_{Cl^-}^{OUT,base} = M_{Cl^-}^{IN,base} \quad (121)$$
$$M_{H^+}^{OUT,base} = M_{H^+}^{IN,base} \quad (122)$$
$$M_{H_2O}^{OUT,base} = M_{H_2O}^{IN,base} + 0.5 \cdot JA \cdot PM_{H_2O} \quad (123)$$
$$M_{1\,triplet}^{OUT,base} = \sum_{i=1}^{n} M_i^{IN,base} \quad (124)$$
$$Q_{1\,triplet}^{OUT,base} = \frac{M_{1\,triplet}^{OUT,base} \cdot 1000}{density_{base}^{out}} \quad (125)$$
$$C_i^{OUT,base} = \frac{M_i^{OUT,base}}{Q_{1\,triplet}^{OUT,base} \cdot PM_i \cdot 10^{-3}} \quad (126)$$
$$M_{Na^+}^{OUT,salt} = M_{Na^+}^{IN,salt} - (M_{Na^+}^{OUT,base} - M_{Na^+}^{IN,base}) \quad (127)$$
$$M_{Cl^-}^{OUT,salt} = M_{Cl^-}^{IN,salt} - (M_{Cl^-}^{OUT,acid} - M_{Cl^-}^{IN,acid}) \quad (128)$$
$$M_{OH^-}^{OUT,salt} = M_{OH^-}^{IN,salt} \quad (129)$$
$$M_{H^+}^{OUT,salt} = M_{H^+}^{IN,salt} \quad (130)$$
$$M_{H_2O}^{OUT,salt} = M_{H_2O}^{IN,salt} \quad (131)$$
$$M_{1\,triplet}^{OUT,salt} = \sum_{i=1}^{n} M_i^{IN,salt} \quad (132)$$
$$Q_{1\,triplet}^{OUT,salt} = \frac{M_{1\,triplet}^{OUT,salt} \cdot 1000}{density_{salt}^{out}} \quad (133)$$
$$C_i^{OUT,salt} = \frac{M_i^{OUT,salt}}{Q_{1\,triplet}^{OUT,salt} \cdot PM_i \cdot 10^{-3}} \quad (134)$$
$$\mathrm{PP} = \frac{(\sum_{j=1}^{3} Q_{1\,triplet}^{IN,j} \cdot \Delta P^j)\, N_{trip}}{eff_{pump}} \cdot 10^{-3} \quad (135)$$

Nomenclature

Symbol	Quantity	Unit
A	Active area of the membrane	m^2
$C_i^{IN,j}$	Inlet concentration of the single ions for each channel	mol/L
$C_i^{m,j}$	Average concentration of the generic ionic species between inlet and outlet in channel j	mol/L
$C_i^{OUT,j}$	Outlet concentration of the single ions for each channel	mol/L
density	Density of all the solutions	Kg/m^3
EMF	Electromotive force	V

F	Faraday constant	C/mol
I_{ext}	Applied electric current	A
I_d	Current density	A m^2
JA	Transmembrane flow rate of ions	Kmol/h
K_w	Inlet ionic water product	mol^2/L^2
M	Mass flow rate	Kg/h
N_{trip}	Number of triplets of the channel	-
P	Gross power needed for the stack	W
PM	Molecular weight	g/mol
PP	Power required for pumping the solutions	kW
Q	Flow rate in each channel of one triplet or total	L/h
R_{int}	Internal resistance of the stack	Ω
N_{trip}	Number of triplets	-
R	Gas constant	J/molK
T	Temperature	ºC
z	Chemical valence of the ion	-
V_{ext}	Voltage needed	V
Subscripts and superscripts		
acid	Acid channel	
base	Base channel	
i	Ion	
j	Channel	
salt	Salt channel	
sol	Solution	
w	water	

3.4.7. Electrodialysis (ED) model

ED is a membrane-based technology that allows the transport of salt ions from one solution another solution by applying an electric potential. In this work, ED aims to concentrate further saline solution. The model is build based on [11] as it is described in **Table 3. 8**. The model calculates the flow rates of dilute and concentrate streams, their ion concentration, and the electricity requirements of the unit.

Assumptions:

- Salinity at outlets ($S_{c,o}$)
- Number of identical parallel cell-pairs (N_{cp})
- Number of computational cells (N)
- Voltage applied across an ED cell-pair (V_{cp})
- Voltage across the electrodes (V_{el})
- Membrane efficiency (Mem_{eff})
- Pressure drop

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Table 3. 8. Equations for ED process unit [12].

Equation	
$S_{c,k+1} = S_{c,k} + \frac{S_{c,o} - S_{c,i}}{N-1}$	136
$S_{c,k+1} = \frac{\dot{N}_{s,d,j} MW_s}{\frac{\dot{N}_{w,d}\, MW_w}{1000}}$	137
$\dot{N}_{s,c,j} = \frac{\dot{m}_{c,j} \cdot S_{c,j}}{1000 \cdot MW_s}$	138
$\dot{N}_{s,c,j+1} - \dot{N}_{s,c,j} = A_{cp,tot,j} \cdot J_{s,j}$	139
$\dot{N}_{w,c,j+1} - \dot{N}_{w,c,j} = A_{cp,tot,j} \cdot J_{w,j}$	140
$N_{cp} = \frac{\sum_{j=1}^{N} A_{cp,tot,j}}{A_{cp}}$	141
$J_{s,j} = T_{s.j} \cdot \frac{i_j}{F} - L_{s,j} \cdot (C_{c,m,j} - C_{d,m,j})$	142
$J_{w,j} = T_{w.j} \cdot \frac{i_j}{F} + L_{w,j} \cdot (\pi_{c,m,j} - \pi_{d,m,j})$	143
$T_s^{cp} = -4 \cdot 10^{-6} S_d^2 + 4 \cdot 10^{-5} S_d + 0.96 \pm 0.04$	144
$T_w^{cp} = -4 \cdot 10^{-5} S_d^2 - 1.9 \cdot 10^{-2} S_d + 11.2 \pm 0.6$	145
$L_S^{cp} = \min\,(2 \cdot 10^{-12} S_d^2 - 3 \cdot 10^{-10} S_d + 6 \cdot 10^{-8},$ $2 \cdot 10^{-12} S_c^2 - 3 \cdot 10^{-10} S_d + 6 \cdot 10^{-8}) \pm 6 \cdot 10^{-9}$	146
$L_w^{cp} = 5 S_c^{-0.416} \pm 2 \cdot 10^{-5}$	147
$\dot{N}_{s,d,j+1} - \dot{N}_{s,d,j} = -A_{cp,tot,j} \cdot J_{s,j}$	148
$\dot{N}_{w,d,j+1} - \dot{N}_{w,d,j} = -A_{cp,tot,j} \cdot J_{w,j}$	149
$Q_{d,J} = \frac{\dot{N}_{w,d,j} MW_w}{\frac{d_w(1 - S_{d,j})}{1000}}$	150
$Q_{c,J} = \frac{\dot{N}_{w,c,j} MW_w}{\frac{d_w(1 - S_{c,j})}{1000}}$	151
$A_{cp,tot,j} = N_{cp} \sum_{j=1}^{N} A_{cp,j}$	152
$A_{mem,total} = 2 \frac{A_{cp,total}}{Mem_{eff}}$	153
$W_{ED,stack} = \sum_{j=1}^{N} i_j A_{cp,j} (N_{cp} V_{cp} + V_{el})$	154
$W_{ED,stack} = \frac{\Delta P_{dil} Q_{dil,in}}{n_{p,ED}} + \frac{\Delta P_{con} Q_{con,in}}{n_{p,ED}}$	155
$W_{ED} = W_{ED,stack} + W_{ED,pump}$	156

Nomenclature

Symbol	Quantity	Unit
A	Area	m^2
C	Molar concentration at the surface of the membrane	mol/m^3
F	Faraday	s A / mol
i	Current density	A/m^2
J	Molar flux	$mol/m^2\ s$

Ls	Salt permeability	m^2/s
Lw	Permeability to water	mol/m^2 s bar
$\dot{m}$	Flowrate	L/h
Mem_{eff}	Membrane efficiency	-
MW	Molecular weight	g/mol
N	Number of computational cells	-
$\dot{N}$	Total molar flow rate	mol/s
Ncp	Number of identical parallel cell-pairs	-
Q	Flow rate	L/h
S	Salinity	kg salt/kg solution
Sc	Schmidt number	-
Sh	Sherwood number	-
Ts	Membrane salt transport number	-
Tw	Membrane water transport number	-
Vcp	Cell pair voltage	V
Vel	Voltage across the electrodes	V
W	Power required	W
Greek symbols		
ΔP	Pressure drop	bar
π	Osmotic pressure at the surface of the membrane	bar
η_{pump}	Pump efficiency	-
Subscripts and superscripts		
c	Concentrate channel	
cp	Cell-pair	
d	diluate	
ED	Electrodialysis	
i	Inlet	
j	computational cell	
k	Index for the number of computational cells	
m	At membrane surface	
mem	membrane	
o	Outlet	
s	Salt	
$total$	total	
w	Water	

3.4.8. Process model validation

The validation of the integrated software tool focused on assessing how well the modelled performance of individual technologies aligns with literature values and expert expectations. The goal was to ensure that the software produces outputs suitable for early-stage, comparative sustainability assessment of desalination and brine treatment systems. Key indicators validated include specific energy consumption (SEC), recovery rates, product quality, and chemical consumption. Among these, SEC was prioritized for systematic validation. This choice was driven by two main reasons:

1. *Relevance*: Energy consumption is a central driver in the economic and environmental assessment conducted in subsequent chapters.
2. *Availability*: SEC is one of the most commonly reported performance metrics in literature, offering a consistent and comparable benchmark across technologies.

To complement the literature-based validation, expert knowledge and pilot-scale results [13] were used to assess recovery behaviour, product quality and other parameters for selected technologies. Feedback from technology experts also helped confirm modelling assumptions for newer or evolving technologies where published data was limited or inconsistent. The literature studies used for comparison have been develeloped from similar research projects focused on seawater brine valorisation for resource recovery, ensuring alignment in system objectives and boundary conditions. **Table 3. 9** gives an overview of the validation of the technical model of each technology with existing models in literature based on the specific energy consumption.

Table 3. 9. Comparison of SEC results with experimental studies from the literature.

Technology	Specific electrical energy consumption (this study)	Specific electrical energy consumption (literature)
NF	1.42 KWhel/m^3 brine intake	1.7 KWhel/m^3 brine intake [2]
MED	1.94 KWhel/m^3 brine intake	1.59 KWhel/m^3 brine intake [2]
TCr	4 KWhel/m^3 brine intake	1.7-6.25 KWhel/m^3 brine intake [2,14]
MF-PFR	0.38 KWhel/m^3 brine intake	2.23 KWhel/m^3 total brine intake [2]
EDBM	4.4 KWhel/ kg of HCl, 4.0 KWhel/ kg of NaOH	3-4KWhel/ kg of HCl [13], 2-3KWhel/ kg of NaOH [13]
ED	312.5 KWh/ton salt	219 KWhe/ ton salt [11]

***Note that for the thermal process units, **MED** and **TCr**, we use the electrical-specific consumption, primarily for pumping, for comparison. For thermal requirements, waste heat (low-quality thermal source) has been used for the calculations.*

Among the validated technologies, most results align reasonably well with literature values. However, notable deviations are observed in the **MF-PFR** and **TCr** units, which are discussed below. For **MF-PFR**, the difference in SEC between this study and the values reported in [2] (previous study from same research group) is primarily due to different assumptions regarding the drum filter's energy consumption. In this work, the drum filter is used to recover hydroxide solids from the slurry, and its energy consumption was estimated using recent experimental data from a pilot-scale setup [13]. These estimates were validated in collaboration with the research group that developed the MF-PFR technology. Nevertheless, [2] does not provide detailed calculations for electricity use, particularly for the drum filter, making it impossible to compare the specific assumptions. Similarly, for the **TCr**, the higher SEC in this study (4 kWhel/m³) compared to literature values (1.7 kWhel/m³) is due to updated assumptions regarding cooling water usage and additional pumping requirements. As with **MF-PFR**, the literature does not disclose calculation methods or process boundaries, limiting the ability to reconcile the values. Importantly, the SEC reported in this thesis aligns more closely with industrial benchmarks for sodium chloride thermal crystallization, which are approximately 6 kWhel/m³. This suggests that earlier estimates may have underestimated energy demands due to simplifications or narrower system scopes. While exact comparisons remain challenging, the results in this study are considered robust for comparative analyses, particularly given the broader process boundaries and updated assumptions used.

3.5. Mathematical description of economic models

The major costs of a desalination plant comprise capital expenditure (CAPEX) and operating expenditure (OPEX).

3.5.1. Capital costs

The CAPEX consists of fixed-capital investment and working capital, and the former one includes hardware costs, costs of buildings, process, and auxiliary, land, working capital and other indirect costs [15].

For the economic analysis of a full-scale desalination plant, the equipment costs of pilot-scale units are scaled-up to a capacity of 3000 m^3/d. The equipment (material) costs of the full-scale plant are derived from the cost of the same equipment in the pilot plant with known capacity using equation 157, known as six-tenths factor rule (m=0.6) [15]. For desalination plants the exponent m is usually closer to 0.8 [16,17], which is used in this work:

$$\frac{Cost\ of\ purchased\ equipment(Plant\ A)}{Cost\ of\ purchased\ equipment(Plant\ B)} = (\frac{capacity\ of\ plant\ A}{capacity\ of\ plant\ B})^m \qquad 157$$

For the calculation of the annualized CAPEX, the amortization factor (α) is used (see equation 158-159) [18–21].

$$Annualized\ CAPEX\ =\ CAPEX\ *\ \alpha \qquad 158$$

The amortization factor (α) is defined by:

$$amortization\ factor\ \alpha\ =\ \frac{i(1+i)^n}{(1+i)^n-1} \qquad 159$$

where i is discount rate, n is plant lifetime (year).

3.5.2. Operating costs

The OPEX refers to expenditure directly generated by manufacturing operations or connected to the equipment of a technical unit. **Table 3. 10** gives an overview of the costs that constitute

OPEX [15]. In this study, the utilities in this system are mainly energy, chemicals, and water costs. The calculation of yearly electrical (C_{el}) and thermal (C_{th}) energy costs follows equations 160–162:

$$C_{el} = Etot_{el} \cdot t_{operation} \cdot P_{el} \quad 160$$

$$C_{th} = Etot_{th} \cdot t_{operation} \cdot P_{steam} \quad 161$$

$$C_e = C_{el} + C_{th} \quad 162$$

Where:

E_{el} and E_{th} are the total energy consumption per operating hour (in kWh/hr), $t_{operation}$ is the total operation time in one year (in hr), P_{el} and P_{steam} are the prices of electricity and steam, respectively (in €/kWh). The calculation of chemicals and water costs is similar to the energy cost, multiplying the amount of consumption every year by their price.

3.5.3. Assumptions on CAPEX and OPEX

Table 3. 10 shows the assumptions that were made to calculate the CAPEX and OPEX of all the scenarios.

Table 3. 10. Assumptions on CAPEX & OPEX [15,22].

CAPEX		Annual OPEX	
Installation	25% of purchased equipment cost	**Maintenance**	3% of the fixed-capital investment
Buildings, process, and auxiliary	20% of purchased equipment cost	**Operating Supplies**	5% of maintenance
Land	6% of purchased equipment cost	**Operating Labor**	15% of annual OPEX
Indirect costs	15% of direct cost	**Direct supervisory and clerical labor**	15% of operating labor
Working capital	20% of total investment cost	**Laboratory charges**	15% of operating labor
		Patents and royalties	3% of annual OPEX
		Fixed charges	5% of annual OPEX
		Plant overhead costs	5% of annual OPEX

The additional assumptions on the economic parameters are reported in **Table 3. 11**.

Table 3. 11. Economic parameters employed in the economic analysis.

Parameter	Value	Units
Discount rate	6%	-

Operating hours	24	hour
Annual working days	300	day
Plant lifetime	20	year
Inflation rate	2%	-

3.6. Limitations

The proposed software is not designed to replace detailed physical models or system dynamics approaches. For applications requiring highly detailed process representations, the software may need to be enhanced to provide more detailed results and optimization opportunities. This work highlights that the proposed software is particularly valuable for evaluating the integration of different processes and preliminary designs, capturing the technical, economic, and environmental impacts of technology integration.

The validation process focused primarily on specific energy consumption (SEC), which was systematically reported in this chapter because it is the most widely available and consistently defined metric in the literature, allowing for clear and direct comparisons. While additional performance indicators such as recovery rates and product quality were internally reviewed and discussed with technology experts and suppliers, these were not systematically presented due to scope and data constraints. Discrepancies from literature values remain for some technologies (e.g., MF-PFR, TCr), largely due to model simplifications, evolving process configurations (e.g., updated energy assumptions for components like the drum filter), or scarce and inconsistent validation data.

These limitations are most relevant for less mature processes or those relying on estimated inputs and should be considered when interpreting performance outputs. While the tool is reliable for comparative scenario analysis and integration studies—as applied in subsequent chapters—its predictive precision is constrained by these assumptions and data limitations.

3.7. Conclusions

A comprehensive open-source software tool in Python designed to simulate and evaluate desalination and brine treatment systems. By addressing the absence of accessible simulation tools in the field, this work contributes a valuable resource for researchers and practitioners. The examples included demonstrating its potential for modelling diverse process configurations and generating critical insights for sustainability and efficiency. The outputs from this software directly support the analyses presented in Chapters 4–7, illustrating its integral role in this thesis and its broader applicability to the scientific community.

While the software was validated using literature values(e.g., specific energy consumption) and further reviewed by technology experts (e.g., specific energy consumption, recovery rates, product quality), discrepancies remain for some technologies, particularly where data is scarce, or model simplifications were required. These deviations reflect broader challenges in modelling emerging or poorly documented processes and underscore the need for caution when interpreting results for such technologies. Nevertheless, these limitations are unlikely to alter the overall conclusions of this thesis, as the tool was primarily used for comparative analysis and scenario exploration, where relative performance and system-level trends are more important than precise absolute values.

Through the software's application, researchers, engineers, and policymakers gain the power to evaluate the resource recovery potential, economics, and greenhouse gas emissions associated with different configuration combinations. Its open-source nature supports transparency and future refinement, positioning it as both a functional decision-support platform and a foundation for continued research into sustainable water treatment systems.

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4

A value-sensitive approach for integrated seawater desalination and brine treatment

ABSTRACT

The transition to seawater desalination integrated with resource recovery, particularly in water- and energy-scarce regions, requires innovative approaches that consider societal benefits and costs. This study goes beyond traditional techno-economic evaluations by employing a Value-Sensitive Design (VSD) approach, which guides the selection of performance indicators and informs the design of technical scenarios for integrated seawater desalination and brine treatment systems. VSD ensures that the scenarios are socially relevant by directly incorporating stakeholder values into the design and assessment process. Four technical scenarios (Sc) were used to evaluate the VSD approach: Sc1) maximum water recovery, Sc2) and Sc3) integrated desalination with brine treatment for maximum resource recovery (using different configurations) and Sc4) electricity-based desalination for chemical recovery. Techno-economic models are implemented using Python to analyse the feasibility and performance of these scenarios. The modeling results indicate that all scenarios achieve zero brine production. However, the trade-offs between resource recovery and greenhouse gas emissions are evident. Increased salt recovery leads to higher CO_2 *emissions (locally) due to electricity consumption. Scenario 1 minimized electrical energy consumption and emissions while maximising water production. Scenarios 2 and 3 performed best in water and high-quality salt production. Despite its higher* CO_2 *emissions, Scenario 4 proved most profitable due to the production of chemicals. These findings highlight the importance of tailoring plant designs to regional needs. By providing a comprehensive understanding of trade-offs, the VSD approach fosters stakeholder dialogue and serves as a valuable decision-analysis tool for designing sustainable desalination systems.*

Keywords: *Desalination, Brine treatment, Resource recovery, Value sensitive design, Sustainability assessment*.

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4.1. Introduction

Desalination is a crucial water treatment technology that provides solutions to water-stressed regions, but the high energy consumption and disposal of the saline by-product, brine, pose significant environmental and social challenges. Zero liquid discharge (ZLD) and Minimal liquid discharge (MLD) systems have been developed to increase water recovery and minimize brine discharge by treating brine streams and recovering water and salts [1]. While ZLD presents an attractive solution, its practical implementation faces challenges, including high energy requirements, high operational costs, the management of solid wastes and the need for advanced technologies capable of handling diverse brine compositions [2].

Seawater is a rich source of valuable and scarce materials, which are lost when they end up in brine discharged from desalination plants [3]. Developments are moving from minimizing brine disposal to recovering valuable resources beyond water, presenting economic and environmental opportunities [4]. Numerous studies have explored technologies for recovering salts like magnesium, calcium, sodium, and metals [5–8]. However, no single technology can recover all valuable materials effectively.

Integrating multiple technologies is necessary for effective multiple-product recovery and improved technological and economic performance [3], but introduces complexity. The transition to resource recovery also introduces societal benefits and costs, as additional processing steps can increase energy use and capital costs, though they may offer economic gains depending on the recovered resources [9]. Evaluating these integrated systems requires approaches that go beyond technical and economic performance [10]. There is no fixed approach to evaluating integrating technologies as it is context-dependent, as goals, target product quality, and quantity [7]. Thus, integrated systems should be designed to meet market demand and meet local requirements, ensuring solutions are technically efficient and socially relevant.

Although sustainability assessments in desalination often address environmental, economic, and social dimensions [11–13], there remains a gap in existing frameworks related to the oversight of brine and resource recovery. ZLD studies typically focus on water and salt recovery from brine using a techno-economic approach, often neglecting social aspects, while the environmental assessments primarily center on energy-related emissions [14–16]. To advance holistic solutions, existing frameworks need to be revised to incorporate societal context, encourage stakeholder participation, and evaluate whether the technological configurations are desirable in specific contexts [17].

Value-sensitive design (VSD) addresses this gap by explicitly integrating societal values into the design and assessment of technological systems. Incorporating social aspects through stakeholders' values, VSD ensures that technological solutions are tailored to the community's specific needs. This alignment enhances both social acceptability and the likelihood of successful implementation [17]. Additionally, recognizing that technical systems cannot be fully understood or designed without considering the stakeholders involved, VSD bridges the gap between technical solutions and social perspectives [18]. Thus, unlike conventional methodologies such as Multi-criteria assessment (MCA) or techno-economic assessments, which focus predominantly on technical and economic parameters, VSD provides a more holistic evaluation by incorporating social, ethical, and environmental dimensions into the process [19–21]. This contrasts with state-of-the-art methods that often marginalize these societal concerns or include them as secondary considerations [17].

The VSD approach is especially effective in co-designing technical scenarios because it engages stakeholders early in the processes, allowing their values to shape key technical variables. For example, prioritizing resource security could lead to scenarios that focus on brine concentration and resource recovery, aligning technical configurations with both community needs and sustainability goals [22,23]. This differs from MCA, which typically involves stakeholders only at the final stage to validate pre-selected alternatives. This co-design approach addresses a key gap in existing sustainability assessments, which often lack clear reasoning behind the selection of alternatives or technical scenarios [24]. In addition, stakeholder values are translated into measurable objectives and performance indicators, making the assessment process transparent and aligned with community priorities.

Given the rapid advancements in seawater desalination and the need to resolve value tensions between societal, environmental, economic and technical goals, this study applies elements of VSD to fill gaps in existing assessment methods and offer insights for the design of socially relevant desalination systems. The study addresses the following key question:

What are the benefits and drawbacks of different technical configurations in integrated resource recovery desalination, vis-à-vis identified values, and how do they apply to different societal contexts?

To answer the questions, we investigate different technical configurations using some of the elements of the VSD approach. Indicators were selected based on values identified in prior research by [25] and technical scenarios were designed to reflect stakeholders' values. Process and economic models were developed to provide the required data for the alternative scenarios. Finally, the alternative technical scenarios were analysed in the context of societal values and placed in relative social contexts. This work provides a novel integration of VSD and soft MCA methodology [26] in the desalination field, offering a valuable decision-support tool.

4.2. Methods

The framework, as previously outlined by [27], consists of six steps: 1) Problem definition, 2) Indicator definition, 3) Design of alternative scenarios, 4) Data acquisition, 5) Assessment indicators quantification, and 6) Performance analysis. In this study, we implement steps 2-6 of the comprehensive methodology illustrated in **Figure 4. 1**. This section describes the methodology and adjustments that followed. It is worth noting that this work does not evaluate the treatment chains in a specific societal context, but the example of Lampedusa and the identified stakeholders' values in that context are used to implement the framework (see Section 4.2.1). Then generalized outcomes and useful insights are used in the discussion (see Sections 4.3.3 and 4.3.4). For this reason, a detailed and specific definition of the problem (step 1) is left out.

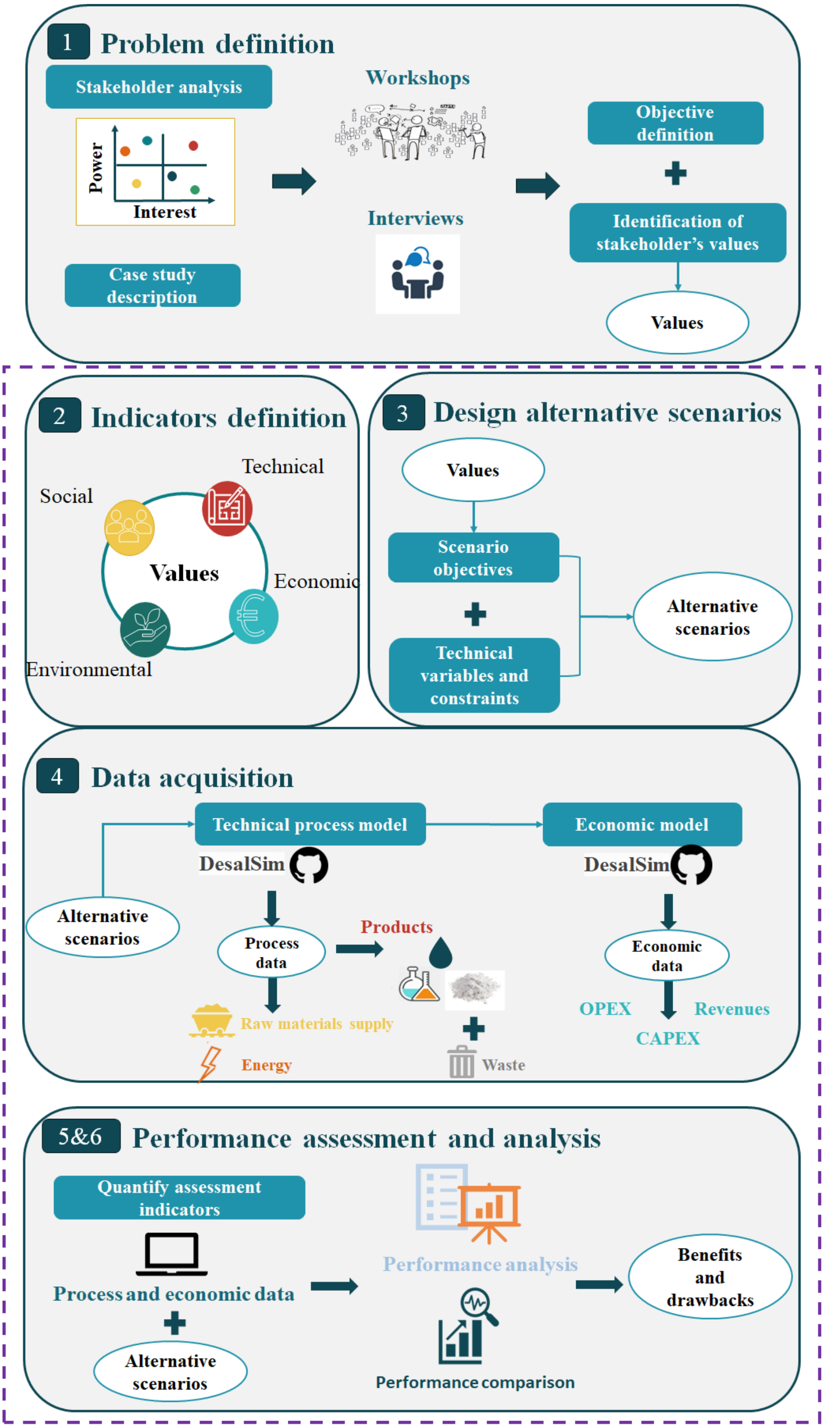

Figure 4. 1. Schematic representation of the followed methodology. The dashed line shows the steps followed in this work.

4.2.1. Problem definition

This work focuses on seawater desalination integrated with a power plant (different owner) on an island or coastal area that depends on external fossil resources for its energy production. The integration aims to increase water availability with the same or similar energy use by capturing waste heat and recovering salts. In particular, the example of Lampedusa, a small island in the Mediterranean Sea, is used to identify the stakeholders' values. The island covers 100% of its water demand through desalination, which can account for around 30% of the total electricity usage for small islands [25]. Building upon prior research by [25] and [28], we incorporate valuable insights into stakeholder values and tensions related to seawater desalination in island contexts. This study did not involve direct interviews or surveys with new stakeholders; instead, it builds on previously published research that identified key stakeholder values. The main identified stakeholder values are:

- Resource security
- Water security
- Energy security
- Affordability
- Protection of the environment, including marine life
- Climate change mitigation
- Efficiency
- Safety

Systems in this societal problem statement present several tensions that need to be considered. **Figure 4. 2** summarises the identified sustainability tensions for integrated desalination and brine treatment systems in islands or coastal areas. A tension arises between water security, energy security, and sustainability. While the system would enhance water availability and self-resilience, it would increase the need for energy imports and compromise energy security. Furthermore, the system's impacts on sustainability aspects, such as brine discharge reduction and increased greenhouse gas emissions due to higher energy use, as well as uncertainties regarding the cost of water, must be assessed. Therefore, a tension arises between water, resource security, and affordability. While brine minimization and water and salts/chemicals recovery will increase, it will also increase the production costs. In this way, how costs are distributed will affect the competitiveness of resource recovery and the affordability of water in a water-scarce region. Although recovery of valuable products will result in extra revenue from selling products, there is a risk of how competitive the solution is. Finally, a tension exists between efficiency and long-term sustainability. Although integrating waste heat promotes energy efficiency, there is a risk of sustaining dependence on fossil fuels, preventing the adoption of renewable energy sources. Limited renewable energy source areas in islands contribute to the reliance on fossil resources, although local planning considers expanding renewable energy. These tensions require further investigation and discussion with stakeholders to ensure sustainable outcomes.

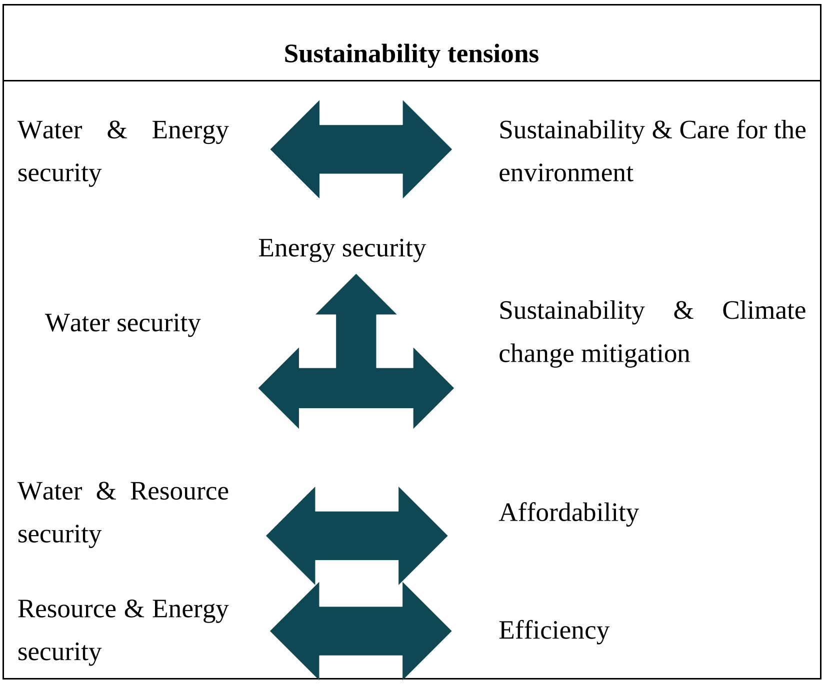

Figure 4. 2. Identified sustainability tensions for integrated desalination and brine treatment systems in islands or coastal areas.

Finally, in the problem definition step, the analysis boundaries need to be defined [17]. This study aimed to design and identify suitable alternatives for various societal contexts, assessing their compatibility and exploring how the development of an integrated system can address identified value tensions. A soft MCA [26] is applied to provide valuable insights and structure knowledge for decision support in desalination projects. Therefore, the analysis boundaries will be limited to technical system evaluation using selected indicators. In this work, we adopt a system-level approach, evaluating technical alternatives as a collective system rather than individual components. By focusing on these specific aspects, we aim to shed light on the potential benefits and challenges of an integrated system and contribute to informed decision-making in the field of desalination.

4.2.2. Define performance indicators

This methodological step outlines how sustainability issues and identified values are transformed into performance indicators. Firstly, the identified values from [9] (see Section

4.2.1) were translated into objectives and then performance indicators. The connection between values, objectives, and indicators can be explained as follows: values guide the selection of the objective used to assess different scenarios, and indicators act as the measurements that evaluate how well those scenarios align with the chosen objective [17]. The indicator database in [27] was used as inspiration for the selection of indicators in this work. To ensure the indicators' relevance and importance in this context, they were shared with a small group of stakeholders consisting of researchers specializing in sustainability, desalination, and resource recovery. This engagement provided valuable input to refine the indicator selection and ensure alignment with stakeholder expectations.

While social indicators are typically crucial in sustainability assessments, the social dimension is embedded within the VSD approach rather than through separate social indicators, as the analysis is not focused on a specific societal context. This approach allows us to integrate social considerations holistically throughout the scenario assessment without limiting them to specific, quantifiable indicators.

4.2.3. Design of alternative scenarios

This section outlines the approach for developing technical scenarios that incorporate stakeholder values identified in the problem definition. While value tensions are acknowledged as a critical aspect of this study (as highlighted in the problem definition), the primary emphasis during scenario development is placed on aligning with these values. This emphasis on alignment stems from the high complexity of the issue. Value tensions will play a crucial role in the subsequent analysis of our results. Therefore, the scenarios are designed to address the value of water, resource, and energy security, climate change mitigation, and environmental protection, particularly concerning marine life and efficiency, while also indirectly considering affordability and safety. **Figure 4. 3** presents the following procedure for the design of the alternative technical scenarios. The design of these scenarios was made on the basis of the value-sensitive design (VSD) approach. The detailed methodology for VSD can be found in [29,30].

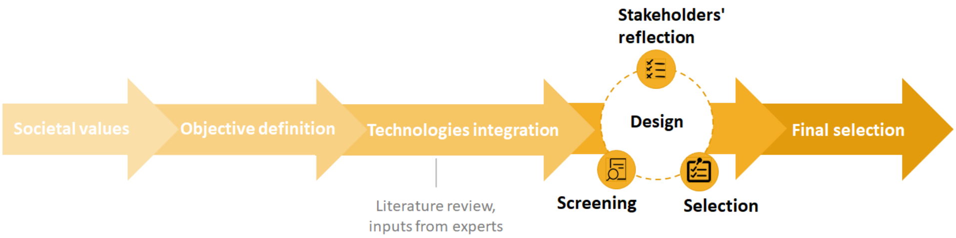

Figure 4. 3. Followed procedure for the design of alternative technical scenarios.

The development of technical scenarios is organised around three main technical scenario variables: process and technology, product and by-products, and raw materials and utilities. The main variables used in this study to generate the scenarios are the intensity of recovery (water focus vs. intense resource recovery) and the type of energy source (thermal or electrical). In particular:

- The intensity of the recovery variable represents the degree of resource recovery within the scenarios, ranging from a focus on maximizing water recovery to intense resource recovery encompassing elements like salts, chemicals, and critical raw materials.
- Energy Source Variable declares the source of energy used within the scenarios, distinguishing between thermal-based technologies and electricity-based technologies, with a potential focus on renewable energy sources.

These key variables are essential in shaping the technical scenarios, but they are intricately linked to the stakeholder values identified in the problem definition. The main identified stakeholder values include:

- Resource security is closely related to the intensity of recovery variable. A higher intensity of resource recovery aligns with resource security by reducing dependence on external resources and enhancing self-sufficiency.
- Water security is directly tied to the intensity of the recovery variable. Greater water recovery ensures water availability, which is crucial for human well-being and economic activities.
- Energy security can be linked to both the energy source variable and the intensity of recovery variable. Integrating thermal-based technologies with waste heat or using renewable energy sources contributes to energy security.
- Affordability is influenced by the intensity of the recovery variable, particularly in scenarios with intense resource recovery, which may affect production costs, revenue, and affordability.
- Protection of the Environment, Including Marine Life, aligns with scenarios that aim for minimal brine discharge, reducing the negative environmental impact and benefiting marine life.
- Climate Change Mitigation is associated with the energy source variable, with scenarios using renewable energy sources contributing to reducing greenhouse gas emissions.
- Efficiency is promoted by scenarios with higher energy and water/production efficiency, which both variables can influence.

- Safety considerations should be integrated into scenarios regardless of the variables, ensuring the well-being of individuals involved in the process.

Additionally, a literature review on technology integration for desalination and brine treatment was carried out to identify the advantages and limitations of the integration. Specifically, studies where at least two technologies were combined to treat seawater or brine streams were selected and analysed. For a comprehensive overview of the integration of technology, including the main products, scale, advantages, and limitations of each study, please refer to **Table S.2** in the Supplementary Information. The performance of technologies in the systems was studied, and data regarding energy consumption and economics were collected and analysed. Note that lab-scale technologies were excluded, focusing exclusively on well-developed technologies with practical relevance. The selected studies were analysed further in terms of the following values:

- Socio-economic values such as development opportunities, energy security, economic value-sharing
- Human-nature interaction such as protection and recovery, efficiency and circularity

Considering the identified values (see problem definition, Section 4.2.1), the objectives, and the insights from the literature review, the technical scenarios were developed. After the preliminary design of the technical scenarios, they were shared with a group of stakeholders in a workshop to ensure the practicality and feasibility of the scenarios. During this workshop, the objective and the technical aspects of each scenario were discussed. Their feedback was incorporated, and changes were made. The technical scenarios are described in Section 4.3.

4.2.4. Data acquisition and quantification of assessment indicators

One of the most important steps in the proposed framework is data acquisition because it is directly related to the accuracy, reliability, and quality of the results. In this work, data will be provided by technical and economic models. The mathematical description, the details of the modelling, the main assumptions, and references are given in Chapter 3 and GitHub repository for the technical process and economic models (https://github.com/rodoulak/Desalination-and-Brine-Treatment-Simulation-.git) developed in the context of this study.

In this section, an overview of the main inputs and outputs for each process unit in the integrated system is given (see **Table 4. 1**). These parameters were selected based on their direct relevance to the system's techno-economic and environmental performance. Additional parameters and assumptions are provided in Chapter 3. All technical process models were implemented in Python. The feed flow rate is the same for all the scenarios, and it is equal to

3000m^3/d. The technical process models were validated with experimental pilot-scale results from the Water Mining project [5] (see Supplementary Information, Section S4). Furthermore, the results of this study align with those of previous research in the literature [7,16]. Especially with work from [16] that was carried out within the Zero Brine project and previous works [31] sharing the same objective as this work, which is technological integration for recovering valuable materials from brine.

Table 4. 1. Main inputs and outputs of each process unit in the integrated system.

Process	Input	Output
Nanofiltration	Feed flow rate [m^3/h]	Permeate flow rate and composition [g/L]
	Ion concentration [g/L]	Concentrate flow rate and composition [g/L]
	Osmotic pressure [bar]	Electrical requirements [kWh$_{el}$]
	Water recovery [%]	Chemicals consumption [L/h]
	Ion rejection [-]	
Multi-effect distillation	Feed flow rate [m^3/h]	Flow rate of water [m^3/h]
	Ion concentration [g/L]	Effluent flow rate and composition [g/L]
	Feed temperature [ºC]	Electrical [kWh$_{el}$] and thermal [kWh$_{th}$] requirements
	Steam temperature [ºC]	Cooling water flow rate [m^3/h]
Thermal crystallizer	Feed flow rate [m^3/h]	Flow rate of water [kg/h]
	Ion concentration [g/L]	Flow rate of NaCl [kg/h]
	Feed temperature [ºC]	Cooling water flow rate [m^3/h]
	Steam temperature [ºC]	Electrical [kWh$_{el}$] and thermal [kWh$_{th}$] requirements
Multi-plug flow reactor	Feed flow rate [m^3/h]	Alkaline solution flow rate [L/h]
	Ion concentration [g/L]	Flow rate of $Mg(OH)_2$ [kg/h]
	Concentration of the alkaline solution (NaOH) [M]	Flow rate of $Ca(OH)_2$ [kg/h]
	Concentration of the acid solution (HCl) [M]	Acid solution flow rate [L/h]
		Effluent flow rate [m^3/h] and composition [g/L]
		Electricity requirements [kWh$_{el}$]
Eutectic freeze crystallizer	Feed flow rate [m^3/h]	Flow rate of Na_2SO_4 [kg/h]
	Ion concentration [g/L]	Flow rate of ice [kg/h]
	Feed temperature [ºC]	Effluent flow rate [m^3/h] and composition [g/L]
		Electricity requirements [kWh$_{el}$]

Electrodialysis with bipolar membranes	Feed flow rate [m^3/h]	Flow rate of acid [m^3/h] and composition [g/L]
	Ion concentration [g/L]	Flow rate of base [m^3/h] and composition [g/L]
	Electric density	Flow rate of salt [m^3/h] and composition [g/L]
		Electricity requirements [kWh_{el}]
Electrodialysis	Feed flow rate [m^3/h]	Flow rate of diluted stream [m^3/h] and composition [g/L]
	Ion concentration [g/L]	Flow rate of concentrate stream [m^3/h] and composition [g/L]
	Electric density	Electricity requirements [kWh_{el}]

Note: The mathematical description, modelling details, and relevant references for the inputs and outputs of each process unit are provided in Chapter 3.

In this study, we have made key assumptions to create a clear framework for our analysis, which are essential for understanding our results and conclusions. It is important to note that the validity and robustness of our findings are contingent upon these assumptions. Variations or deviations from these assumptions could impact the outcomes of our analysis. The key assumptions for our analysis are the following:

i. Waste heat availability at zero economic cost: Given its status as a by-product of electricity generation, we assume waste heat from integrated power and desalination plants is available at zero economic cost.
ii. Negligible emissions from waste heat: In our analysis, we do not consider emissions arising from waste heat. Waste heat, a by-product of electricity generation, is primarily intended for electricity generation, and any emissions associated with it are deemed negligible.
iii. Exclusive use of grid electricity or direct power plant output: we exclusively consider two electricity sources, the grid and direct power plant output for combined facilities, facilitating clear source differentiation in our assessment.
iv. European Union (EU) average emission factor for electricity: we consider the EU average emission factor for electricity as a standardized basis for our CO_2 emissions calculations.

Economic models were developed in order to evaluate the economic performance of the alternative scenarios. The economic model consists mainly of capital expenditure (CAPEX) and operating expenditure (OPEX). Specifically, CAPEX consists of fixed-capital investment and working capital, and OPEX refers to expenditure directly generated by operating the plant [32]. The main inputs of the economic models are:

- Equipment cost
- Mass flow rates (from technical models)
- Energy and utility consumption (from technical models)
- Selling price of products (from literature)
- Price of energy and utilities (from literature)

Note that in the assessment of economic viability for scenarios, we assumed established market demand and potential off-takers for the recovered salts and chemicals, as their profitability hinges on market uptake. A detailed explanation of the economic models and the assumptions that were made, as well as the input data from the literature, are given in Chapter 3 (see also GitHub repository). The two models were coupled, and the main outputs of the technical models for each scenario became the inputs for the respective economic model of the scenario. Finally, the selected indicators are determined using data from technical and economic models. These models provide the necessary input parameters, such as mass flow rates, energy consumption, equipment costs, and product selling prices, which are essential for accurately assessing each indicator. This ensures that the indicators, initially defined in the indicator selection step (see Section 4.2.2 and 4.3), are grounded in robust and comprehensive data. After the quantification of the selected indicators, the performance analysis can carried out where the benefits and drawbacks of the different technical configurations relative to the identified values are evaluated (see **Figure 4. 1**).

4.3. Results and discussion

4.3.1. Define performance indicators

Following the methodology described in Section 4.2.2, the performance indicators are defined below, and they are summarised in **Table 4. 2**. The detailed description (and mathematical formulation) of these indicators is provided in the Supplementary Information (see Section S1).

The value of water security is quantified through the system's water production quantity, emphasizing the importance of measuring product outputs and recovery efficiency. Energy consumption, critical for energy security considerations, is evaluated using indicators for electrical and thermal energy consumption. The value of resource security is quantified through the system's salt production quantity. System efficiency, crucial for overall effectiveness and the value of efficiency, is assessed through two specific indicators: overall brine production and resource efficiency.

This study used indicators to evaluate the affordability of integrated systems comprehensively, considering the entire integrated process rather than evaluating each individual component separately. Production efficiency measures the monetary value of all the recovered products relative to the total annual cost of the integrated system. The production efficiency indicator can accommodate different metric units, which is particularly important in multi-product systems. This indicator, along with the selected CAPEX and OPEX indicators, provides a comprehensive assessment of the economic dimension, ensuring that affordability is sufficiently addressed.

To evaluate climate change mitigation and the carbon footprint resulting from energy consumption, we have selected CO_2 emissions as an indicator for this specific stage of the analysis. It's important to note that in this phase, we focus solely on operational CO_2 emissions and do not consider the broader life cycle impacts of the system. Specifically, we use the average CO_2 emission rate from electricity use in the European Union for our calculations. At this stage, renewable energy sources are not included in electricity production, but they will be considered in a subsequent phase of the analysis. In terms of care for the environment and specifically related to brine disposal, aquatic eco-toxicity was selected to quantify the potential impacts of brine discharge on the marine environment. It was calculated based on the final concentration (concentration of salt ions, chemicals, metals) of the brine stream [33]. Water footprint is an indicator of resource efficiency. This indicator provides insights into the system's efficiency in utilizing water resources, aligning with the value of care for the environment and resource conservation. Finally, to assess the environmental impact and ensure safety from chemical use in the system, human toxicity was chosen as an indicator.

4

Table 4. 2. The main values identified and the indicators used to operationalize them in view of sustainability assessment.

Value	Objective	Indicator	Units
Energy security	Improve energy performance	Energy consumption	kWh
Water security	Increase water recovery	Quantity of water produced	m^3/year
Resource security	Increase resource recovery	Quantity of salt produced[1]	Ton/year
Efficiency	Increase efficiency	Resource efficiency	%
		Brine production	ton/year
Affordability	Increase the economic viability of the plant	CAPEX	€
		OPEX	€/year
	Increase profitability	Production efficiency	€/€

[1] In this paper, the term "Salt produced" refers to various types of salts (NaCl, $Mg(OH)_2$, Na_2SO_4 etc) recovered through the integrated seawater desalination and brine treatment processes

Climate change mitigation	Minimize climate change impact	Carbon dioxide emission	Kg CO_2-Equ
Care for the environment	Minimize resource utilization	Water footprint	m^3/year
	Minimize the aquatic eco-toxic impact of brine disposal	Eco-toxicity	Kg of brine/kg of seawater
Safety	Use of chemicals	Human toxicity	-

4.3.2. Description of alternative scenarios

While all scenarios share the common goal of increasing water recovery and reducing brine discharge (compared to typical seawater desalination), they do so differently. Note that the mainstream entering all the treatment chains is seawater (same flow rate and concentration), and all the scenarios aim for either zero-liquid discharge or minimal-liquid discharge. In this way, the scenarios address the value of protection of the environment regarding marine life. The scenarios are summarized in **Table 4. 3** and a detailed description of the design of each scenario is given below and in Supplementary Information (see Section S5).

Scenario 1: Water recovery

Scenario 1 focuses on water security and energy security values by maximizing water recovery while minimizing energy requirements by using waste heat from a nearby power plant. This scenario does not focus on recovering salts or chemicals but rather on ensuring water availability through the recovery of water. The brine discharge is expected to be zero. This scenario generates a mixed salt stream, which cannot be used and is considered a solid waste that must be disposed of properly. Scenario 1 is a typical Zero liquid discharge system that was reported and assessed several times in the literature (see Section S2; **Table S.2** in Supplementary Information). Nanofiltration (NF) is used as pre-treatment to Multi-Effect Distillation (MED) to increase the efficiency of the desalination process, avoid scaling, and further concentrate the NaCl stream. Energy security is ensured by integrating thermal-based technologies such as MED and Thermal Crystallizer (TCr) with available waste heat, which can be sourced from a nearby power plant. While it is true that thermal desalination processes like MED are generally more energy-intensive compared to membrane-based technologies like Reverse Osmosis (RO), their advantage lies in their compatibility with the utilization of excess heat energy.

Based on these considerations, Scenario 1 consists of three process units: NF, MED and TCr (see **Figure 4. 4**). The seawater stream first goes to the NF unit and is separated into two different streams: one high in monovalent ions and one in multivalent ions. The former is directed to a process line of conventional units, including the MED unit that obtains water from the evaporation process. The NF unit is used as pre-treatment for MED to increase the performance of the unit. Following this unit, the stream goes to the thermal crystallizer and is mixed with the latter stream from NF, which is high in multi-valent ions, to finally obtain water and mixed salt (low-purity NaCl crystals).

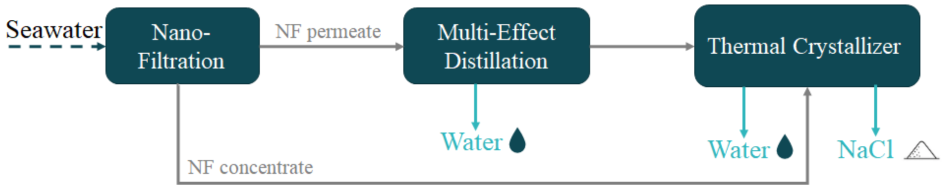

Figure 4. 4. Process flow diagram of Scenario 1.

Scenario 2: Desalination and resource recovery

Scenario 2 focuses on water security and resource security values by recovering multiple high-value materials. For this reason, the NF concentrate treatment line from scenario 1 is extended by integrating various technologies. The integration of technologies will affect the efficiency of the system. Literature showed that NF can be used as a pre-treatment step to separate the monovalent ions and multivalent ions from brine and increase the efficiency of the MED unit (see Section S2; **Table S.2** in Supplementary Information). Another advantage of this separation is the recovery of the multi-valent ions in the form of salt or chemicals. The use of multiple technologies is required to achieve high recovery of valuable products, including Magnesium (Mg), which is one of the Critical Raw Materials (CRMs) defined by the European Union (EU) [16]. Mg precipitation and crystallization from brine streams have been studied in the literature, and pilot-scale plants have been tested [34–36]. This crystallization step can be combined with Electrodialysis with Bi-polar Membrane (EDBM) to recover chemicals (HCl, NaOH) from the brine feed, contributing to the economic feasibility and circularity of the plant (innovative circular economy). Additionally, the effectiveness of using Eutectic Freeze Crystallization (EFC) as pre-treatment to EDBM has been studied to recover more products (Na_2SO_4 and water) and concentrate further the effluent from the precipitation process to increase EDBM efficiency [37], The recovery of Mg and Ca will also increase the efficiency of EFC, the quality of the products, and, therefore, their affordability.

The main desalination and brine concentration technology used in Scenario 2 is MED, while NF is used as a pre-treatment. MED can be used to recover water and concentrate the brine solution further and it is commonly combined with a thermal crystallizer in ZLD or MLD systems to recover the remaining amount of water and salt crystals [38,39]. Besides water and resource security, Scenario 2 aims to ensure energy security by integrating thermal-based technologies such as MED and TCr with waste heat (from power plants) to cover the thermal energy requirements.

Based on the above information, Scenario 2 consists of six process units (see **Figure 4. 5**). The seawater stream first goes to the NF unit and is separated into two different streams: one high in monovalent ions and one high in multivalent ions. The former is directed to a process line of conventional units, including the MED unit that obtains water from the evaporation process. Following this unit, the stream goes to a thermal crystallizer to finally obtain NaCl crystals and water. The latter stream from NF, high in multivalent ions, is directed to a treatment line comprising three innovative units for the recovery of magnesium and calcium in the form of hydroxide, Na_2SO_4 and water in the form of ice, and HCl and NaOH from the remaining NaCl-rich solution The recovered HCl and NaOH are reused in the treatment chain.

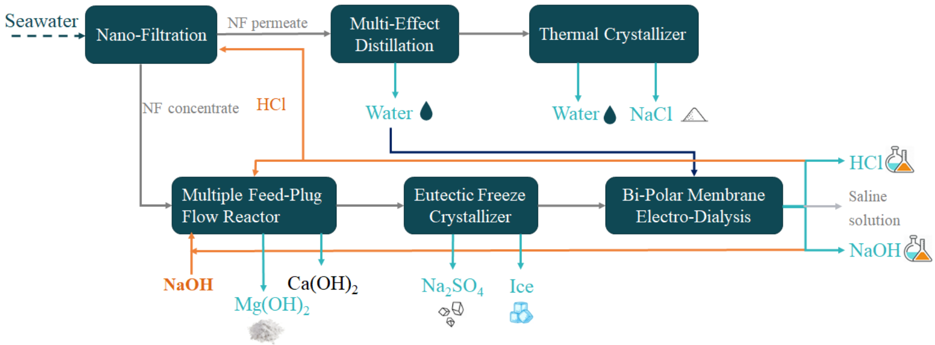

Figure 4. 5. Process flow diagram of Scenario 2.

Scenario 3: Integrated RO and brine treatment plant

Scenario 3 aims to ensure water availability and resource security by recovering multiple high-value materials. Specifically, in Scenario 3, the objective is to maximize water and resource recovery from seawater brine by integrating various technologies with a typical desalination plant that uses RO. Unlike Scenario 2, which is integrated with a MED plant, Scenario 3 is designed to be integrated with an existing RO plant (with 40% recovery). RO brine contains a large amount of water, this water can be recovered in a MED unit. All other aspects of Scenario 3 remain identical to those in Scenario 2 (see **Figure 4. 6**).

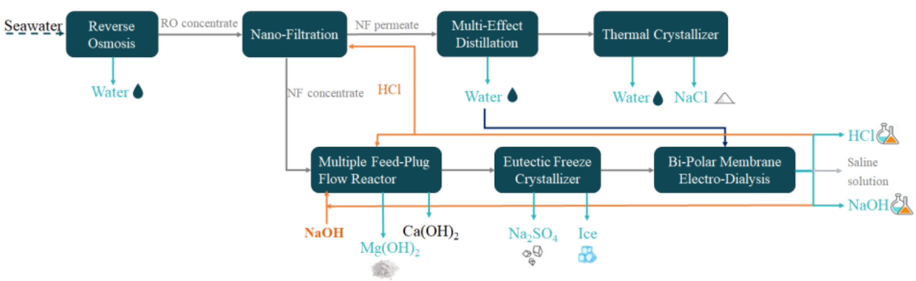

Figure 4. 6. Process flow diagram of Scenario 3.

Scenario 4: Electricity-based desalination and chemical recovery

The objective of Scenario 4 is to balance water and resource recovery. Specifically, this scenario focused only on the recovery of high-value materials such as Mg to increase the economic feasibility and long-term sustainability of the plant. Additionally, the internal production and consumption of chemicals from seawater brine could also contribute to those values and enhance the circularity of the plant. Electrodialysis (ED) can be used as pre-treatment to the EDBM unit to increase efficiency by concentrating the feed stream [40]. Additionally, [37] showed that the presence of sulphate ions does not significantly affect the purity of the obtained products but significantly reduces the specific energy consumption of EDBM. Overall, there is no brine discharge from the system since the exit flow streams from ED and EDBM are low salinity streams (diluted brines), and they could be recycled back into the system or discharged. Regarding the energy aspect, in this scenario, only electricity is used to cover the energy requirements of the treatment chain. This scenario addresses the values of energy security and climate change mitigation by using renewable energy and maybe the lack of waste heat (long-term sustainability). Therefore, only electricity-based technologies are used in the design of this scenario (see **Figure 4. 7**).

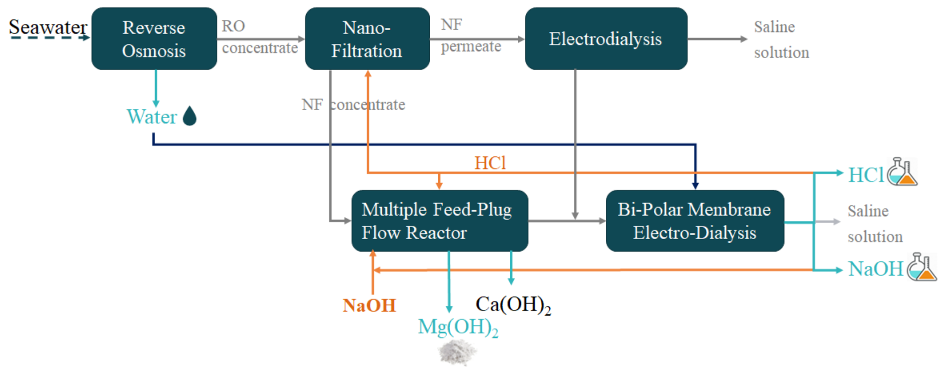

Figure 4. 7. Process flow diagram of Scenario 4.

Based on these, Scenario 4 consists of five process units (see **Figure 4. 7**) and it represents an MLD system aiming to maximize water and valuable resources recovery from brine. The seawater stream first goes to the RO unit that recovers 40% of the water, followed by the NF unit that separates monovalent and multi-valent ions. The monovalent-rich stream is further concentrated using ED, while the multivalent stream is processed to recover magnesium and calcium as hydroxide precipitates. The remaining solution, combined with the NaCl-rich stream from ED, is fed into the EDBM unit to recover valuable chemicals such as HCl and NaOH. Additionally, the low-concentration saline solution can be recycled back into the treatment chain.

Table 4. 3. Overview of the alternative technical scenarios.

Scenario	Objective	Technologies	Recovered products
1	Maximize water recovery and minimize brine discharge	NF, MED, ThCryst	Water, Mixed salts
2	Desalination and brine treatment for recovery of water and valuable products and minimizing brine discharge	NF, MED, ThCryst, MFPR, EFC, EDBM	$Ca(OH)_2$, HCl, Ice, $Mg(OH)_2$, NaCl, NaOH, Na_2SO_4, Water
3	Integrated RO plant with brine treatment for recovery of water and valuable products and minimizing brine discharge	RO, NF, MED, ThCryst, MFPPR, EFC, EDBM	$Ca(OH)_2$, HCl, Ice, $Mg(OH)_2$, NaCl, NaOH, Na_2SO_4, Water
4	Integrated RO plant with brine treatment focusing on chemical recovery, using only electricity-based desalination	RO, NF, ED, MFPR, EDBM	$Ca(OH)_2$, HCl, $Mg(OH)_2$, NaOH, Water

ED: Electrodialysis; EDBM: Electrodialysis with bipolar membranes; EFC: Eutectic freeze crystallization; MED: Multi-effect distillation; MFPR: Plug-flow reactor; NF: Nanofiltration; RO: Reverse Osmosis; ThCryst: Thermal crystallizer.

4.3.3. Performance assessment

In this section, we present a critical analysis of the performance of the four designed scenarios, each developed to enhance water recovery and reduce brine discharge compared to typical seawater desalination processes (see Section 4.2.3). The performance analysis is oriented around the identified value tensions (see Section 4.2.1, **Figure 4. 2**). All scenarios were designed to achieve *'zero brine production'*, effectively eliminating concentrated brine discharge (see **Table 4. 4**), and the modeling results confirm that this was achieved in all cases, resulting also in zero marine eco-toxicity potential. Scenarios 2, 3 and 4 produce a low-salinity solution of Na, Cl, and K, which it is possible to recycle this low-salinity stream back into the system or safely discharge it. For the sake of simplicity in this study, we have not considered the recirculation of these streams. Human toxicity potential due to chemical consumption is negligible across all scenarios, as only antiscalants, HCl, and NaOH are used. Note that other valuable trace elements, such as lithium or rare earth elements, are excluded from the analysis due to their low concentrations and the additional complexity required for recovery, which is beyond the scope of this study.

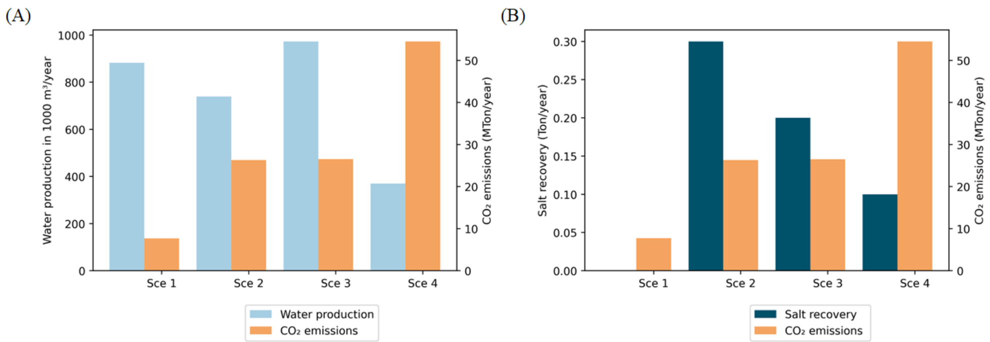

Figure 4. 9. Performance of integrated desalination and brine treatment systems in relation to CO_2 emissions from electricity consumption and (A) Water production, (B) Salt recovery.

Figure 4. 9 illustrates the trade-off between avoiding the environmental impacts of brine discharge and GHG emissions associated with the energy requirements of ZLD systems (see assumptions, Section 4.2.4). The increased salt recovery in Scenarios 2 and 3 results in 71% higher CO_2 emissions than Scenario 1 (water recovery scenario). This means that recovering multiple products and enhancing resource security value comes with different environmental costs and potential conflicts with values related to climate change mitigation and

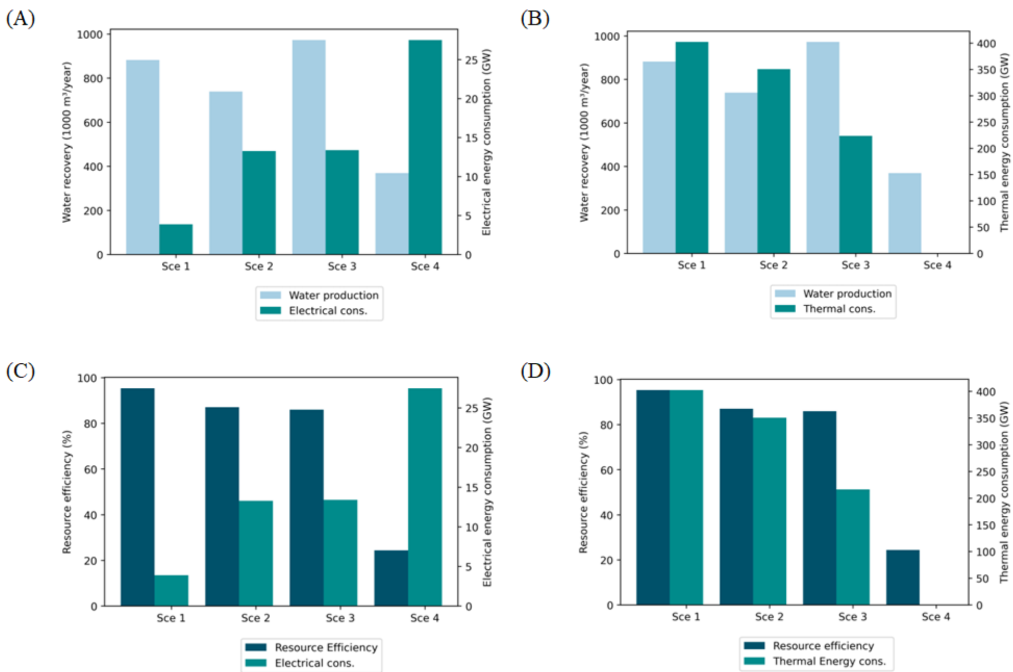

Figure 4. 8. Performance of integrated desalination and brine treatment systems in relation to electrical and thermal energy consumption and water production (A), B)), resource efficiency (C), D)).

environmental protection. Additionally, the use of thermal-based technologies and available waste heat sources, like Scenario 1, leads to lower CO_2 emissions. In contrast, Scenario 4 focuses on chemical production (lower water and salt production) with only electricity-based technologies that consume higher amounts of electricity and zero amounts of thermal energy, which implies 86% higher CO_2 emissions than Scenario 1 and 52% higher than Scenarios 2 and 3. This comparison is based on specific assumptions. Scenario 4 exclusively relies on grid electricity, and the emissions will largely depend on the local energy mix used to generate electricity. These emissions could be mitigated by integrating renewable energy sources, which will be considered in future studies.

Figure 4. 8 illustrates the results for water, recovery and overall resource efficiency versus electrical and thermal energy consumption. Resource efficiency in this context refers to the ratio of mass of valuable materials output, such as water, salts, and chemicals, to material input (see **Table 4. 3** and Section S1.3 in Supplementary Information). The comparison reflects the tension between the values of water, overall resource security and energy security. While the systems would enhance water availability and self-resilience, they increase the energy requirements, compromising energy security. Scenario 1, designed to align with stakeholder values of energy efficiency and security, achieves the lowest electrical energy requirements by utilizing waste heat (**Figure 4. 8A** and **B**). However, it doesn't perform the best in water production (9% lower than Scenario 3), which is the main objective of this scenario. Regarding the overall resource recovery, **Figure 4. 8** shows that the production of high-quality products in Scenarios 2 and 3 comes with high energy costs. Waste heat use reduces electricity intensity by 86% and 52%, compared to Scenario 4, which only uses electricity-based technologies. From an energy efficiency point of view, Scenario 1 performed better in terms of electrical energy consumption and water production, but Scenario 1 is less self-resilient. The use of available waste heat by coupling the desalination plant with a power plant to cover the thermal energy requirements and fewer electricity-dependent technologies can decrease the dependency on energy imports or additional energy sources. Although integrating waste heat promotes energy efficiency, there is a risk of sustaining dependence on fossil fuels, preventing the adoption of renewable energy sources.

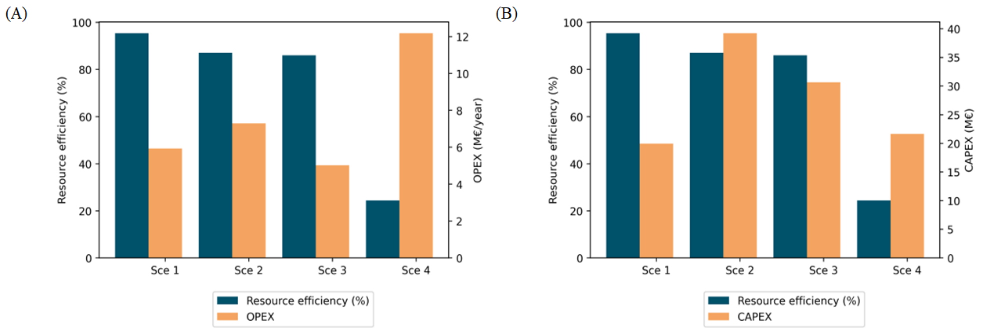

Figure 4. 10. Performance of integrated desalination and brine treatment systems in relation to resource efficiency (%) and (A) OPEX, (B) CAPEX.

The tension between resource recovery for water and resource security and associated costs is illustrated in **Figure 4. 10**. Scenarios 1-3 achieve high resource efficiency (86%-95%), which comes with high economic costs. Contrarily, Scenario 4, with a focus on chemical production and the use of only electrical-based technologies, has the highest OPEX because of the high electrical energy consumption and the low resource efficiency. The OPEX in scenario 4 is 40-59 % higher than in the other scenarios. The integration of technologies to recover multiple valuable products effectively results in a high investment cost, specifically for Scenarios 2 and 3 (Sc2: 49% higher than Sc1, 22% higher than Sc3, 45% higher than Sc4, Sc3: 35% higher than Sc1 and 29% higher than Sc4). An opportunity to deal with this tension is to consider alternative energy sources to decrease energy costs and, therefore, the OPEX. Regarding CAPEX, alternative approaches or designs for the production of the same products could be explored. These technologies will become more cost-effective without compromising resource efficiency as designs evolve, and advancements reduce initial high costs. Scenario 3 offers an additional benefit compared to Scenario 2 by integrating the brine treatment system with an existing RO plant. This integration enhances the system's overall efficiency and resource utilization. It enables the utilization of existing infrastructure, which means lower investment costs.

The tension between water, resource security, and profitability is given in **Figure 4. 11**, which displays resource recovery efficiency and production efficiency for the four scenarios. The production efficiency reveals the monetary value of all the recovered products relative to the total annual cost and, therefore, provides insights into the affordability of the production of multiple products. The higher the production efficiency, the more profitable and competitive the solution. Despite the high resource efficiency and the low OPEX of Scenario 1, its low revenue relegates it to the least profitable. This is because water is the only product of the system. The high resource efficiency of Scenario 1 means that most of the compounds are recovered but in the form of mixed salt, which means low product quality and, thus, low economic value. Scenario 4 presents the largest OPEX, and despite the high investments required, this scenario is potentially more profitable and has higher production efficiency thanks to the possibility of recovering and selling Mg and chemicals (NaOH, HCl). Scenario 3, while having a similar OPEX to Scenario 1, offers higher profitability due to revenue from selling salts and chemicals, offsetting production costs. Scenarios 2 and 3 have the most affordable water.

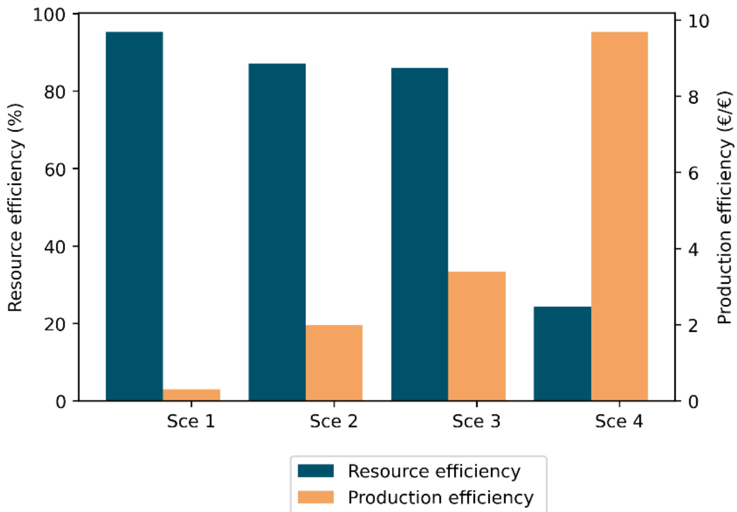

Figure 4. 11. Performance of integrated desalination and brine treatment systems in terms of resource efficiency and production efficiency.

In resource recovery, Scenarios 2 and 3 excel in water and high-quality salt production. Scenario 3 yields a 9% increase in water production compared to Scenario 1. Although Scenarios 2 and 3 have similar designs, they differ in water and salt recovery. Scenario 3 produces the most desalinated water (24% more than Scenario 2), while Scenario 2 has the highest number of high-quality salts and chemicals. Scenario 4 prioritises chemical recovery, resulting in low water and salt recovery and overall resource efficiency compared to the other scenarios (only 24% resource efficiency). To accurately reflect Scenario 4's performance in its target area (chemical recovery), the output-specific resource efficiency metric (see Supplementary Information, Section S1) is applied. This metric focuses on the recovery efficiency of the targeted chemicals such as NaOH, HCl, and $Mg(OH)_2$, rather than water or general salt recovery. Using this indicator, Scenario 4 achieves an output-specific resource efficiency of 92%, reflecting its high performance in recovering valuable chemicals, despite its lower overall resource recovery rate (measured in terms of water and salts).

This distinction highlights that while Scenario 4 performs less effectively in general resource efficiency compared to Scenarios 1, 2 and 3, its focus on chemical recovery makes it a strong candidate for regions or industries where chemicals like NaOH and HCl are of primary importance. Thus, Scenario 4's lower overall resource efficiency is offset by its high efficiency in producing specific valuable products tailored to meet specific industrial demands.

Table 4. 4. Summary of results of the evaluation of technical scenarios.

	Scenarios			
Indicator	**Scenario 1: Water Recovery**	**Scenario 2: Desalination and resource recovery**	**Scenario 3: Integrate RO plant with brine treatment**	**Scenario 4: Electricity-based desalination and chemical recovery**
Energy consumption (GWh)	3.9	13.3	13.4	27.5
Quantity of water produced (1000 m^3/year)	881.7	738.8	972.9	369.7
Quantity of salt produced (Ton/year)	0.0	0.3	0.2	0.1
Resource efficiency (%)	95.4	87.1	86.0	24.4
Brine production (ton/year)	0.0	0.0	0.0	0.0
CAPEX (M€)	20.0	39.2	30.6	21.7
OPEX (M€/year)	5.9	7.3	5.0	12.2
Production efficiency (€/€)	0.3	2.0	3.4	9.7
Carbon dioxide emission (MTon CO_2-Equ)	7.7	26.3	26.5	54.5
Water footprint (1000 m^3/year)	0.0	267.1	248.0	688.5
Eco-toxicity (Kg of brine/kg of seawater)	0.0	0.0	0.0	0.0
Human toxicity (-)	0.0	0.0	0.0	0.0

Figure 4. 12 summarises the alignment of the four designed scenarios against stakeholder values, including water security, resource security, efficiency, affordability, and environmental impact. By aligning each scenario with specific societal values our approach provides a more nuanced understanding of the scenarios' real-world implications. As shown in **Figure 4. 12**, Scenario 1 strongly aligns with values of water security, energy security, and efficiency due to its use of waste heat and lower electrical energy consumption. However, with water as the only valuable product and the generation of solid waste, its alignment with affordability is weaker, reflecting potential cost concerns.

	Alignment of technical scenarios with stakeholders' values			
Stakeholders' values	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Water security	● Strong	● Strong	● Strong	● Weak
Resource Security	● Weak	● Strong	● Strong	● Strong
Energy Security	● Strong	● Strong	● Strong	● Moderate
Affordability	● Weak	● Moderate	● Moderate	● Strong
Protection of the environment	● Moderate	● Strong	● Strong	● Moderate
Climate change mitigation	● Strong	● Moderate	● Moderate	● Weak
Efficiency	● Moderate	● Moderate	● Moderate	● Weak

● Strong alignment ● Moderate alignment ● Weak alignment

Figure 4. 12. Qualitative performance assessment of scenarios for sustainable seawater desalination. This figure presents an overview of the four designed scenarios (Sc1: Water recovery, Sc2: Desalination for resource recovery, Sc3: Integrated RO and brine treatment plant, and Sc4: Electricity-based desalination and chemical recovery) relative to identified stakeholder values. A dark teal dot denotes strong alignment, a light teal dot denotes moderate alignment, and a turquoise dot denotes weak alignment.

Scenarios 2 and 3 excel in both water and high-quality salt production, demonstrating strong alignment with resource security and circular economy values. The increased energy requirements may pose challenges in terms of sustainability and energy security, potentially conflicting with stakeholder values associated with climate change mitigation and environmental protection. The potential economic viability and resource efficiency of these scenarios may support their alignment with affordability and efficiency, provided that energy challenges are adequately addressed.

While Scenario 4 aligns with resource security values, it also involves higher electricity consumption and increased CO_2 emissions, challenging climate change mitigation values. The lower production of water and salt results in a weaker alignment with water security. The economic viability and resource efficiency of Scenario 4's chemical production show a strong alignment with affordability value and a weak alignment with efficiency value.

4.3.4. Societal context and scenario suitability

In addition to assessing each scenario's performance, it is crucial to evaluate its suitability within specific societal contexts. The benefits and drawbacks of each scenario may vary based on the unique characteristics and priorities of the society in which they are implemented. Based on these benefits and drawbacks, we discuss which scenario is suitable for a specific context.

For the sake of having low CO_2 and GHG emissions, it is desirable to implement electricity-based systems in areas where renewable energy sources are available or in areas where there are no restrictions for the deployment of renewable energy systems due to extensive land use. The use of waste heat results in lower (direct) GHG emissions. However, the risk of sustaining dependence on fossil fuels is higher with the utilization of waste heat to cover the thermal energy requirements of the systems. Ensuring flexibility in energy integration is crucial to avoid dependency on fossil fuels (long-term sustainability). To mitigate these risks, it is recommended to establish a flexible integration approach between thermal equipment and waste heat. This approach would involve obtaining thermal energy directly from renewable energy sources, such as solar hybrid systems or solar collectors, to supply the MED and thermal crystallizer units [41,42].

Based on the reported results and the above analysis, Scenario 1 is particularly suitable in regions where water scarcity is a critical issue and the primary goal is to maximize water production. Examples included small islands, the Mediterranean or the Aegean Sea, or arid coastal areas, where tourism is the main industry. For instance, in Lampedusa, a small island in the Mediterranean Sea, desalination often covers 100% of the water demand due to limited freshwater sources [25]. Additionally, it is applicable in regions where the economic context is characterized by limited industrial activities or markets for by-products like salts/chemicals. In this context, water is the only valuable product due to the high demand. Those areas are often characterized by limited access to renewable energy sources due to land constraints; thus, the allocation of the energy sources is primarily for meeting the basic requirements of the local community, leaving limited capacity for producing additional products from recovered resources. Therefore, despite the higher profitability of Scenarios 2-4 from recovered resources, it can't compensate for the additional energy requirements in energy scarcity regions and the lack of local demand for the resources. Finally, utilizing waste heat from existing power plants helps lower the additional energy needs for extra water and the direct GHG emissions, making it environmentally viable in regions with limited land for renewable energy installations.

Scenario 4 focuses on chemical production using electricity-based technologies, making it suitable for coastal areas or larger islands with more electricity sources or no critical land limitations for applying solar or wind energy. However, the economic viability of Scenario 4 heavily relies on the presence of established markets or potential off-takers for the produced chemicals such as Mg, NaOH, and HCl. In regions where there is a strong market demand for these chemicals, this scenario not only offers a technically feasible solution but also supports local economies by integrating into existing supply chains. This consideration is crucial for the realistic implementation of resource recovery operations and underscores the importance of aligning technical solutions with market demands and societal needs.

In the case of regions with high industrial activities where there is a demand for high-quality salts and chemicals, Scenarios 2 and 3 are the most suitable since water and seven additional high-quality products are recovered from seawater desalination. The additional products would enhance/promote the circular economy and industrial symbiosis, bringing additional benefits to the local economy and community. The presence of industries that can utilize the recovered salts and chemicals helps justify the higher CAPEX and OPEX. The local production and consumption of those products could also prevent risks of future short supply chains. In the case of an existing RO plant, the investment cost is lower, and the implementation of the brine treatment chain would eliminate stakeholder's concerns about brine discharge and its potential environmental impact on marine life.

4.3.5. Discussion, limitations and future work

This study demonstrated the integration of stakeholders' values into the design and assessment of integrated seawater desalination and brine treatment systems, using a VSD approach. Unlike traditional evaluations in the desalination field that mainly prioritize economic gains or technical performance, this work integrates environmental, social, and ethical aspects that are often overlooked in the design assessment via VSD, providing a more holistic evaluation beyond evaluating indicators. The design of alternative technical scenarios can become very challenging and complicated, especially when technologies are integrated into a system. However, prioritizing the identified values, technical variables and constraints, and stakeholders' knowledge in the design of the scenarios promotes the development of solutions that are not only technically feasible but also socially acceptable and sustainable in the long run. This approach bridges the gap between technical feasibility and societal relevance by using stakeholders' values for scenario design and indicator selection and by validating the techno-economic models with stakeholders' knowledge, fostering more informed decision-making.

The methodology demonstrates the need to tailor desalination and brine treatment systems to the specific values, concerns, and expectations of different communities. It is informed by the example of Lampedusa and the values identified in previous work. The results reveal that in regions like Lampedusa, where water scarcity is acute and industrial activity is minimal, prioritizing water production directly addresses local needs, and resource recovery is not desirable. In more industrialized coastal areas, like larger islands or areas in the Mediterranean Sea, the focus on resource recovery and circular economy principles can support local industries and enhance economic resilience.

Analysing the tensions between scenarios through VSD fosters essential stakeholder dialogue, enabling the exploration of trade-offs and the identification of context-specific solutions. Discussing the performance results with relevant stakeholders allows the identification of general patterns and insights that can guide future designs based on regional differences, influenced by factors such as climate, economy, and cultural norms. For example, stakeholders in densely populated urban areas may prioritize efficient water production to meet high demand, while those in rural communities may prioritize environmental sustainability and local resource management. Scenarios tailored to address water scarcity in arid regions may prioritize water production and energy efficiency, while those in coastal areas may focus on environmental conservation and minimizing ecological impact.

The adaptability of these scenarios is a key finding, as it provides decision-makers with a range of options depending on their priorities, regional needs and constraints. The findings suggest that future desalination projects should prioritize early and continuous stakeholder engagement to ensure that technological solutions are not only technically and economically viable but also align with the societal values of the communities they serve. Policymakers should consider these insights when drafting regulations that support sustainable and socially responsible resource recovery.

Beyond the context of this study, our methodology holds valuable insights for technological developments in the field of integrated seawater desalination and brine treatment systems. By emphasizing the trade-offs and potential benefits of different scenarios, our approach provides a roadmap for researchers and engineers to refine and innovate technologies that address critical societal and environmental challenges.

Limitations

While this study successfully integrates technical and social dimensions through the VSD approach, several limitations should be noted:

- Stakeholder Engagement: The stakeholder values used were derived from prior research rather than direct engagement through interviews or surveys. While these values are reliable within the context of previous research, the incorporation of broader engagement to capture diverse perspectives and validate the values in specific contexts would enhance the robustness of the analysis.
- Validation of Technical Scenario Design: The technical scenarios were designed based on stakeholder values, but further rounds of empirical validation with stakeholders are needed to assess the practical implications and feasibility of the proposed designs. Additional workshops and feedback sessions would help refine these scenarios.
- Energy Use Assumptions: The reliance on grid electricity with EU average emissions factors is a simplification. This approach does not account for the variability in energy mixes or the potential use of renewable energy sources, which could significantly alter the emissions outcomes. Therefore, the results should be interpreted with the understanding that alternative energy sources could yield different environmental impacts.

Future work

Future work should apply this methodology to specific locations, incorporating broader stakeholder engagement through interviews or surveys to identify and validate values in a particular context. Empirical validation with stakeholders will provide valuable insight into scenario performance and real-world feasibility. Additionally, comparing scenarios with linear production systems that produce the same products using LCA methodology will assess the potential environmental benefits of resource recovery systems.

Exploring alternative energy sources will help evaluate the impact of the energy mix on identified tensions (water, resource security, and energy security) and provide insights into how renewable energy can mitigate CO_2 emissions. Expanding this framework to diverse geographic regions and cultural settings will ensure its relevance across societal contexts.

Finally, integrating system dynamics with the VSD approach could offer a more comprehensive understanding of the problem statement for resource recovery systems. While VSD effectively aligns technical configurations with societal values and stakeholder needs, system dynamics can increase understanding of the scope and complexity of the problem and trust in model results [43]. This combination would support more informed and collaborative decision-making.

4.4. Conclusions

In recent years, the integration of desalination with brine treatment technologies has been increasingly studied, aiming to develop sustainable solutions for resource recovery from seawater. This study used four technical configurations to evaluate a Value-Sensitive Design (VSD) framework, demonstrating the importance of tailoring systems to specific societal and regional needs. Each scenario offers unique benefits and trade-offs, highlighting the need to balance water and resource recovery with energy consumption and environmental impacts.

Using the identified values from the example of Lampedusa island, the proposed technical scenarios reveal emerging trade-offs around seawater desalination and brine treatment, highlighting the importance of considering multiple perspectives in their design. Scenarios that prioritize water and salt recovery align with water and resource security values but require higher energy input, raising concerns about their economic and environmental sustainability. In contrast, scenarios utilizing existing waste heat or focusing on chemical production offer greater energy efficiency but may limit broader resource recovery or lead to higher CO_2 emissions. These findings underscore the importance of tailoring solutions to regional conditions and energy availability, ensuring that technological advancements are sustainable and contextually appropriate.

This study serves as an example for supporting decision-making and guiding the development of sustainable solutions for resource recovery from seawater. By using the VSD methodology, we gain insights that go beyond traditional techno-economic evaluations by incorporating societal values, ethical considerations, and stakeholder perspectives. This holistic approach is designed to support the development of solutions that are technically and economically viable, as well as socially acceptable, proactively addressing potential societal resistance and ethical dilemmas. As we move forward, embracing methodologies that incorporate societal aspects beyond social indicators will be crucial in ensuring that technological advancements contribute effectively to sustainable and equitable resource management.

4.5. Supplementary information

See documentation.

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5

Economic evaluation of water and resource recovery plants: A novel perspective on levelized cost

ABSTRACT

Water treatment facilities are bound to incorporate resource recovery in the near future, necessitating novel economic assessments that capture the full economic potential of these systems. This study evaluates three cost calculation methods—Non-allocation, Economic allocation, and Dual allocation— to improve the accuracy of the Levelized Cost for multi-product desalination and brine treatment plants. The methods were tested across three technical scenarios: Sc1) maximum water recovery, Sc2) integrated desalination with brine treatment for resource recovery and Sc3) electricity-based desalination for chemical recovery. Results reveal that the traditional Non-allocation method tends to overestimate production costs by uniformly applying fixed costs across products, leading to inflated levelized costs. The Economic allocation approach reduces the levelized costs of water and other recovered products by up to 81%, enhancing competitiveness with conventional production methods. The Dual allocation approach is most effective for recovered salts and chemicals, ensuring fair cost distribution and fostering competitiveness with linear systems. Sc2 is the most economically feasible under both novel approaches due to its balanced mix of high-value products and moderate operational costs. These findings suggest that cost calculation methods should align with plant objectives: Economic allocation for scenarios prioritizing water recovery and Dual allocation for maximizing the value of salts and chemicals. This study provides a foundation for tailored economic assessments and guides plant design and investment decisions.

Keywords: *Economic assessment; Levelized cost; Desalination; Brine treatment; Resource recovery.*

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5.1. Introduction

Seawater is a rich source of valuable and rare materials [1]. The integration of desalination and brine treatment technologies holds promise for water sustainability and the advancement of circular economy principles by recovering materials like NaCl and $Mg(OH)_2$ [2]. In recent years, there has been a notable shift towards integrating these technologies to achieve Zero Liquid Discharge (ZLD), ensuring both water sustainability and economic feasibility. As resource recovery gains prominence, traditional economic assessment tools, which focus solely on water production, are no longer sufficient. New tools are required to evaluate the economic feasibility of multi-product systems and to support investment decisions by fairly comparing recovered materials with their equivalent conventional products [2,3].

Historically, desalination plants have been evaluated based on water production costs using metrics such as unit cost [4–6], production cost [7], water cost [8–10] and levelized cost of water [11–14]. With a growing emphasis on circular desalination, the Levelized Cost of Water (LCW) has been modified. [15] included the environmental and social costs of the plant in the calculation of LCW. In renewable energy-powered desalination plants, the costs and benefits of water and energy cogeneration are integrated into LCW [16–18].

For the assessment of brine treatment plants, [19] introduced the levelized cost of the by-product, NaCl crystals, and the Levelized Brine Cost [20], considering concentrate brine as a by-product. These approaches modified the traditional Levelized Cost (LVC) calculation to account for revenues generated by by-products, thus providing a more comprehensive view of economic feasibility. [21] further advanced this concept by evaluating the economic feasibility of multi-product systems through the Levelized Cost Index, which includes a specific cost index for each product.

Despite these advancements, there remains a significant gap in how costs are allocated across technologies in multi-product systems where water and other valuable products are recovered. Current methods typically load the total annual cost uniformly over each product, often failing to capture the complex interdependencies among technologies and operational synergies within multi-product systems, such as shared infrastructure and complementary processes, where one technology may serve as a pre-treatment for another. This simplification can reduce the accuracy of feasibility assessments by inflating costs for some products and undervaluing others, potentially leading to unprofitable plants and skewing investment decisions.

This study addresses this gap by introducing two novel cost allocation methods—the Economic allocation and Dual allocation approaches. Unlike existing methods, these approaches incorporate operational synergies and technological interconnections, ensuring fairer cost distribution and more accurate economic assessments. In particular, this study aims to investigate how different cost calculation methods influence the levelized cost of products in a multi-product desalination and brine treatment plant. The study compares traditional and the two novel cost allocation methods to clarify their impact on the economic feasibility of resource recovery.

To evaluate the effectiveness of these methods, we developed economic models for integrated desalination and brine treatment systems. Inspired by existing calculation methods in the literature [21,22], the theoretical background on joint costs [23], other domains such as life cycle assessment [24], and the need to evaluate the economic benefits of resource recovery plants, we introduced two novel calculation methods for levelized cost. Using varied technical scenarios that represent different operational conditions and objectives, we assessed the performance of each method in delivering representative economic outcomes.

This study bridges methodological rigor with practical applications, advancing the understanding of fair cost allocation in multi-product systems. By optimizing resource recovery and economic feasibility, it supports the transition toward a circular economy. The insights gained can directly inform process design, investment decisions and policy frameworks, promoting sustainable resource recovery strategies in water-scarce regions and industries reliant on high-value materials.

5.2. Case study description

In this study, a case of integrated desalination and brine treatment plants aiming to recover valuable materials such as water, salts, and chemicals, as shown in **Figure 5. 1** is used primarily to demonstrate the application of novel cost allocation methods. Although the study does not focus on a specific real-world site, it is informed by real-world cases and prior research, particularly the example of islands and coastal regions that rely on desalination as their primary freshwater source [25].

Building on prior research on treatment chains for resource recovery from brine effluent [2,13,26], this hypothetical but practical case simulates an integrated desalination-brine treatment system with a feed flow rate of 3000 m^3/d (capacity of a desalination plant on an island), reflecting real-world resource challenges [27]. The technical scenarios in this study test varying objectives and cost allocation methods, offering insights into the broader applicability of the calculation methods.

5.2.1. Definition of scenarios

In this work, technical scenarios are analysed to evaluate the calculation methods based on varying objectives for the studied plant configuration. Although all scenarios aim to increase water recovery and reduce brine discharge compared to typical seawater desalination, they differ in their specific objectives [27]. These technical scenarios aim to recover water, salts (NaCl, $Mg(OH)_2$, Na_2SO_4) and chemicals (HCl, NaOH) from seawater, as shown in **Figure 5. 1**.

- **Scenario 1 (Water recovery):** focuses on maximizing water recovery and minimizing brine discharge without the recovery of additional products, simulating a case where the primary objective is potable water production with minimal environmental impact.
- **Scenario 2 (Integrated RO plant with brine treatment):** integrates the Reverse Osmosis (RO) desalination plant with the brine treatment plant to optimize both water and salt recovery and minimize brine discharge.
- **Scenario 3 (Electricity-based desalination with chemical recovery):** integrated RO plant with brine treatment focusing on chemical recovery, such as HCl and NaOH, using only electricity-based desalination.

Each of these scenarios aligns with different real-world recovery objectives, from basic water recovery to comprehensive chemical extraction, thus offering a robust framework for assessing the economic implications of each configuration. Further details on the design, motivation and simulations of these scenarios can be found in Supplementary Information (see Section S1) and Chapter 4.

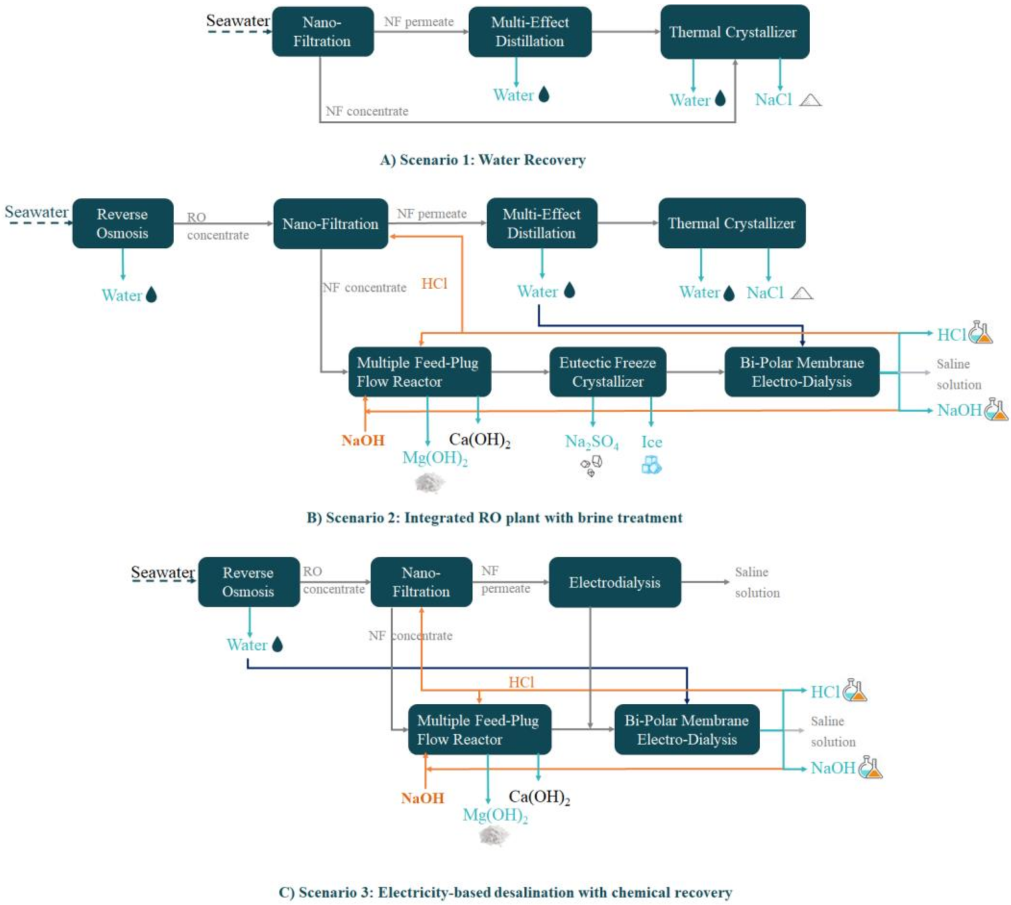

Figure 5. 1. Process diagram of the three scenarios illustrating the integrated desalination and brine treatment systems used in the present study [27].

5.3. Material and method

Levelized cost is the price at which a product should be sold to cover all production costs and reaches break-even costs [13]. Until now, it is expressed as the ratio of all the capital and operating expenses and the revenues coming from the by-products of the plant over the economic life to the overall production of a product over the same period [13,18]. The purpose of this work is to investigate the influence of different cost calculation methods on the levelized cost of the products in a multi-product desalination and brine treatment plant. Input assumptions like capacity costs, maintenance, marginal operating costs, or average capacity factor vary by study and are critical to the calculation [28]. We applied the traditional approach alongside two novel methods under the same conditions to provide a baseline for comparison. This approach ensures that any observed differences in levelized cost are due to the methodologies themselves rather than external variables.

The different calculation methods are designed to evaluate the influence on the LVC when the by-products are not considered as by-products anymore but as valuable products of the plant (multi-functional system). Another parameter that is taken into account is the consideration of brine as a resource and not as a waste and how this would change the economic evaluation in the future. The different methodological approaches followed in this work are illustrated in **Figure 5. 2**. Below, a detailed explanation of three calculation methods is given.

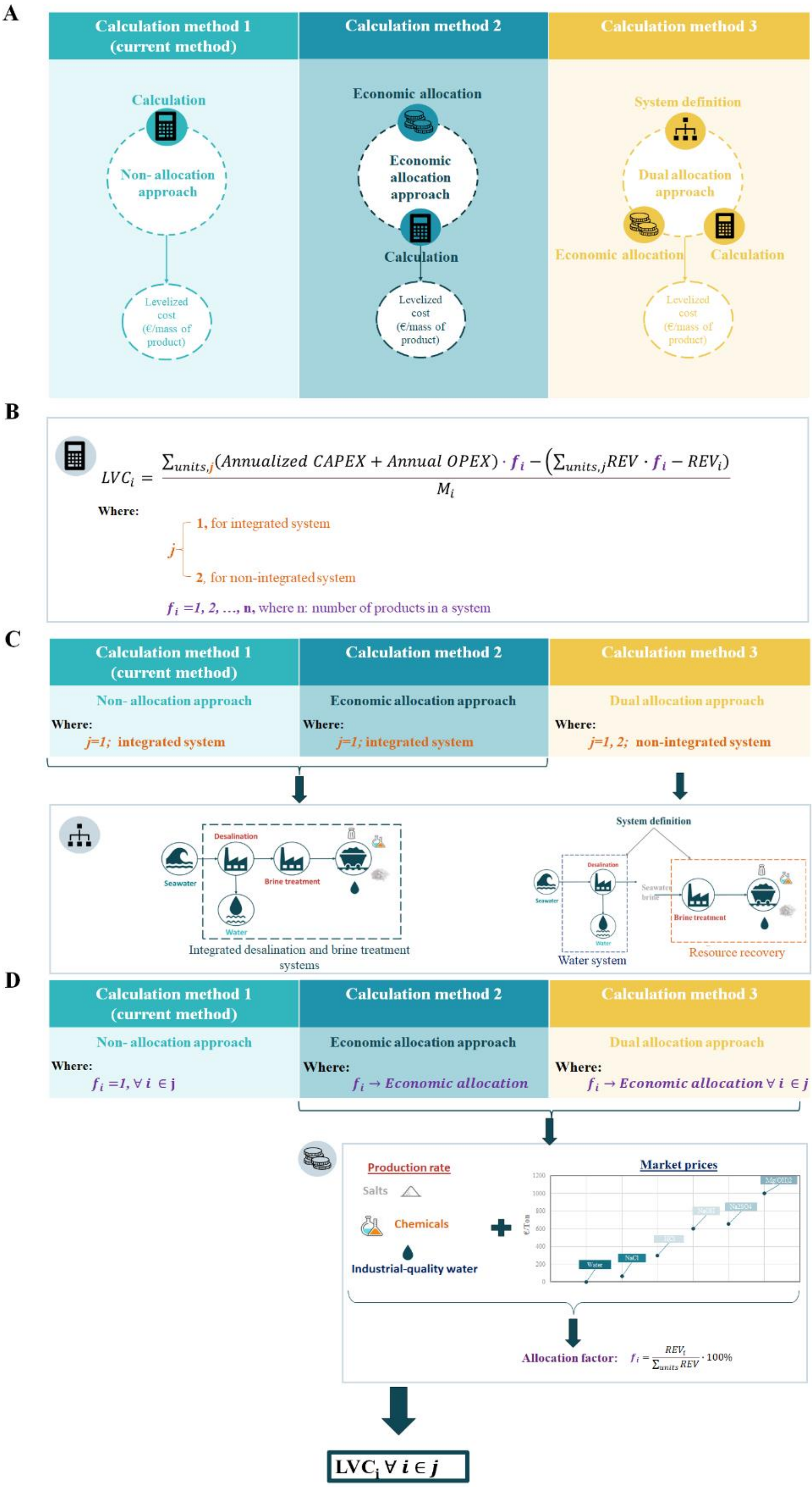
A
Calculation method 1 (current method)
Calculation method 2
Calculation method 3
Calculation
Non- allocation approach
Levelized cost (€/mass of product)
Economic allocation
Economic allocation approach
Calculation
Levelized cost (€/mass of product)
System definition
Dual allocation approach
Economic allocation
Calculation
Levelized cost (€/mass of product)
B
$LVC_i = \frac{\sum_{units,j}(Annualized\ CAPEX + Annual\ OPEX)\cdot f_i - \left(\sum_{units,j} REV \cdot f_i - REV_i\right)}{M_i}$
Where:
j
1, for integrated system
2, for non-integrated system
f_i =1, 2, …, n, where n: number of products in a system
C
Calculation method 1 (current method)
Calculation method 2
Calculation method 3
Non- allocation approach
Economic allocation approach
Dual allocation approach
Where:
j=1; integrated system
Where:
j=1; integrated system
Where:
j=1, 2; non-integrated system
Desalination
Seawater
Brine treatment
Water
Integrated desalination and brine treatment systems
System definition
Desalination
Seawater
Seawater brine
Brine treatment
Water
Water system
Resource recovery
D
Calculation method 1 (current method)
Calculation method 2
Calculation method 3
Non- allocation approach
Economic allocation approach
Dual allocation approach
Where:
f_i =1, ∀ i ∈ j
Where:
f_i → Economic allocation
Where:
f_i → Economic allocation ∀ i ∈ j
Production rate
Salts
Chemicals
Industrial-quality water
Market prices
€/Ton
Water
NaCl
Allocation factor: $f_i = \frac{REV_i}{\sum_{units} REV} \cdot 100\%$
LVC$_i$ ∀ i ∈ j

Figure 5. 2. Schematic diagram illustrating the methodology for calculating the levelized cost of products using three different calculation methods: Non-allocation, Economic allocation, and Dual allocation. (A) Overview of the three methodological approaches, including data and technical configurations inform the calculations; (B) Overview of the methodological approach adopted in this study for the calculation of the levelized cost of each product; (C) The methodological approach for system definition in Dual allocation approach: water system and resource recovery system; (D) Overview of the methodological approach adopted in this study for the calculation of the allocation factors, including production rates, market prices and the annual revenues of the products.

5.3.1. Economic model: Definition of input/outputs

For the calculation of the LVC, economic models were developed based on previous work [27]. The main purpose of these models is to provide the necessary data for LVC calculations. Interested readers can refer to the GitHub repository for the technical process and economic models (https://github.com/rodoulak/Desalination-and-Brine-Treatment-Simulation-.git). **Table 5. 1** shows the most relevant inputs and outputs of the economic model used in this study for the economic assessment of the technical scenarios. The mathematical description and the main assumptions can be found in Chapter 3 and the Supplementary Information (see Sections S2, S3). It is important to note that the main focus of this work is not the detailed calculation of major costs and revenues in desalination and brine treatment processes. **Table 5. 2** shows the annual production rate of each product across the three technical scenarios. Further technical details, including input data on products' flow rates and quality, as well as the energy, chemical, and water requirements, are available in Section S4 (Supplementary Information). To simplify the calculation of LVC, it is assumed that the production rates and operational costs are constant over the years.

Table 5. 1. Main inputs and outputs of the economic model for the economic assessment of the technical scenarios.

	Input	Output
Economic model	Equipment cost	Capital cost (CAPEX)
	Product mass flow rates	Operating cost (OPEX)
	Quality of products	Revenues
	Energy consumption	
	Chemical consumption	
	Cooling water requirements	

Table 5. 2. Summary of the annual production rate of each product across the three technical scenarios.

Product	**Scenario 1**	**Scenario 2**	**Scenario 3**
Water (m^3/year)	8.82E+05	9.73E+05	3.70E+05
NaCl (Ton/year)	2.69E+04	2.32E+04	N/A
$Mg(OH)_2$ (Ton/year)	N/A	2.55E+03	2.55E+03
Na_2SO_4 (Ton/year)	N/A	2.91E+03	N/A
NaOH (Ton/year)	N/A	N/A	8.49E+03
HCl (Ton/year)	N/A	1.63E+03	1.15E+04

5.3.2. Calculation method 1: Non-allocation approach

The first calculation method is the commonly used approach based on the definition of the LVC without any allocation method. According to the knowledge of the authors of this article, the latest modification of the calculation method for the levelized cost of products in a multi-product plant, as described by [21], is expressed in eq. 1. In their study, [21] considered the Annualized costs of the different units and the revenues of the multiple products in the calculation of the LVC. The following calculation is carried out for each product in the plant.

$$LVC_i = \frac{\sum_{units}(Annualized\ CAPEX + Annual\ OPEX) - (\sum_{units} REV - REV_i)}{M_i} \qquad \text{eq. 1}$$

Where LVC is the Levelized cost of the i^{th} product in the plant (€/Ton or €/m^3), CAPEX is the capital cost of each unit/technology within the plant (€/year), OPEX is the operating cost of the unit (€/year), REV is the revenue from the i^{th} product of the unit/technology (€/year) and M is the annual production rate of the interested i^{th} product (Ton/hr or m^3/hr).

5.3.3. Calculation method 2: Economic allocation approach

The Economic allocation method suggests the consideration of the by-products as the main products and the distribution of the cost based on their economic value. In the context of integrated desalination and brine treatment plants that prioritize resource recovery, the emphasis shifts from brine minimization to the recovery of valuable, high-quality products. In this case, each unit or technology essentially functions as a 'pre-treatment' for the subsequent one. Consequently, capital and operating expenses, as well as revenues, need to be fairly distributed among all products in a multi-product plant (multi-functional system). This cost allocation is essential to avoid arbitrary distribution, which could misrepresent the economic value of individual products. To handle multi-functionality, Economic allocation is employed according to the life cycle assessment ISO standard [24,29] and life cycle costing [30], allocating a higher cost (or impact) to products generating the highest revenues. By considering the economic value of each product, this method ensures a rational and fair distribution of costs, aligning with the plant's overall objective—whether it prioritizes brine minimization or resource recovery.

Accordingly, the Economic allocation method used in this work considers the contribution of the products in the calculation, as is shown in eq. 2. In particular, Economic allocation is considered for the distribution of the entire plant's annualized costs and revenues.

$$LVC_i = \frac{\sum_{units}(Annualized\ CAPEX + Annual\ OPEX) \cdot f_i - (\sum_{units} REV \cdot f_i - REV_i)}{M_i} \quad \text{eq. 2}$$

Where f_i is the economic allocation factor of the i^{th} product, representing the proportion of costs allocated to the i^{th} product. The economic allocation factor is calculated based on the economic value of the products (see **Table S3**) and, therefore, the revenues associated with that product (see results in **Table 5. 3**).

The economic allocation factor of the i^{th} product (f_i) is calculated:

$$f_i = \frac{REV_i}{\sum_{units} REV} \cdot 100\% \quad \text{eq. 3}$$

The revenues associated with selling a specific product is calculated as follows:

$$REV_i = M_i \cdot t_{operation} \cdot SP_i \quad \text{eq. 4}$$

Where REV is the revenue from the i^{th} product of the unit/technology (€/year), M is the annual production rate of the interested i^{th} product (Ton/hr or m^3/hr), $t_{operation}$ is the total operation time in one year (in hr), and SP_i is the selling price of the i^{th} product (in €/Ton or €/ m^3).

Table 5. 3. Economic allocation factors for Scenarios 1, 2 and 3, based on revenues used in the second calculation method.

	Revenues (€/year)			**Economic allocation** (%)		
Product	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Scenario 1**	**Scenario 2**	**Scenario 3**
Water	8.82E+05	9.73E+05	3.70E+05	33.21%	13.01%	3.11%
NaCl	1.77E+06	1.53E+06	N/A	66.79%	20.51%	N/A
$Mg(OH)_2$	N/A	2.55E+06	2.55E+06	N/A	34.16%	21.52%
Na_2SO_4	N/A	1.90E+06	N/A	N/A	25.38%	N/A
NaOH	N/A	0.00E+00	5.30E+06	N/A	0.00%	44.66%
HCl	N/A	5.19E+05	3.64E+06	N/A	6.94%	30.71%

5.3.4. Calculation method 3: Dual allocation approach

Inspired by the industrial symbiosis concept, defined as the collective approach to competitive advantage through the exchange of materials, energy, water, and by-products among traditionally separate entities [31], the Dual allocation method suggests the division of the treatment chain into distinct sub-systems: the water recovery sub-system and the resource recovery (or brine mining) sub-system. By applying this concept to the proposed desalination and brine treatment plant, the Dual allocation method lays the groundwork for potential separation in the future, emphasizing adaptability, resource efficiency, and the achievement of competitive advantages through symbiotic relationships between water and resource recovery systems. The resource recovery sub-system will operate as a stand-alone plant, using desalination brine as feedstock.

By distinctly accounting for water and resource recovery processes, the method ensures that each is evaluated on its economic merits independently, which allows for more context-specific cost distribution. This distinction is crucial for fair comparisons with conventional production systems and significantly influences decision-making, particularly regarding water pricing. Unlike the Economic allocation method, which can inflate water costs by factoring in brine treatment expenses, the Dual allocation method isolates these costs, preventing distortions. For example, the additional expenses of brine treatment or product recovery can affect the final price of water. As water is the primary objective of the proposed systems, distinguishing between water recovery and resource recovery ensures a transparent, unbiased comparison in economic assessments.

According to the above principles and building upon the Economic allocation method, the Dual allocation method first separates the annualized costs and revenues into distinct sub-systems. The division of the treatment chain into the water recovery and resource recovery sub-systems is not predetermined; rather, it depends on the unique characteristics of each case study. For the calculation of the products in the water recovery sub-system, only the Annualized CAPEX and OPEX of the technologies in that sub-system are considered. Similarly, for the revenues of the additional products in that sub-system. Then, the economic allocation factor is applied, as in calculation method 2 (see Section 5.3.3).

$$LVC_i = \frac{\sum_{units,j}(Annualized\ CAPEX + Annual\ OPEX) \cdot f_i - (\sum_{units,j} REV \cdot f_i - REV_i)}{M_i} \qquad \text{eq. 5}$$

Where j is the number of the sub-system (water or resource recovery systems), and f_i is the economic allocation factor of the i^{th} product. In cases like the water recovery sub-system, where only water is produced, cost allocation becomes straightforward, as all costs are attributed solely to water production. This simplicity contrasts with more complex systems that require careful allocation of shared costs among multiple products (resource recovery system). The economic allocation factor is calculated based on the revenues associated with that product using eq. 3 (see results in **Table 5. 4**).

Table 5. 4. Economic allocation factors for Scenarios 1, 2 and 3 based on revenues used in the third calculation method for resource recovery sub-systems.

	Revenues (€/year)			**Economic allocation** (%)		
Product	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Scenario 1**	**Scenario 2**	**Scenario 3**
Water system						
Water	5.53E+05	8.24E+05	3.70E+05	100%	100%	100%
Resource recovery						
Water	3.29E+05	1.49E+05	N/A	15.63%	2.24%	N/A
NaCl	1.77E+06	1.53E+06	N/A	84.37%	23.05%	N/A
$Mg(OH)_2$	N/A	2.55E+06	2.55E+06	N/A	38.39%	22.21%
Na_2SO_4	N/A	1.15E+06	N/A	N/A	28.53%	N/A
NaOH	N/A	0.00E+00	5.30E+06	N/A	0.00%	46.10%
HCl	N/A	1.09E+06	3.64E+06	N/A	7.80%	31.69%

In this work, the economic value of the concentrate streams (brine) is assumed to be zero. This assumption is made because, at this stage, brine is considered waste with no current economic value. Brine is considered as by-product that can be used as a feedstock in a separate brine treatment plant for resource recovery. The potential economic costs of purchasing this feedstock should be considered in the operating costs of the plant. Additionally, in this particular approach, the water system does not include any treatment or handling of the brine. This ensures that the costs associated with handling and treating the brine are not included in the final cost of water, maintaining the independence between the water recovery and brine treatment systems. This approach aligns with the industrial symbiosis concept, where waste from one process becomes input for another, promoting resource efficiency and economic viability.

5.4. Results and discussion

5.4.1. Levelized Cost: Results and Implications

The analysis of levelized costs across different scenarios reveals key insights into the impact of cost calculation methods. **Figure 5. 3** provides a comprehensive overview of the levelized cost of key products across different technical scenarios using three different calculation methods. The results are compared with constant market prices for each product, which serve as reference values for assessing economic feasibility. These reference values differ for each product to reflect their specific market conditions. The results indicate significant variation in levelized costs within the same scenario depending on the calculation method applied. For example, the levelized cost of water varies significantly when desalination and resource recovery systems are separated (calculation method 3: Dual allocation approach), especially in Scenarios 1 and 2, when the water production process consists of multiple technologies. Note that in the Dual allocation approach, the price of water comes from the water system, while the prices of other products come from the resource recovery system. Water from the resource recovery system is not included in this comparison and analysis of the results.

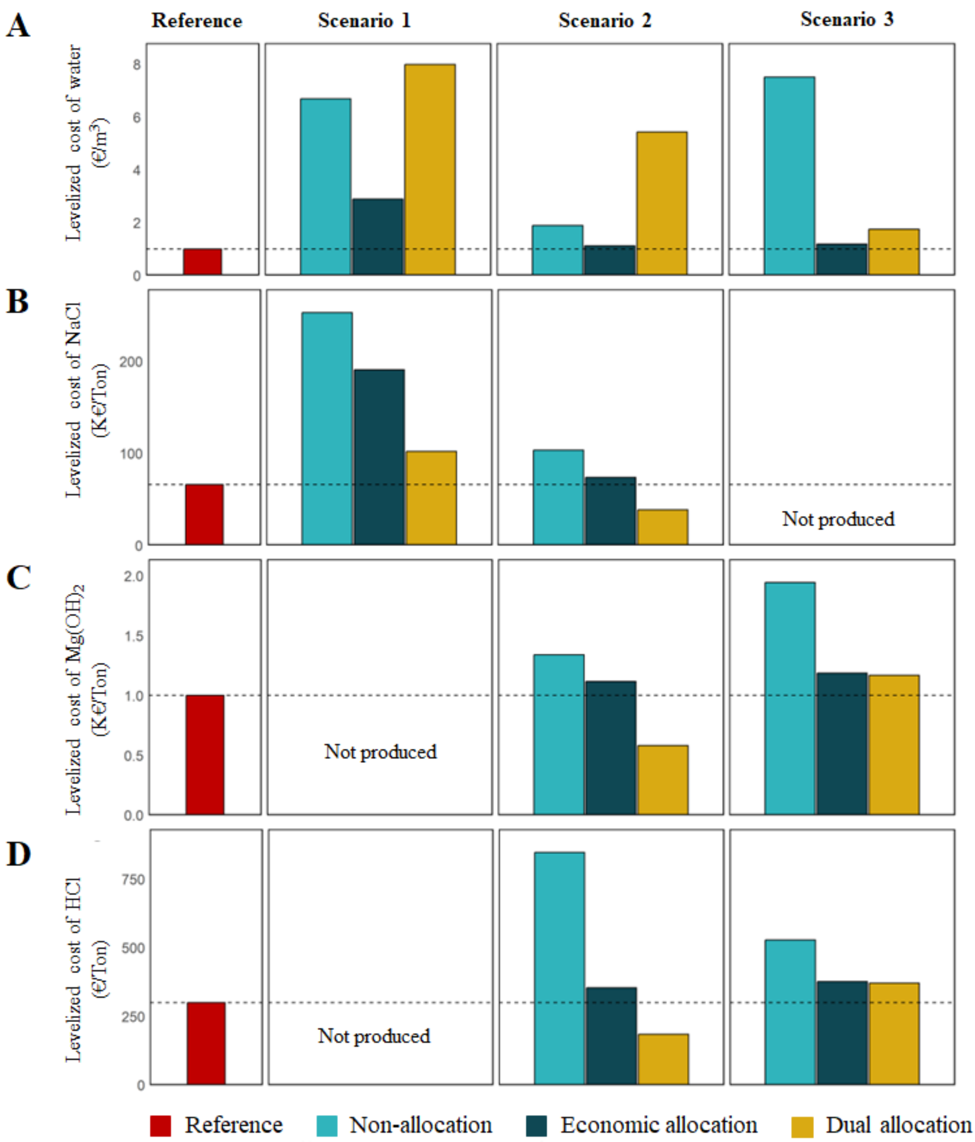

Figure 5. 3. Levelized cost of selected products (A) Water, (B) Sodium Chloride (NaCl) (C) Magnesium Hydroxide ($Mg(OH)_2$), and (D) Hydrochloric acid (HCl) using the three different calculation methods for each scenario. The Red bar denotes the specific cost of each product from the literature that is used as a reference for a comparison with the conventional systems. The Turquoise denotes the Levelized cost of each product using the Non-allocation approach. The dark teal denotes the Levelized cost of each product using the economic allocation approach. The yellow denotes the Levelized cost of each product using the Dual allocation approach.

The Economic allocation approach significantly reduces LVCs compared to the Non-allocation approach. For water, the reduction is particularly notable—57% in Scenario 1, 41% in Scenario 2, and 84% in Scenario 3. Sodium chloride (NaCl) costs also see substantial decreases of 25% and 28% in Scenarios 1 and 2, respectively. These reductions have important implications for plant design and the implementation of circular economy principles. The Dual allocation approach further reduces NaCl costs by 60% and 63% in Scenarios 1 and 2, respectively, suggesting that separating resource recovery from desalination enhances market competitiveness. Overall, **Figure 5. 3** reveals that the Non-allocation approach generally results in the highest levelized costs, while the Dual allocation approach, in most cases, achieves the lowest costs for recovered salts and chemicals. This cost distribution based on product value enhances competitiveness with conventional production systems.

Comparing the LVC of the key products using the three calculation methods with the reference market prices, Economic allocation results in competitive prices in Scenario 2 (12%-18% higher than reference), while the Dual allocation approach results in even more competitive prices for salts and chemicals (39-42% lower than reference price). Scenario 1 shows no competitive results across any methods, while Scenario 3 sees the Economic allocation method as being more competitive for water production, with both novel methods performing similarly for other products compared to market prices. Although total annual costs are theoretically constant across all methods, the Non-allocation approach tends to overestimate them. This reduction in LVCs, particularly in high-value products like NaCl, enhances market competitiveness and could significantly influence investment decisions and the overall economic feasibility of integrated desalination and brine treatment plants.

To effectively interpret the results of levelized cost calculations (**Figure 5. 3**), decision-makers must examine the costs of different products in combination. This holistic approach provides a more nuanced understanding of how changes in the levelized cost of one product may influence other products within the same scenario. Detailed results for each scenario and product can be found in Supplementary Information Sections S5 and S6.

Figure 5. 4 presents the total annual revenues for each scenario, using the levelized cost of the products calculated from the three different methods as the selling price. These revenues are compared with those from selling products at market prices (reference bar). The Non-allocation method yields significantly higher revenues in Scenarios 1 and 3 due to the higher levelized cost of products calculated by this method (see **Figure 5. 3**). However, lower revenues using the LVC as a selling price do not necessarily mean lower overall profitability. The LVC represents the breakeven price. If the selling price exceeds the LVC, it results in higher revenues. Thus, a lower LVC indicates greater competitiveness with conventional production methods and more potential for profit. Conversely, when the LVC is much higher than the market price, the potential for additional profit is limited. This also supports the hypothesis that separating the resource recovery system from the desalination plant enhances competitiveness in the market.

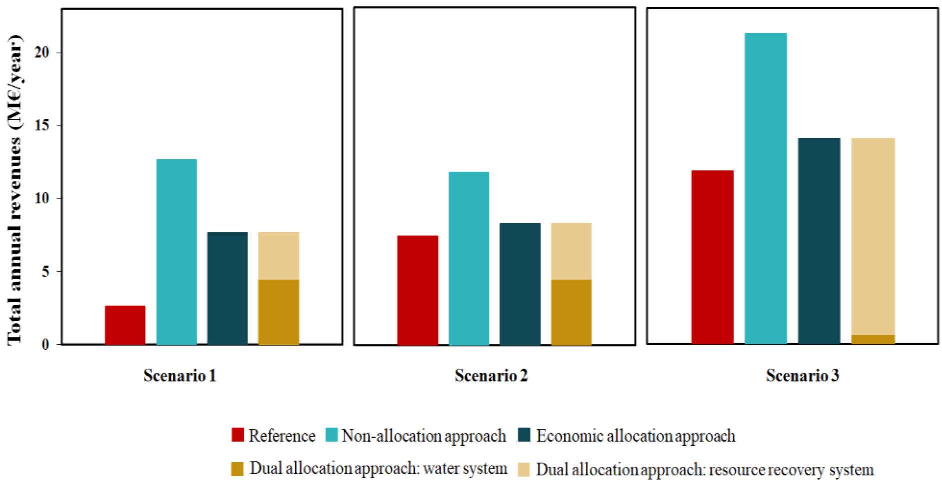

Figure 5. 4. Total annual revenues for each technical scenario from selling products using their levelized costs as a selling price. The red bar (reference) represents the revenues from selling products using the market price of each product.

To understand why the Non-allocation approach generally results in the highest LVC and provide a detailed comparison of the total annual production costs calculated using the two different methods (Non-allocation and Economic allocation), **Figure 5. 5** illustrates the breakdown of costs per product and for the entire plant in Scenario 2. **Figure 5. 5A** clearly demonstrates that the Non-allocation approach results in an overestimated total annual production cost of 3.45 M€/year because it applies fixed annual costs (CAPEX and OPEX) uniformly across all products, only adjusting revenues of the by-products. Under the Non-allocation method, the first term in the LVC calculation remains the same for all products, leading to a significant multiplication of total annual costs. This leads to an inflated overall production cost and, therefore, higher levelized costs for each product. In contrast, **Figure 5. 5B** illustrates how the Economic allocation approach distributes costs more proportionally based on the revenues coming from each product. This method avoids the overestimation seen in the Non-allocation approach by using allocation factors that ensure the cost assessment

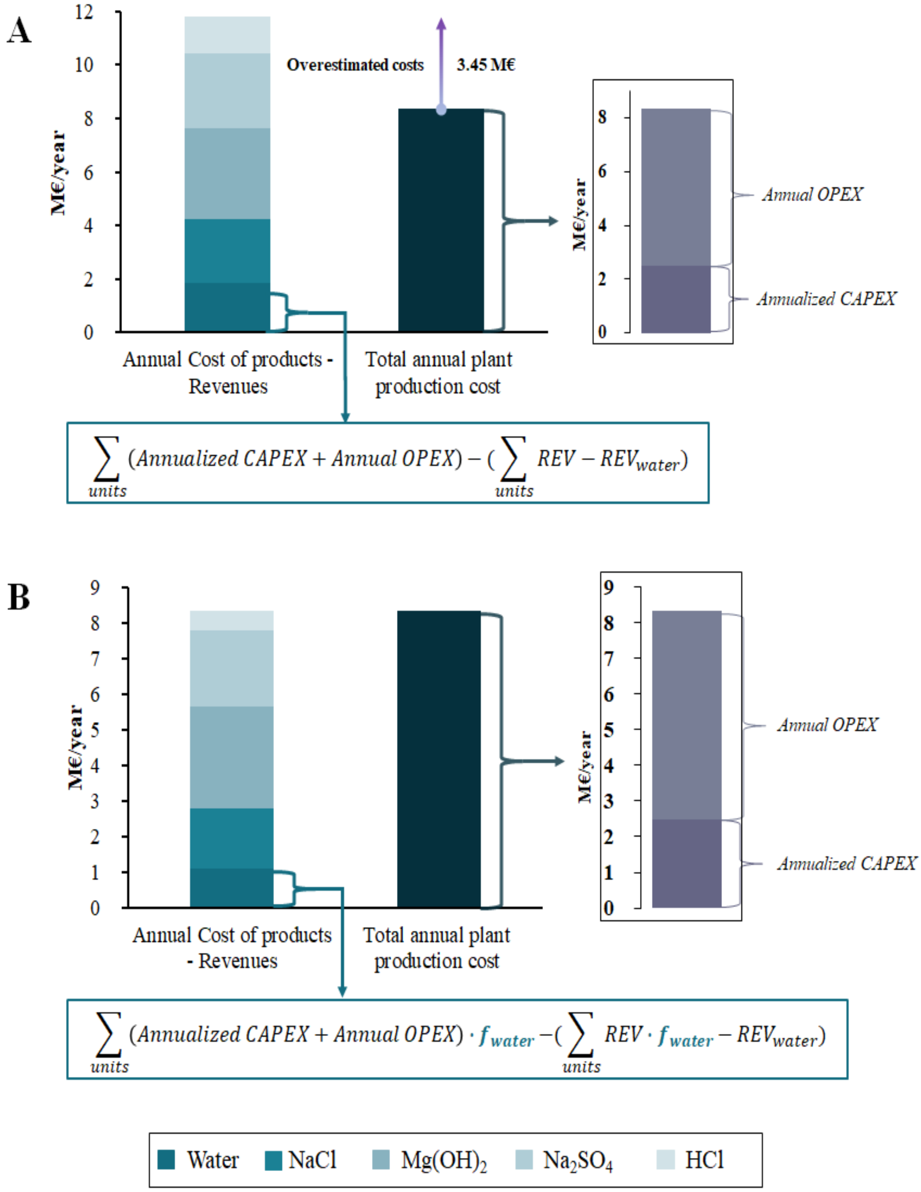

Figure 5. 5. Comparison of total annual production costs calculations per product and for the entire plant in Scenario 2 using two different calculation methods: (A) Non-allocation approach and (B) Economic allocation approach. The small bar charts on the right side of each subfigure illustrate the breakdown of the Annualized CAPEX and Annual OPEX contributing to the total annual plant production cost.

reflects the true economic contributions of each product. The allocation factor corrects the overestimation by aligning the total production costs with the revenues of the products; the numerator in the levelized cost equation reflects the actual production cost. Detailed results for the other two scenarios can be found in Section 5.6, S6 (see **Figure S.3, Figure S.4**).

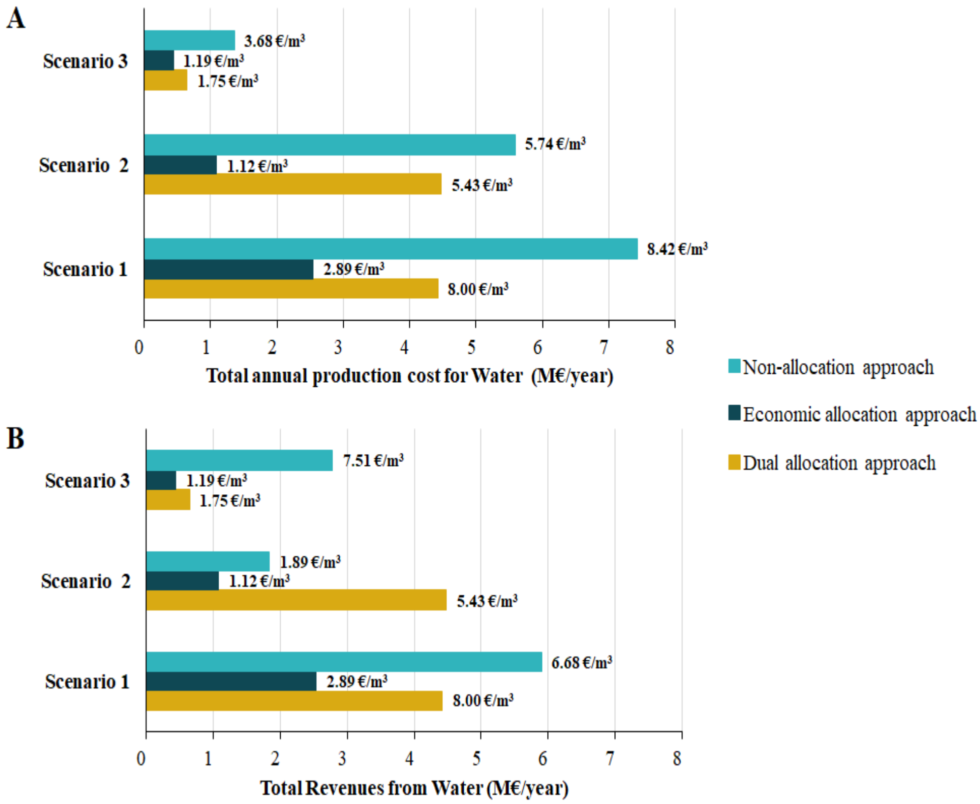

Figure 5. 6. (A) The total annual cost for water production using the three calculation methods, with specific €/m³ values shown for each method. (B) Annual revenues from selling water at a levelized cost price using the three calculation methods with specific €/m³ values shown for each method.

Figure 5. 6 further examines the impact of the calculation methods on the Levelized Cost of Water. **Figure 5. 6A** illustrates how the total annual costs of water, and thus the LVC, vary depending on the calculation method, with the corresponding specific €/m^3 values clearly labeled. The Economic allocation method achieves an 81% reduction in the annual costs of water compared to the traditional Non-allocation method. This reduction results from reallocating costs to higher-value products and avoiding overpricing. In this context, overpricing refers to an artificially higher value assigned to a product due to disproportionately loading costs onto it beyond its actual production cost. This overpricing effect is evident when comparing the significant difference between the annual costs in **Figure 5. 6A** and the revenues from selling water at the LVC in **Figure 5. 6B**. In contrast, the other

two methods (Economic allocation and Dual allocation approaches) show better alignment between costs and revenues (see specific €/m^3 values), indicating that the LVC is accurately calculated to achieve break-even. This alignment suggests that any increase in the selling price beyond the LVC will directly enhance profitability, validating the effectiveness of Economic allocation in reflecting the true economic potential of water production. The detailed results for each product across the three calculation methods are provided in Supplementary Information (see Section S6, **Table S.11-Table S.13**).

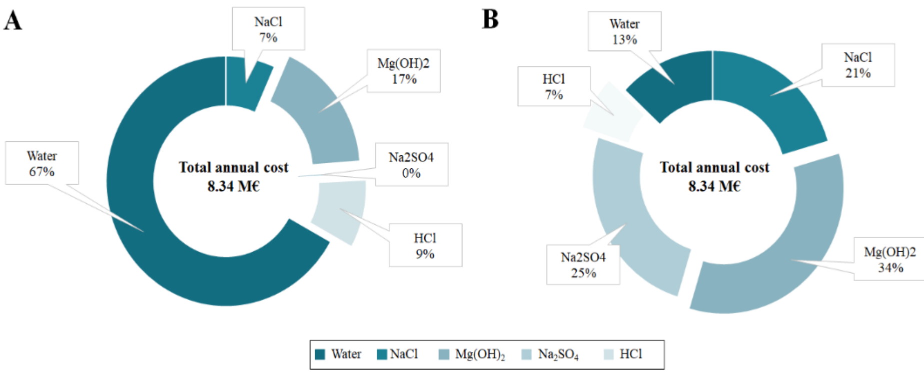

Figure 5. 7. Distribution of total annual production cost for scenario 2 using two different calculation methods: (A) Non-allocation approach, (B) Economic allocation approach.

Figure 5. 7 shows how the annual production costs (sum of annualized CAPEX and OPEX) are distributed across the recovered products in Scenario 2 using the Non-allocation approach (**Figure 5. 7A**) and the Economic allocation approach (**Figure 5. 7B**). To make this comparison, the Non-allocation approach involves process-level distribution, considering the cost of each unit to produce a specific product. This approach differs from other calculations for Non-allocation in this work (see **Figure 5. 3-Figure 5. 6**), as it aims to assess the impact of non-allocating the annual production cost based on revenues while maintaining the same annual production costs (without overestimation). Breaking down the annual production cost using the Non-allocation approach shows that 67% of costs are loaded on water due to its large production rate. In contrast, the Economic allocation method distributes costs more equitably among products with higher market value, assigning only 13% to water. This highlights a major drawback of the traditional Non-allocation method: it tends to overprice the main product, water, by uniformly applying fixed costs across all products. Detailed results for the other two scenarios can be found in Section S6 (see **Figure S.1, Figure S.2**).

5.4.2. Sensitivity analysis

A sensitivity analysis is performed to evaluate the effect of product market prices (see Section 5.4.2.1) and operating costs (see Section 5.4.2.2) on the calculation of the levelized cost of products using the three different calculation methods.

5.4.2.1. Effect of water market price

To analyse the effect of water price on the levelized cost of different products in the integrated desalination and brine treatment technical designs, the following water price scenarios were considered:

- **Baseline:** Standard scenario with no change in water market prices (reference value).
- **WMP+25:** Water market price increased by 25%.
- **WMP-25:** Water market price decreased by 25%.

Note that in this context, *water market price* refers to the regulated baseline cost of water production. This analysis examines how changes in production costs affect the economic viability of resource recovery.

Figure 5. 8 provides an overview of the sensitivity of the levelized cost of key products across various scenarios and the three calculation methods in response to changes in water market price (+ or - 25 %). It also illustrates how these changes impact the levelized cost of water (**Figure 5. 8B**) and $Mg(OH)_2$ (**Figure 5. 8C**) in Scenarios 2 and 3.

The Non-allocation approach shows a consistent response to changes in water market price across all scenarios. Generally, the levelized cost of water increases or decreases proportionally to price fluctuations, reflecting the method's straightforward nature. Changes in the price of water have a uniform influence on the cost of products across different scenarios, with Scenario 2 having the most widespread impact.

The Economic allocation method is highly sensitive to changes in water market price, especially in scenarios with high external water usage and low water production, like Scenario 3. A 25% price change leads to a 26% fluctuation in the levelized cost of water in Scenario 3. Scenario 2 shows a 22% increase in LVC with a 25% WMP rise and a 23% decrease with a 25% reduction. This pattern is consistent across products, though the magnitude of change varies depending on the allocation factors and the proportion of water usage. The greater sensitivity in this method highlights how water prices directly impact cost distribution, particularly in more complex or water-intensive scenarios.

The Dual allocation approach provides a contrast between the water and the resource recovery systems. The water system remains stable across all scenarios, unaffected by water market price changes due to the absence of water consumption and by-products. In contrast, the resource recovery system is highly sensitive to water market price changes. In Scenario 2, a 25% increase in WMP leads to a 27% rise in the levelized cost of water, while a similar decrease causes a 26% reduction. This method's stability in the water system, coupled with sensitivity in the resource recovery system, highlights the advantage of separating the integrated systems into the water system and resource recovery system, as it allows for more precise cost management and less volatility in the overall LVC.

In Scenarios 2 and 3, the LVC of water (see **Figure 5. 8B**) under the Non-allocation approach shows limited sensitivity to WMP changes, with increases of 4% and 9%, respectively, for a 25% increase and corresponding decreases for a 25% WMP reduction. This uniform response occurs because water price affects both the annual production costs and revenues, leading to a proportional change in LVC across these scenarios. Scenario 3 is slightly more sensitive due to its higher water consumption and, thus, higher operating costs. The Economic allocation approach is more sensitive in both scenarios, with LVC changes of ±22% in Scenario 2 and ±26% in Scenario 3. The Dual allocation approach shows stability in the water system component of both scenarios, with no impact from WMP fluctuations due to the absence of direct water usage and by-products affecting revenues. However, in the resource recovery system, Scenario 2 shows a ±27% increase or decrease in LVC of water with a 25% change in WMP, highlighting the critical role of water price in cost distribution.

For $Mg(OH)_2$ (see **Figure 5. 8C**), the Non-allocation approach shows low sensitivity to WMP changes, with LVC variations of ±5% in Scenario 2 and ±3% in Scenario 3. This is because water price has a minimal effect on the overall production cost of $Mg(OH)_2$ in these scenarios. The Economic allocation method similarly shows low sensitivity, with only ±2% LVC change due to higher allocation factors for $Mg(OH)_2$. The Dual allocation approach also demonstrates limited sensitivity for $Mg(OH)_2$, particularly in Scenario 2, where LVC change is aligned with changes in annual production costs. The small difference in allocation factors of water and $Mg(OH)_2$ compared to the baseline water price scenario ensures that water market price fluctuations have a minimal effect on $Mg(OH)_2$ LVC, maintaining a stable cost structure.

Overall, the water price sensitivity mainly affects more complex systems with significant water usage. Non-allocation approach, while straightforward, may oversimplify the impacts, whereas the Economic allocation method captures these effects in more detail but at the cost of greater variability. The Dual allocation approach provides more stability in cost distribution by isolating the water system from resource recovery processes. Detailed results for all products are given in Supplementary Information (see Section S7).

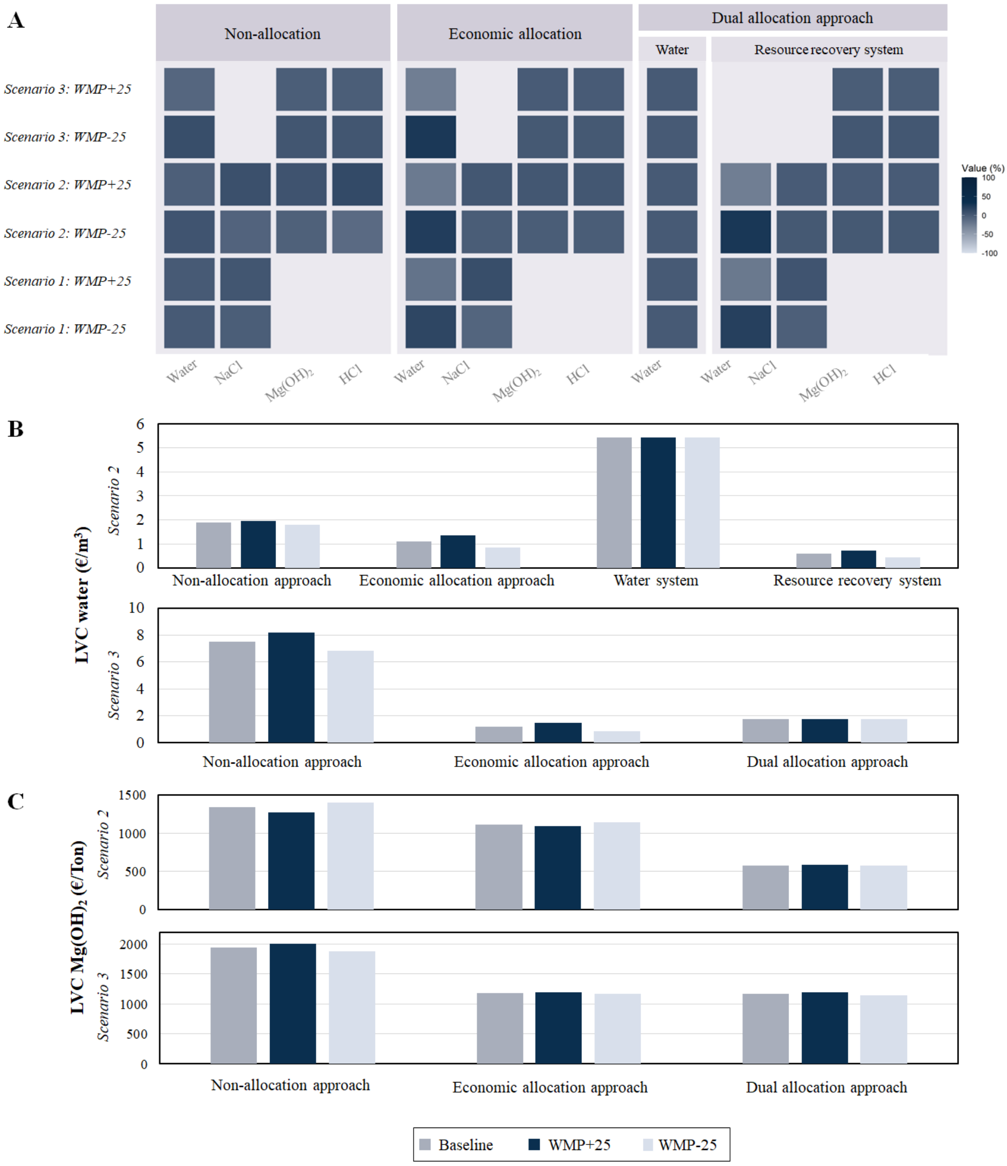

Figure 5. 8. Impact of water price variations on the Levelized Cost of key products across different scenarios and calculation methods: (A) The heatmap illustrates the percentage change in the Levelized Cost of water and other recovered products under two different water price scenarios (WMP+25, WMP-25) and three calculation methods: Non-allocation, Economic Allocation, and Dual allocation approach. Darker and lighter shades indicate a higher percentage change (positive or negative), highlighting the sensitivity of specific products and methods to water price fluctuations. Each column represents a different product, and the rows correspond to the specific scenario and price variation. (B) Bar charts illustrate the change in the Levelized Cost of Water in Scenarios 2 and 3 under varying water prices. (C) Bar charts illustrate the change in the Levelized Cost of $Mg(OH)_2$ in Scenarios 2 and 3 under varying water prices.

5.4.2.2. Effect of electricity (operating) costs

To analyse the effect of electricity price on the levelized cost of different products in the integrated desalination and brine treatment technical designs, the following electricity price scenarios were considered:

- **Baseline**: Standard scenario with no change in electricity market prices (reference value).
- **EMP-25:** Electricity Market Price decreased by 25%.
- **EMP+25:** Electricity Market Price increased by 25%.

Figure 5. 9 provides an overview of the sensitivity of the levelized cost of key products across various scenarios and the three calculation methods in response to changes in water market price (+ or - 25 %). It also illustrates how these changes impact the levelized cost of water (**Figure 5. 9B**) and $Mg(OH)_2$ (**Figure 5. 9C**) in Scenarios 2 and 3.

The Non-allocation method (current method) is the most sensitive to electricity price changes, particularly in Scenario 3. A 25% change in electricity market price (EMP) increase results in a 17% increase in LVC of water for Scenario 2, while Scenario 3 experiences a dramatic 93% increase, reflecting its heavy reliance on electricity (see **Figure 5. 9B**). This high sensitivity reveals the instability of the Non-allocation method in energy-dependent scenarios like Scenario 3.

In contrast, the Economic allocation method shows more balanced responses to electricity price variations, mitigating the impact of electricity price changes by distributing costs based on the economic value and revenue of each product. Since the allocation factors and revenues remain constant across the sensitivity analysis, the variation in the levelized cost of products is directly aligned with changes in operating costs alone. Scenario 2’s LVC of water rises by 4% with a 25% EMP increase, while Scenario 3's LVC of water increases by 18%. This approach provides more stable and predictable cost estimates, particularly in energy-intensive scenarios like Scenario 3.

The Dual allocation approach shows the least sensitivity to EMP changes. In Scenarios 2 and 3, water system LVC changes are limited to ±5% and ±7%, respectively, with a 25% EMP variation, demonstrating resilience to price fluctuations. These changes directly relate to the annual operating cost fluctuations because the water system calculations remain unaffected by other variables, such as allocation factors or revenues from by-products. In the resource recovery system, the LVC of water shows moderate sensitivity to EMP changes, with a ±2% change in Scenario 2 reflecting a more stable response due to the balanced distribution of costs and revenues. Scenario 3, being more energy-intensive, exhibits a greater sensitivity with a ±19% change in LVC, indicating the significant impact of EMP fluctuations in scenarios with higher energy demands. Scenario 1 is the least affected by EMP variations, with modest fluctuations (5-6%), indicating a stable cost structure.

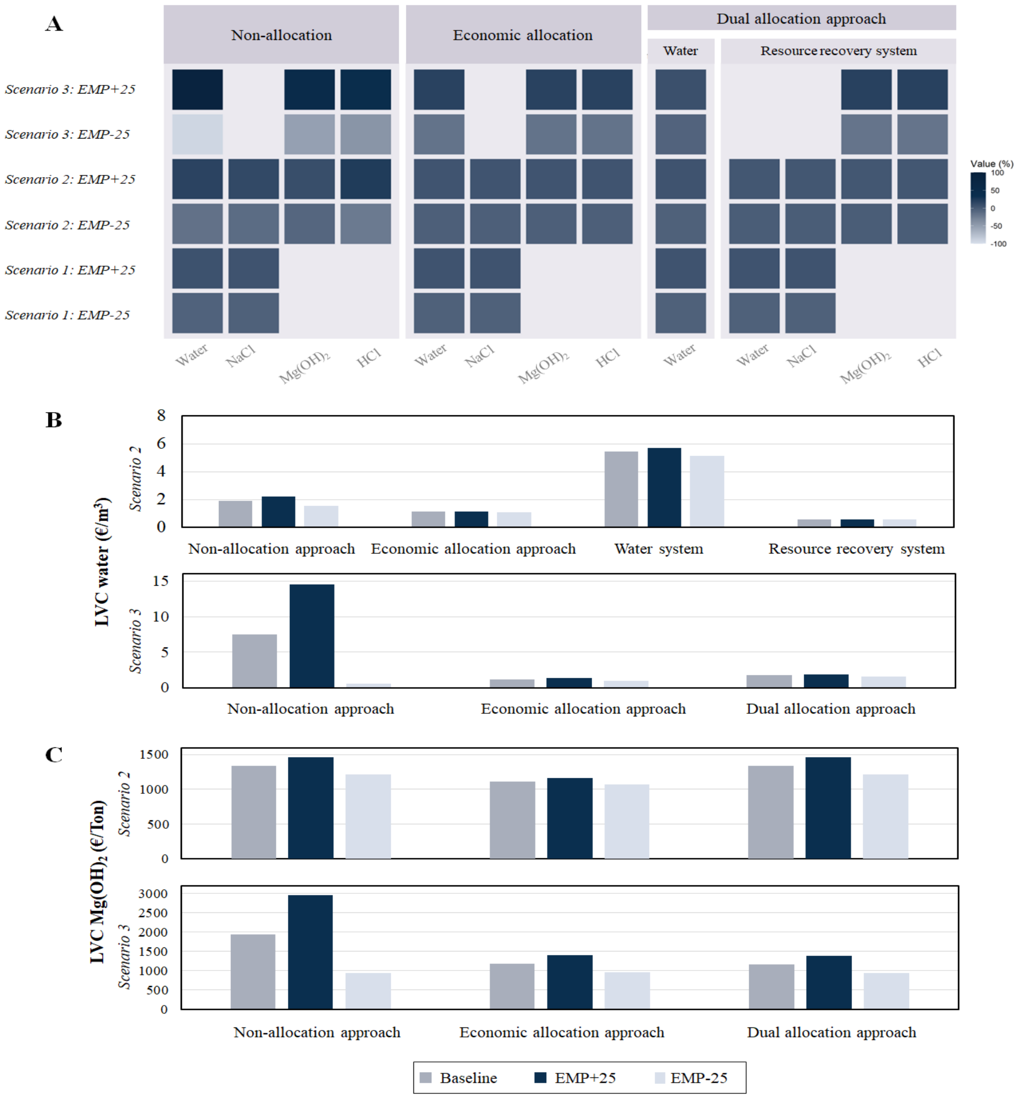

Figure 5. 9. Impact of electricity price variations on the Levelized Cost of key products across different scenarios and calculation methods: (A) Heatmap displaying the percentage change in the Levelized Cost of water and other recovered products under two electricity price scenarios (EMP+25 and EMP-25) across three calculation methods: Non-allocation, Economic Allocation, and Dual allocation approach. Darker shades indicate greater sensitivity to electricity price fluctuations, with each column representing a different product and each row corresponding to a specific scenario and price variation. (B) Bar charts illustrate the change in the Levelized Cost of water in Scenarios 2 and 3 under varying electricity prices. (C) Bar charts illustrate the change in the Levelized Cost of $Mg(OH)_2$ in Scenarios 2 and 3 under the same conditions.

For $Mg(OH)_2$ (**Figure 5. 9C**), Scenario 3 shows a 52% LVC increase under the Non-allocation method with a 25% EMP rise, while the Economic and Dual allocation methods limit this to ±18% and ±19%, respectively. Scenario 2 shows moderate sensitivity, with LVC increasing by 9% (with a 25% rise in EMP) under the Non-allocation method, while the Economic allocation and Dual allocation approaches provide more stable responses (±4% and ±2%, respectively). Scenario 2's inclusion of more products highlights the effectiveness of these novel methods in mitigating the impact of energy price variations.

Overall, the Economic and Dual allocation methods provide more reliable and stable cost estimates, particularly for high-revenue products like $Mg(OH)_2$, making them preferable for scenarios sensitive to electricity price fluctuations. Detailed results for all products are given in Supplementary Information (see Section 5.6, S7).

5.4.3. Discussion and reflection on the different calculation methods

Desalination plants traditionally prioritize water production, especially in water-scarce regions where they are typically constructed [8]. However, as s seawater brines are increasingly seen as valuable resources rather than waste, the economic evaluation of resource recovery and the consideration of potential revenues from the sale of recovered resources become increasingly critical [32]. This study explores how different cost calculation methods influence the levelized cost of water and other recovered products, offering insights that could significantly impact political and investment decisions related to desalination and resource recovery.

The results underscore the importance of selecting an appropriate cost calculation method in the local socio-economic context. This choice directly affects the economic viability of the plant and its competitiveness with conventional salt and chemical production systems. A key finding of this study is the overpricing issue linked to the traditional Non-allocation method. By uniformly applying fixed annual costs (annualized CAPEX and OPEX) across all products, this method overestimates costs. As a result, it inflates the levelized cost of water and other recovered products, making the system less competitive compared to linear systems, brine disposal systems [33].

The Economic allocation and Dual allocation approaches introduced in this study address these issues by ensuring a fairer distribution of costs, reflecting the true economic value of each product rather than just the production rate [34]. The Economic allocation method reduces the levelized cost of water by up to 81% compared to the traditional Non-allocation method. This reduction in water costs can profoundly influence investment decisions and operational strategies [35] and encourage the adoption of technologies that maximize the recovery of high-value by-products, ultimately improving overall plant profitability. The Dual allocation method isolates the water recovery and resource recovery processes, allowing for more accurate cost distribution by ensuring that water costs are not inflated by additional brine treatment steps.

Accurate cost allocation is essential for realistic economic assessments in resource recovery systems, where design choices are driven by local needs, values, and profitability. The critical decision in resource recovery systems is not just about building a desalination plant but determining the extent of resource recovery—whether to focus solely on salt or extend to HCl and $Mg(OH)_2$. This study shows that using fairer cost allocation methods, such as Economic allocation or Dual allocation, supports more informed decisions on economically viable resource recovery. While the traditional approach may work for basic desalination, assessing the full economic potential of seawater, brine valorisation requires choosing the right cost allocation method to justify more extensive recovery systems.

Although Economic allocation is sometimes considered too arbitrary, in multi-product systems, it is often considered the most practical because the market prices reflect the functionality of a material quality [36]. Similar to other resource recovery studies, cost allocation plays a crucial role in achieving fair assessments. As with allocating upstream burdens when waste is treated as a resource [37], or distributing fuel consumption between heat and electricity in cogeneration, careful allocation ensures accurate comparison and efficiency in multi-product systems [38].

Our analysis reveals that the economic feasibility of resource recovery systems can vary significantly depending on the cost calculation method applied. For instance, Scenario 2, which appeared economically unfeasible under the traditional Non-allocation method, becomes viable when the Economic allocation approach is employed. This approach significantly reduces the levelized cost of key products, including water, making the scenario competitive with conventional production methods. When comparing the three scenarios using the different calculation methods, it is clear that Scenario 2 emerges as the most economically feasible under both the Economic allocation and Dual allocation approaches, primarily due to its balanced mix of high-value products and moderate operational costs. Scenario 3, while still competitive, benefits more from the Dual allocation approach, which minimizes costs associated with resource recovery. Scenario 1, however, faces challenges across all methods due to the lower market value of its products.

While both novel methods offer improved cost distribution, they come with challenges. The complexity of the Economic allocation method lies in determining accurate market values for each product, particularly in fluctuating markets. This complexity was evident in the sensitivity analysis, which showed significant variations in the levelized cost of water and other products, with changes in water prices causing up to ±26% fluctuations and electricity prices causing up to ±18% fluctuations. These sensitivities highlight the difficulty of maintaining stable cost estimates in systems heavily influenced by market-driven factors. Similar challenges are faced in renewable energy projects, where market price fluctuations for market share can significantly impact economic viability [28].

Integrated systems, such as those involving water and brine treatment, present additional challenges. Defining system boundaries of water and brine treatment systems—as in the Dual allocation approach—can be complex and subjective, leading to potential inconsistencies in cost allocation. This challenge is not unique to resource recovery systems, but it is also observed in other multi-product systems, such as desalination combined with Concentrated Solar Power (CSP) [16]. In such cases, while the Levelized Costs of Water and Electricity are determined separately, the process is more straightforward due to clearer system boundaries and well-established methods. In such cases, thermoeconomic methods apply effectively, using exergy to allocate costs between energy and water. For brine treatment systems that do not produce energy as a co-product, thermoeconomic methods are less applicable, as their exergy-based approach does not align with systems where non-energy resources like salts and chemicals are the primary outputs.

Future research should explore the impact of financial incentives, such as tax breaks or subsidies, on the economic viability of resource recovery systems. Additionally, developing dynamic assessment models to account for fluctuating market conditions, such as variable water and energy prices, could provide more adaptive and accurate economic evaluations, reflecting the variability and risks faced by such projects. As the industry shifts toward viewing brine as a resource rather than waste, economic assessments must evolve to reflect this change, potentially leading to a reassessment of cost allocation strategies.

Although this study employs generalized scenarios to evaluate the proposed cost allocation methods, the methodologies are designed to be adaptable to real-world applications. By incorporating region-specific data—such as local market prices, energy costs, or policy-driven incentives—they can be tailored to address diverse operational and economic conditions. This flexibility ensures their practical relevance in varied contexts, including industrial desalination systems, water-scarce regions, or areas with high demand for specific recovered products.

The proposed calculation methods represent a step forward in addressing the complexities of resource recovery systems, although they may not apply universally. They serve as a pioneering attempt to emphasize the need for objective-oriented and context-specific cost allocation, considering the unique characteristics and economic values of the recovered products. As the first of its kind reported in resource recovery literature, this approach should be viewed as a starting point for future investigations, encouraging the development of more robust methodologies tailored to the complexities of resource recovery.

5.5. Conclusions

This study contributes to the ongoing discussion on assessing the economic performance of resource recovery plants by introducing two novel calculation methods—the Economic allocation and the Dual allocation approaches. Compared to the Non-allocation method (current practice in literature), the Economic allocation approach significantly reduces water levelized costs by up to 81% and NaCl costs by up to 28%, while the Dual allocation approach further reduces NaCl costs by over 60%. Such reductions highlight the practical benefits of tailored cost methods in supporting circular economy goals and market viability.

The traditional Non-allocation method tends to overestimate production costs (up to 3.45 M€/year) due to uniform cost application, leading to inflated product prices, which emphasizes the need for refined allocation. By redistributing costs to higher-value products, the Economic allocation approach assigns only a minimal percentage to water costs, compared to the heavy loading seen with Non-allocation. This work underscores the ability of the methods to provide a more competitive economic outcome through fair cost distribution. The sensitivity analysis reveals the significant impact of fluctuating water and electricity prices on the levelized costs, emphasizing the necessity of adaptable, context-specific cost methods aligned with individual plant goals. These insights are critical for guiding investment and operational strategies in resource recovery plants, ensuring that decisions are economically sound and aligned with market realities.

While these innovative methods improve decision-making, it is essential to acknowledge potential debates, particularly with the Dual allocation approach. This method raises questions on cost allocation in multi-product systems, thereby serving as a starting point for future studies. Future research should refine these methodologies, address their limitations, and propose alternatives. The aim is not to establish a fixed calculation approach but to inspire critical thinking and develop robust methodologies for resource recovery in multi-product settings.

5.6. Supplementary information

See documentation.

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6

LCA methodological choices and environmental impacts performance of an integrated seawater desalination and brine treatment system

ABSTRACT

As water research and industry shift towards resource recovery plants, comprehensive assessment methods are essential to capture potential impacts. This study evaluates the environmental performance of integrated desalination and brine treatment systems in Cyprus using life cycle assessment (LCA). Five impact categories were analyzed: climate change, human toxicity, marine ecotoxicity, water depletion, and fossil depletion. Conventional desalination was compared with three resource recovery scenarios: Sc1) maximum water recovery using waste heat (WH), Sc2) integrated desalination plant with brine treatment using WH, Sc3) electricity-based desalination with chemicals recovery. Methodological choices—two functional units (1m³ seawater and 1m³ desalinated water) and three approaches to address multifunctionality (system expansion, mass, and economic allocation)—proved crucial for assessing these complex systems. Sc3 showed a 59% higher impact using 1m³ desalinated water as the functional unit, while excluding WH altered impacts by up to 89%. Resource recovery systems outperformed conventional systems, highlighting the need for integrated practices.

Keywords: *Life Cycle Assessment; Desalination; Brine treatment; Resource recovery.*

Submitted as: R. Ktori, J.A. Posada, M.C.M. Van Loosdrecht, D. Xevgenos, LCA methodological choices and environmental impacts performance of an integrated seawater desalination and brine treatment system.

6.1. Introduction

Desalination is a crucial water treatment technology addressing water scarcity in regions that face significant challenges due to its substantial energy needs and the disposal of brine, a saline waste stream. Zero liquid discharge (ZLD) and resource recovery practices from seawater brine are considered an opportunity for decreasing the environmental impact of desalination [1]. Beyond water recovery, extracting valuable products from seawater can substitute traditional materials mining, reducing the environmental impact compared to conventional salt, metal and chemical production. Optimal recovery strategies for high-quality and multiple products are documented in the literature [1–3]. However, a comprehensive environmental assessment of multi-product ZLD systems, specifically tailored to address the complexities of resource recovery in desalination, remains underdeveloped [4].

Life Cycle Assessment (LCA) is a powerful tool for evaluating environmental impacts at different stages of technology development, from planning and conceptual design to operational phases [5]. Integrating LCA early in technology development could optimize processes, enhance understanding of design implications, and enable cost-effective redesign of products and processes [6,7]. However, accurately quantifying impacts in emerging technologies like ZLD is challenging due to limited data on material and energy flows [6,8].

While LCA has been applied extensively to desalination technologies since the 1990s, primarily to examine and compare various desalination technologies [9–12], most studies focus on single-output systems or renewable energy integration [13–15], with limited attention to multi-product resource recovery. Recent studies have addressed some aspects of brine management and resource recovery [6,16,17], yet the integration of desalination and brine treatment remains an emerging area that combines established desalination technologies with newer resource recovery advancements [18,19]. Although assessing the environmental impacts of these emerging technologies at various stages of development poses uncertainties, it is essential for guiding investment, research, and development [7,17].

How effective are current assessment methods for evaluating the integration of technologies and systems in the early stages of development [20]? Historically, these studies have utilized an attributional modeling approach. However, modifications are needed for resource recovery systems in the field of desalination. Some initial steps have been taken by [21], who examined whether and to what extent the environmental impacts of Reverse Osmosis (RO) vary due to different Life Cycle Impact Assessment methods. [16] studied the effect of allocation type (mass and economic allocation) on the environmental impacts of brine treatment systems.

Existing LCAs on desalination largely overlook key methodological challenges specific to multi-product ZLD, such as an adequate selection of functionality and related functional units, managing multi-functionality, as well as other aspects like systems comparability, data availability, and uncertainty [8,22], which may result in misleading impact assessments and conclusions. The implications of data availability are beyond the scope of this work, as it focuses on comparative environmental performance using consistent data sources and assumptions across all scenarios. This gap limits the ability of current LCA approaches to guide investment and development in integrated desalination and resource recovery systems.

The novelty of this study lies in addressing these methodological gaps through an LCA specifically tailored for integrated, multi-product ZLD systems, focusing on resource recovery. This research seeks to determine how different methodological choices, such as functional unit selection, allocation methods, and energy source inclusion, affect environmental assessments. By developing a refined LCA for integrated ZLD systems, this study provides new insights into the environmental trade-offs and potential benefits of resource recovery strategies in desalination. Based on the above, the following research questions are formulated:

- *How do key methodological decisions such as functional unit, allocation and energy source influence the results and decisions within the context of an integrated desalination and brine treatment systems?*
- *What are the environmental benefits and disadvantages of integrated desalination and brine treatment systems compared with both conventional seawater desalination and salt production systems?*

To address these questions, LCA analyses are conducted on a conventional RO desalination plant and three resource recovery-oriented ZLD systems at a demonstration scale in Cyprus. This assessment aims to reveal critical insights into methodological choices for resource recovery systems, identify environmental performance hotspots, and inform more sustainable design strategies for desalination and brine treatment systems.

6.2. Materials and methods

This paper applies the LCA method, standardized through the ISO14040, and makes use of the software SimaPro and the Ecoinvent v.3.8 database to conduct the LCA. The methodological framework applied in this work is illustrated in **Figure 6. 1**. The main characteristics of the case study and the technical scenarios are described in Section 6.2.1. After the case studies description, this section presents the “Goal and Scope”, Life Cycle Inventory”, “Life Cycle Impact Assessment”, and “Interpretation" steps (see Section 6.2.2).

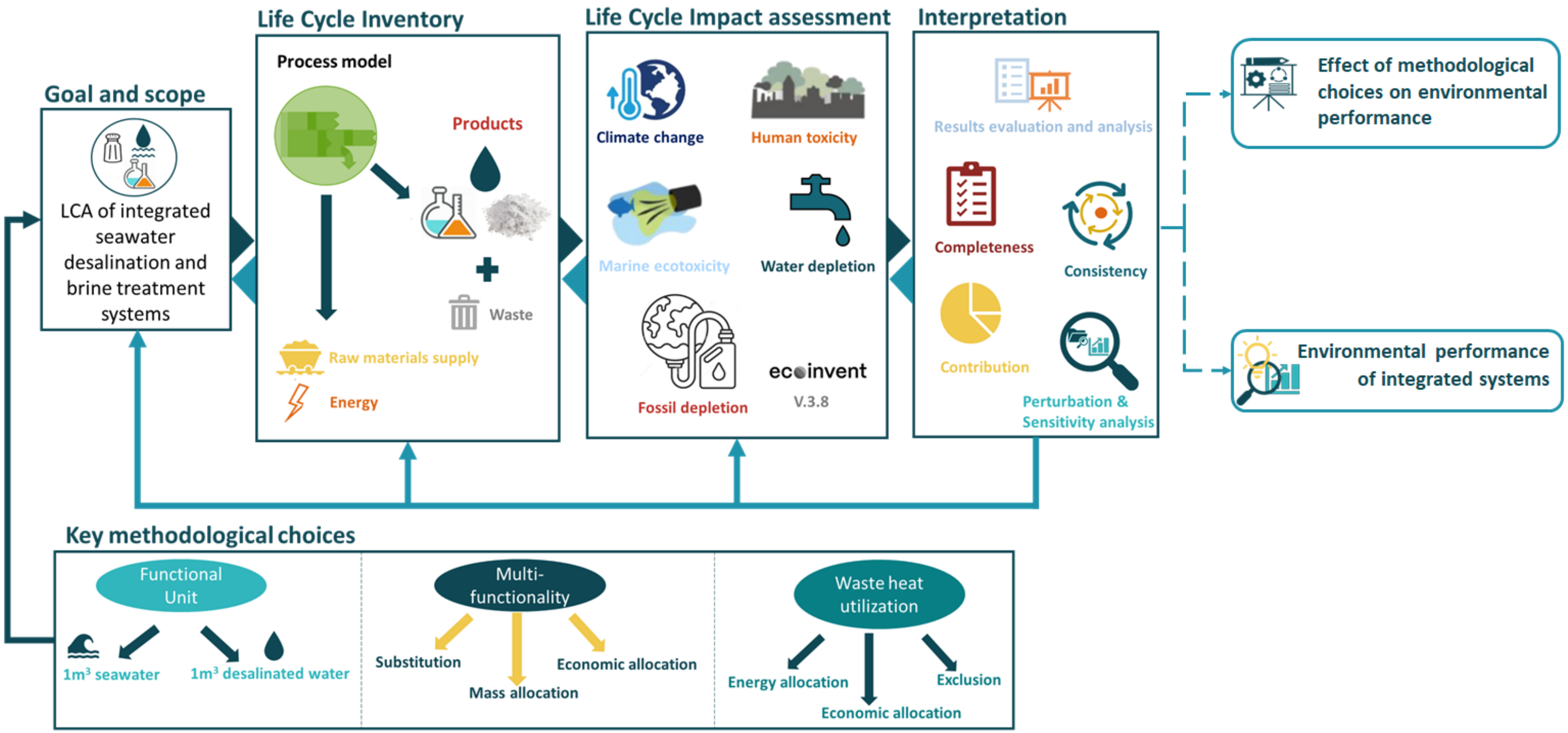

Figure 6. 1. Life Cycle Assessment (LCA) for integrated seawater desalination and brine treatment systems: an overview of methodological approach, related steps and key choices. Key methodological choices related to the functional unit, multifunctionality and the inclusion of waste heat utilization in the background system made in the goal and scope. Light blue line arrows denote feedback loops in the methodological steps and revisions in the methodological choices.

6.2.1. Case study description

Cyprus is considered a relevant geographical case study as it heavily relies on seawater desalination for the majority of its drinking water supply. In 2018, 72.9% of drinking water in Cyprus was desalinated water [23]. Currently, five large-scale (capacity >15,000 m^3/d) desalination plants are supplying drinking water to municipalities in Cyprus, while approximately 24 small-scale (output water <2,500 m^3/d) desalination units are used by other sectors, such as power stations, industry and military purposes. The total installed capacity of the large-scale desalination plants in Cyprus is 235,000 m^3/d, which results in approx. 103 million m^3/year of brine effluent as well [23]. The current brine management option is limited to disposing of the brine back into the marine environment.

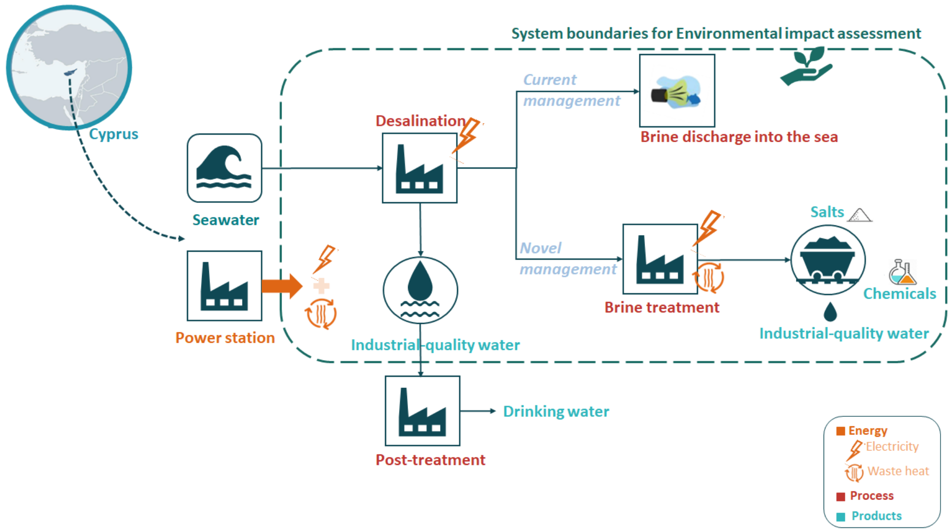

Figure 6. 2. Schematic description of the case study used in this work: integrated desalination and brine treatment plants aiming to recover resources in Cyprus. The green dashed line shows the System boundaries: Cradle-to-gate. Red colour denotes processes, orange colour denotes energy, and turquoise colour denotes output products.

In this work, innovative designs for integrated desalination with brine management and resource recovery are evaluated and compared with benchmark systems, including Seawater Reverse Osmosis (SWRO) for water production and conventional salt and chemical production. The methodological approach described in **Figure 6. 1** has been applied for integrated desalination and brine treatment plants aiming to recover valuable materials such as water, salts, and chemicals. This is illustrated in **Figure 6. 2**, which refers to the case study description and system boundaries. A detailed illustration of the process diagram of the three scenarios and the system boundaries of integrated desalination and brine treatment systems is available in Supplementary Information I (see Figure S.1). Specifically, brine disposal is replaced with brine treatment techniques consisting of at least one technology in brine minimization and several technologies in brine treatment for resource recovery, such as NaCl, $Mg(OH)_2$, and chemicals (HCl, NaOH). Regarding the energy sources, the desalination plants can be integrated with power plants that depend on external fossil resources for power production. Part of the systems integration, in this paper, is the recovery of the available waste heat and utilize it in the desalination plant.

In this study, technical scenarios are employed to evaluate the results and gain insights into different levels of complexity for the studied plants. While all scenarios share the common goal of enhancing water recovery and minimizing brine discharges compared to conventional seawater desalination (see **Figure 6. 2**), they differ from each other on their specific objectives, namely: maximize water recovery (Scenario 1) utilizing waste heat for thermal requirements, integrate existing RO plant with brine management technologies utilizing waste heat for thermal requirements (Scenario 2) and integrate RO plant with electricity-based technologies for chemical recovery (Scenario 3). **Table 6. 1** provides an overview of the three technical scenarios (based on the four cases reported by [4] (see Chapter 4), outlining their objectives, technologies involved, and products recovered. The technical scenarios are designed to recover industrial-quality water, salts (NaCl, $Mg(OH)_2$, Na_2SO_4), and chemicals (HCl, NaOH) from seawater. The feed flow rate remains consistent across all scenarios, set at 60,000 m^3/d (capacity of large desalination plants in Cyprus). The process flow diagrams of the technical scenarios are given in Supplementary Information I (see Figure S.1). For an in-depth explanation of the technical scenario design, including simulation details (like mass and energy balances, refer to [4] (see Chapter 4). Each technical scenario outlined in **Table 6. 1** is systematically compared with the conventional methods of producing the same products. These conventional methods typically involve mining or industrial chemical processes for salts and chemicals, and SWRO for water. For detailed descriptions of these conventional processes, please refer to Section S4 of Supplementary Information I.

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Table 6. 1. Overview of technical scenarios.

Scenario	Objective	Technologies	Products
1	Maximize water recovery and minimize brine discharge	NF, MED, TCryst	Water, Mixed salts
2	Integrated RO plant with brine treatment for recovery of water and valuable products and minimizing brine discharge	RO, NF, MED, TCryst, MFPPR, EFC, EDBM	$Ca(OH)_2$, HCl, Ice, $Mg(OH)_2$, NaCl, NaOH, Na_2SO_4, Water
3	Integrated RO plant with brine treatment focusing on chemical recovery, using only electricity-based desalination	RO, NF, ED, MFPR, EDBM	$Ca(OH)_2$, HCl, $Mg(OH)_2$, NaOH, Water

ED: Electrodialysis; EDBM: Electrodialysis with bipolar membranes; EFC: Eutectic freeze crystallization; MED: Multi-effect distillation; MFPR: Plug-flow reactor; NF: Nanofiltration; RO: Reverse Osmosis, ThCryst: Thermal crystallizer.

Note that the three technical scenarios produce industrial-quality water, which requires post-treatment for drinking water purposes (see **Figure 6. 2**). Additionally, the recovered water is recycled internally in the other processes. However, recycling may not be feasible if the required amount of water exceeds the production capacity, as in Scenario 3 (detailed mass flows for each scenario can be found in the Inventory tables provided in Section S3 Supplementary Information I).

6.2.2. Life cycle assessment (LCA)

6.2.2.1. Goal and scope definition

This LCA study aims to evaluate the environmental performance of three different designs. The focus is on desalination and brine treatment systems with the goal of resource recovery. **Table 6. 2** summarises the main LCA components and choices for the goal and scope definition. As explained in the case study description (see Section 6.2.1), all technical scenarios aim to treat seawater to primarily produce water and treat brine at different stages, producing additional water with salts and chemicals.

To ensure a consistent and comparable FU base across the three scenarios, the functional unit (FU) chosen in this work is '*1m^3 of seawater input at the plant*'. This choice diverges from the conventional practices, where either '*1m^3 of desalinated water*' is considered as the FU in the evaluation of desalination plants [12,24,25], or '*1m^3 of brine input at the plant*' is considered as the FU in the assessment of brine treatment systems [16]. In the case of integrated desalination and brine treatment systems, which are multiproduct systems with different secondary objectives (see **Table 6. 1**), water production depends on the specific secondary objective of each scenario. This means that in some scenarios, water may not be the primary product as other objectives take precedence. Hence, the comparison between the scenarios is not focused on the final products basket but on the rater of the environmental performance of integrated systems and their potential environmental benefits. Furthermore, it is worth noting that, in addition to considering *'1m^3 of seawater input at the plant'* as the primary FU, we also assess the system using '*1m^3 of desalinated water*' as an alternative FU. This alternative FU highlights the importance of methodological decisions, which will be thoroughly analysed in Section 6.2.2.5 and Section 6.3.3 to assess its implications and potential effects on the comparison between scenarios. Note that the results obtained using *'1m^3 of seawater input at the plant'* as the functional unit will be discussed in Sections 6.3.1 and 6.3.2, shedding light on the environmental performance and resource recovery potential of the integrated desalination and brine treatment systems. Additionally, the results obtained with the use of '*1m³ of desalinated water*' as the functional unit are provided in Supplementary Information II (see Sections S1and S2).

Table 6. 2. Overview of the main LCA components and choices for the evaluation.

LCA aspect	Case study
Goal and Scope	Evaluate the environmental performance of integrated desalination and brine treatment systems in Cyprus, considering the conditions in 2021-2022. Three different technical configurations (scenarios) with different objectives (see **Table 6. 1**) are evaluated.
Functional unit*	1m³ of seawater feed
Allocation	Economic allocation at two points: i) for products' distribution, and *ii*) for energy sources when using waste heat.
System boundaries	Cradle-to-gate, for upstream processes, desalination and brine treatment
Data quality	Process Simulation data validated by primary data from pilot scale testing.
Impact categories	ReCiPe midpoint (H) method V1.13 / Europe Recipe H

**The alternative FU of '1m³ of desalinated water' is also considered for comparative purposes, and its related results are presented in Supplementary Information II.*

The system boundaries—Cradle-to-gate—considered comprise only the production phase of the upstream processes for utilities (e.g., electricity and waste heat) generation, chemicals production and the core processes of the designed scenarios for desalination and brine treatment systems (see **Table 6. 1**). The environmental impacts associated with waste heat generation are considered within the system boundaries. Waste heat (WH) is produced as a byproduct of various industrial processes, such as electricity production from natural gas compressor stations. Almost 50% of the global energy consumed is wasted in the form of WH [26]. However, this waste heat can be used for other purposes, such as desalination, as it operates at a lower temperature range below the boiling point of water. This makes the WH a valuable resource for driving thermal processes [27]. In existing works in literature, where waste heat is utilized to cover energy requirements in desalination or brine management systems, waste heat is excluded from the analysis, and the economic and environmental impacts associated with it are deemed negligible [6,28].

Since the proposed integrated systems are multifunctional (*i.e.*, several products are simultaneously generated, see Figure S.1 in Supplementary Information I), and considering that the materials here co-produced are minerals (which otherwise would be obtained through multifunctional traditional linear large-scale extraction processes), the allocation method is applied here to address such multifunctionality. In particular, mass and economic allocation are both applied not only to distribute the overall environmental burdens of the integrated systems accordingly but also to analyse the effects of such methodological choice. However, the results are shown in Section 6.3 are based on economic allocation. shows the market prices and the resulting mass and economic allocation factors for all products from Scenarios 2 and 3 (see Supplementary Information I, Section S2 for Scenario 1). Both the mass and economic allocation factors are calculated using the output flow rates reported in **Table 6. 4** as part of the life cycle inventory (LCI), as shown in Section 6.2.2.2.

Table 6. 3. Products market prices and Mass and Economic allocation factors for Scenarios 2 and 3.

Compound	Price (€/Ton)	Mass allocation factors [%]		Economic allocation factors [%]	
		Scenario 2	Scenario 3	Scenario 2	Scenario 3
Water	1	95.1	N/A	2.7	N/A
NaCl	66 [3]	3.3	N/A	6.1	N/A
$Mg(OH)_2$	1000 [3]	0.4	11.1	10.2	2.0
$Ca(OH)_2$	125[3]	0.1	2.6	0.3	0.1
Na_2SO_4	116 [29]	0.4	N/A	2.3	N/A
HCl	5780 [29]	0.7	49.6	78.4	51.0
NaOH	7200 [29]	0.0	36.7	0.0	46.9

6.2.2.2. Life cycle inventory

Technical process models, developed using the open-source software explained in Chapter 3, were employed to generate the inventory for data on mass and energy flows. The software, available at the GitHub repository (https://github.com/rodoulak/desalsim), facilitated the creation and implementation of these models. **Table 6. 4** presents the inventory data for scenarios 1-3. For data collection for background systems such as electricity supply, waste heat generation, and chemical production, the database Ecoinvent database v.3.8 (system process) is used. Additionally, the inventory for the process of producing *'high voltage electricity production by oil in Cyprus'* has been revised to include the co-production of waste heat from the system. The assumptions section (see Section 6.2.2.3) provides a detailed explanation of this addition and its allocation factor. **Table S7**, **Table S9** and Section S3 (see 6.5.1) present the inventory data per '*$1m^3$ of seawater feed*' for scenarios 1-3, including the background processes and the intermediate streams. Inventory data per '*$1m^3$ of desalinated water*' for scenarios 1-3 can be found in Supplementary Information I (see Section S3, **Table S.8**, **Table S.10** and **Table S.12**).

Note that the three scenarios produce water of industrial-grade quality, which necessitates post-treatment in order to meet the standards required for drinking water. The water recovered from these processes is subsequently reused internally (see Figure S.1 in Supplementary

Information I, section 6.5.1). However, in the instance where the amount of water required exceeds the production capacity, such as in Scenario 3, recycling may not be a viable option.

Table 6. 4. Inventory data per '1m^3 of seawater feed' for scenarios 1-3.

Compound	Units	Scenario 1	Scenario 2	Scenario 3
		Inputs		
Electricity	kWh/FU	4.302	7.853	10.433
Wasted heat	kWh/ FU	447.362	248.624	N/A
NaOH	kg/ FU	N/A	0.403	N/A
Water*	kg/ FU	N/A	N/A	352.189
Antiscalant	l/ FU	0.002	0.060	0.060
		Outputs		
Water*	m^3/ FU	0.980	0.616	N/A
NaCl	kg/ FU	29.857	25.813	NA
$Mg(OH)_2$	kg/ FU	NA	2.838	2.838
$Ca(OH)_2$	kg/ FU	NA	0.661	0.661
Na_2SO_4	kg/ FU	NA	5.534	NA
HCl	kg/ FU	NA	3.782	12.715
NaOH	kg/ FU	NA	N/A	9.397

**Industrial-quality water. FU: '1m^3 of seawater feed'.*

Note that although uncertainty analysis is important in LCA research, it is beyond the scope of this study. As the same data sources and assumptions are used consistently across all scenarios, a uniform level of uncertainty is assumed, enabling direct comparisons of environmental impacts.

6.2.2.3. Assumptions

The following assumptions have been considered:

- Environmental impacts related to energy losses and the use of cooling water are not considered. This decision is based on both the minimal energy losses observed and the challenges posed by limited data availability and reliability in quantifying these impacts. Consequently, the analysis only includes the energy required for pumping these streams within the electricity requirements for the associated processes [4].

6

- Waste heat is integrated into the system by adjusting the Ecoinvent database. Economic allocation is employed to distribute the environmental impact between electricity and waste heat in energy production from oil in Cyprus, ensuring a comprehensive assessment of the system. Although the primary objective of the power plant is electricity production, it is important to note that waste heat utilization doesn't come with zero environmental impact. The allocation factors for electricity and waste heat are provided in **Table 6. 5**. In order to calculate the economic allocation factor of waste heat, firstly, the economic value of the waste heat was calculated using the eq. 1 from [30]:

$$\text{Waste heat cost } (\text{US\$}/MWh_{th}) = 10.7 \ln P_{steam} + 24.2 \qquad \text{eq. 1}$$

  Then, the ratio between the economic value of electricity and waste heat in work by [31] was determined for the year 2019. This value was then used as a fixed parameter to calculate the economic value of waste heat based on the economic value of electricity in 2023, according to Eurostat, (2023). Once the economic value of both energy sources was determined for 2023, an economic allocation between the two energy sources was calculated. For detailed calculations, please refer to Supplementary Information I in Section S2.

Table 6. 5. Emission factor for waste heat based on economic allocation.

Type of energy	**Economic value (per 1KWh)**	**Reference**	**Economic allocation**	**Emission factor ($kgCO_2eq/kWh$)**	**Reference**
Electricity	0.192	(Eurostat, 2023)	85.11%	0.664	[23]
Waste heat	0.034	(own calculation, Section 6.5.1 S2)	14.89%	0.116	(own calculation, Section 6.5.1 S2)

- To integrate the waste heat into the inventory, the electricity dataset represents the production of high-voltage electricity at a grid-connected oil power plant. Emissions are generally calculated/estimated based on European quality fuel oil type S. This implies that the electricity is not sourced from the grid. Therefore, for the baseline analysis, 0% renewable energy sources (RES) are assumed due to simulation constraints. This percentage will change only in the Sensitivity analysis (for more details, see Section 6.2.2.5 and 6.3.4).
- Ice produced in Scenario 2 is considered water, and no post-treatment is taken into account.

- Treated brine outflow streams (*e.g.,* RO-outflow, NF-retentate) are considered waste streams and therefore, their economic value is set as zero.
- The remaining saline solutions, such as discharge saline stream from EDBM in Scenarios 2 and 3 (see **Figure S.1** in Supplementary Information I) have lower salinity (as NaCl) -22g/l and 20g/l respectively- than seawater (40g/l). This means that they can be recirculated back into the systems.
- The environmental impacts due to infrastructure construction, maintenance and demolition are considered negligible (system boundaries).

6.2.2.4. Life cycle impact assessment

The ReCiPe method is utilised for the environmental life cycle impact assessment. The specific characteristics and challenges of Cyprus, such as local environmental conditions and resource constraints, directly inform the selection of midpoint-level indicators, as outlined in Section 6.2.1. Specifically, the following five impact categories were selected to capture the most significant environmental concerns associated with integrated desalination and brine treatment systems (as shown in **Figure 6. 1**):

- Climate change (kg CO_2 eq): Assess the carbon footprint of desalination and brine treatment processes, addressing their energy and materials intensity.
- Human toxicity (kg 1,4-DB eq): Assess the potential effects of chemicals consumption from the integrated systems,
- Marine ecotoxicity (kg 1,4-DB eq): Assess the potential toxicity in the marine environment,
- Water depletion (m^3): Assess the depletion of water resources to understand the sustainability implications of these process systems, and
- Fossil depletion (kg oil eq): Assess the depletion of fossil resources associated with desalination and brine treatment processes, promoting energy security and the transition towards renewable alternatives.

6.2.2.5. Interpretation

The interpretation phase includes various analyses to understand the influence of key methodological choices and assumptions on the results. These choices are treated as Methodological Options (A, B, C, etc.), with corresponding actions used to analyze their impact. Scenario analyses are employed to explore the effects of different system design choices, such as energy mix and technology integration (e.g., waste heat recovery), rather than addressing variability in data inputs (see **Figure 6. 1**). **Table 6. 6** provides an overview of the methodological choices and assumptions identified in this study and the corresponding actions taken to evaluate their effects.

Table 6. 6. Summary of the methodological choices and assumptions identified in this study and corresponding actions.

Methodological choices and assumptions	Corresponding action or analysis to evaluate the effect of key methodological choices
Comparison with conventional production systems (Product basket)	Convert systems into comparable systems: Compare multi-product ZLD systems with the conventional production of all the products within a scenario. Conduct a 1:1 comparison of scenarios and a 1:1 comparison of products, after economic allocation. For conventional processes of the recovered products, see Section 6.5.1 S4, **Table S.15**.
Functional unit	Conduct an LCA using two functional units as scenario analysis and compare the results to determine their influence on the outcome and conclusion.
Handling of multifunctional systems and comparison with conventional systems	
- System expansion/Substitution	Expand the system boundaries and compare the results with a *products-basket* approach to determine the influence on the outcome.
- Allocation: Mass and Economic	Run the two different allocation models as scenarios and compare the results to determine their influence on the outcome and conclusion.
Inclusion of waste heat in the analysis	Conduct a scenario analysis using three different allocation approaches: economic, energy, and one that excludes waste heat.
Energy mix: energy policy for renewable energy transition	Conduct a sensitivity analysis using a baseline scenario and three different energy policy scenarios: e-55, eCSP-55, and eCSP-100.

6

Methodological option A: Effect of functional units

To analyse the impact of the FU on the results in resource recovery systems, LCA is conducted for two functional units: *1m³ seawater fed* and *1m³ desalinated water output* (see Section 6.2.2.1). Inventory data per '*1m³ of desalinated water output*' for scenarios 1-3 can be found in Supplementary Information I (see Section S3, **Table S.8**, **Table S.10** and **Table S.12**). This methodological option examines how the choice of the functional unit affects the results and conclusions.

Methodological option B: Effect of the multifunctionality approach

After selecting the functional unit, the approach to handling multi-functionality in systems with multiple products follows. This paper compares three multifunctionality approaches applied to the three resource recovery desalination systems for the five selected impact categories at the midpoint level. This methodological option explores three approaches: economic allocation, mass allocation, and system expansion, comparing their effects on environmental impacts (see illustration in Section 6.5.1 S2, **Figure S.2**).

- Substitution is solving multifunctionality through the subtraction of avoided burdens related to the co-products that are not part of the FU [32]. Note that the additional amount of recovered water compared to the conventional SWRO plant (with 40% efficiency) is considered in the co-products of each scenario, and thus the credits from this avoided are included. Specifically, in this analysis, inventory modeled in global (GLO) and inventory for the regional markets for Europe (REW) were used for conventional production, and the credits from the avoided products (see Section 6.5.1 S4, **Table S.15**).
- Economic and mass allocation is solving multifunctionality by dividing the inputs and outputs of the process or system between its products according to allocation criterion [32]. In this work, economic allocation is respective to the economic value of the products and the mass allocation to the volumetric flowrate of the products (see **Table 6. 3** and Section 6.5.1, S2).

Methodological option C: Effect of allocation in alternative energy sources

Waste heat is often overlooked in previous works in literature, considering zero environmental impacts for that energy stream. To analyse the effect of the inclusion and allocation factors concerning energy sources like waste heat, three different methodological options are considered: 1) Economic allocation (see **Table 6. 5**), 2) Energy allocation (see **Table 6. 7** and Supplementary Information I, **Table S.6**), and 3) Non-allocation (non-inclusion, zero environmental impacts). Note that the economic allocation approach is used to input the energy source in the SimaPro database for other analyses in this work besides this scenario analysis.

Table 6. 7. Energy allocation factors for Cyprus based on [23].

Type of energy	Energy value (ktoe)	Energy allocation
Oil for electricity production	1030	100%
Electricity	355	34.47%
Waste heat	675	65.53%

Sensitivity analysis: Effect of energy mix on the environmental impact

To analyse the effect of the energy mix on the environmental impacts of the three technical scenarios, a sensitivity analysis is conducted regarding energy policy, following the European Green Deal guidelines [33]. In 2021, the European climate law was approved, incorporating into EU regulations the goal of achieving climate neutrality by 2050 (i.e., eliminating net greenhouse gas emissions), as well as an interim objective of reducing net emissions by 55% by 2030 compared to 1990 levels. Specifically, the 55% reduction target set for 2030 has been used as a benchmark for the energy scenarios. These regulations, which set targets for emission reductions, form the basis for our analysis. To test the integrated desalination and brine treatment technical designs, the following energy scenarios were considered:

- **Baseline:** most updated available energy data for Cypurs in 2021, based on the electricity mix from oil power plant using fuel oil type S (0% RES), using EU and global averages from the Ecoinvent database.
- **e-55:** 55% of electrical energy comes from renewable energy sources, specifically from solar systems (Photovoltaic (PV)). According to [34], PV is expected to be the dominant renewable technology, followed by wind. For simplicity, only one renewable source is chosen: solar (PV) over wind.
- **eCSP-55:** 55% of electrical and thermal energy comes from renewable sources, specifically solar systems (Concentrated Solar Power (CSP) and PV). CSP is chosen to provide high heat, thus covering the thermal energy requirements and replacing waste heat. Additionally, CSP can be combined with existing fossil fuel sources, enhancing its versatility [35].
- **eCSP-100:** 100% of electrical and thermal energy comes from renewable energy sources, specifically from solar systems (Concentrate Solar Power (CSP) and PV).

For the sensitivity analysis, *1 m^3 of seawater* fed is used as functional unit, while for multifunctionality, two approaches are considered: *system expansion* and *economic allocation*. Finally, the environmental burden from the waste heat is calculated based on *economic allocation*.

6.3. Results and discussion

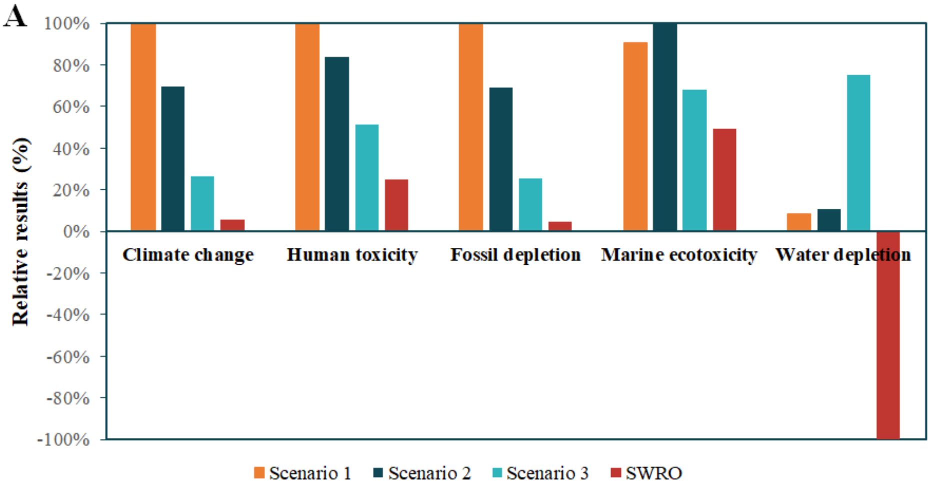
The LCA-based environmental impact analysis is divided into four parts. In the first part, the performances of the three scenarios across the five environmental impact categories are analysed and compared with the conventional desalination system. In the second part, the hotspots are identified, and the energy and chemicals contributions to the impact categories are analysed and discussed. In the third part, the effects of methodological decisions, such as the functional unit and allocation, on the results are analysed (see Section 6.3.3). In the fourth part, the sensitivity analysis on different energy sources is performed using a specific set of methodological choices, including a functional unit of 1 m³ of desalinated water, an economic allocation method, and a substitution approach for handling multi-functionality.

6.3.1. Life cycle assessment for scenarios and reference system

6.3.1.1. Results from LCA for 1m³ seawater as functional unit

Figure 6. 3 presents the LCA relative impact scores (in figure) and absolute (in table) results for each resource recovery scenario and SWRO with 1m³ of seawater fed as functional unit. All resource recovery scenarios result in higher environmental impacts in each of the four impact categories compared to the SWRO, as expected due to the integration of multiple technologies to minimize brine disposal and/or to recover valuable products. These integration strategies increase energy and chemicals consumption, leading to higher environmental impacts in comparison to the conventional desalination plant. It is worth noting that the difference between resource recovery scenarios and the SWRO for Marine ecotoxicity is much smaller than for the other four impact categories. For example, the difference between Scenario 3 and SWRO is only 0.03kg 1,4-DB eq (28% relative impact score). This is because the brine disposal in the SWRO system directly impacts the marine ecosystems. Additionally, the SWRO system results in a negative value for the water depletion impact category, indicating a net reduction in water depletion. This negative value results from the fresh water produced in the desalination process. This reduction was not considered for the other three scenarios because of simulation constraints. Thus, the water depletion category reflects the impact of water consumption in the three multi-product ZLD systems, but the net value is not calculated or shown in **Figure 6. 3**, affecting the interpretation of the results.

A



B

Impact category	Scenario 1	Scenario 2	Scenario 3	SWRO
Climate change (kg CO_2 eq)	39.96	27.89	10.52	2.24
Human toxicity (kg 1,4-DB eq)	3.18	2.66	1.64	0.79
Fossil depletion (kg oil eq)	12.02	8.34	3.09	0.57
Marine ecotoxicity (kg 1,4-DB eq)	0.10	0.11	0.08	0.05
Water depletion (m^3)	0.05	0.06	0.44	-0.58

Figure 6. 3. Life cycle impacts: (A) Relative impact score (%)for the three scenarios and the SWRO for 1 m^3 seawater fed as functional unit; (B) Absolute results for the three scenarios and the SWRO for 1 m^3 seawater fed as functional unit.

These findings emphasize the importance of informed decision-making in desalination plant design and the development of environmental policies, particularly in the context of multi-product complex systems. Resource recovery scenarios show higher environmental impacts than conventional RO desalination due to increased energy and chemicals use, but a fair comparison, including the production of extra products (e.g. NaCl, $Mg(OH)_2$), is essential to avoid misleading conclusions and decisions.

When comparing only the resource recovery scenarios, Scenario 3 results in the best environmental performance concerning all impact categories but water depletion, while Scenario 1 results in the worst environmental performance. Thermal and electrical energy sources are the main inputs in all technologies (see **Table 6. 4**), which means that all environmental impact categories are dominated by energy consumption. Only Multiple Feed Plug Flow Reactor (MF-PFR) (as seen in Scenario 2 and 3) and, to a lesser extent, membrane technologies use chemicals. Lastly, the significant external water usage in the Electrodialysis with Bipolar Membranes (EDBM) unit for the production of chemicals contributes to water depletion in Scenario 3 (see **Table 6. 4**). This highlights a potential trade-off within Scenario 3, as water production is the primary objective of desalination plants in Cyprus. Note that water production is not accounted for in assessing water depletion for these resource reciovery scenarios. The environmental impact results using '1m^3 desalinated water' as functional unit are presented in Supplementary Information II (see Section 6.5.2, **Figure S.3**).

6.3.1.2. Comparative environmental impact analysis of conventional and resource recovery systems

The environmental impact results of the production of recovered products in each technical scenario are compared per category with respect to the conventional production of the recovered products. **Figure 6. 4** represents a products basket approach (without any allocation), where the conventional and multi-product ZLD systems are compared based on the recovered products to evaluate the environmental advantages and disadvantages of recovering, besides water, multiple products from seawater.

Recovering salts and chemicals in Scenarios 2 and 3 significantly reduces overall environmental impacts for all assessed impact categories compared to the traditional production systems. For example, climate change impact is 70% and 89% lower in the resource recovery systems for Scenario 2 and 3, respectively, in comparison to the conventional production processes (see **Figure 6. 4A**). Similarly, the reduction in environmental impacts for each product basket is between 70-95% in the other impact categories for Scenario 2 and 44-96% for Scenario 3 (see **Figure 6. 4 B, C, D, E**). Scenario 3 shows that using only electricity-based technologies and recovering chemicals from seawater brines may result in significant environmental benefits compared to traditional production systems.

Thermal desalination and minimization of brine disposal with no additional recovery of production (scenario 1) results in a higher overall impact than conventional desalination systems. This is because of the higher energy requirements for water recovery. Although the ZLD system recovers more water than conventional desalination systems (with 40% water recovery efficiency), the environmental impacts are higher for Climate change and Fossil depletion than those of the conventional system. It is worth noting that Scenario 1 performs better in Human toxicity and Marine ecotoxicity compared to the conventional system, because of the reduction of brine disposal. Supplementary Information II contains the relative impact scores for both FU (see Section 6.5.2, S1).

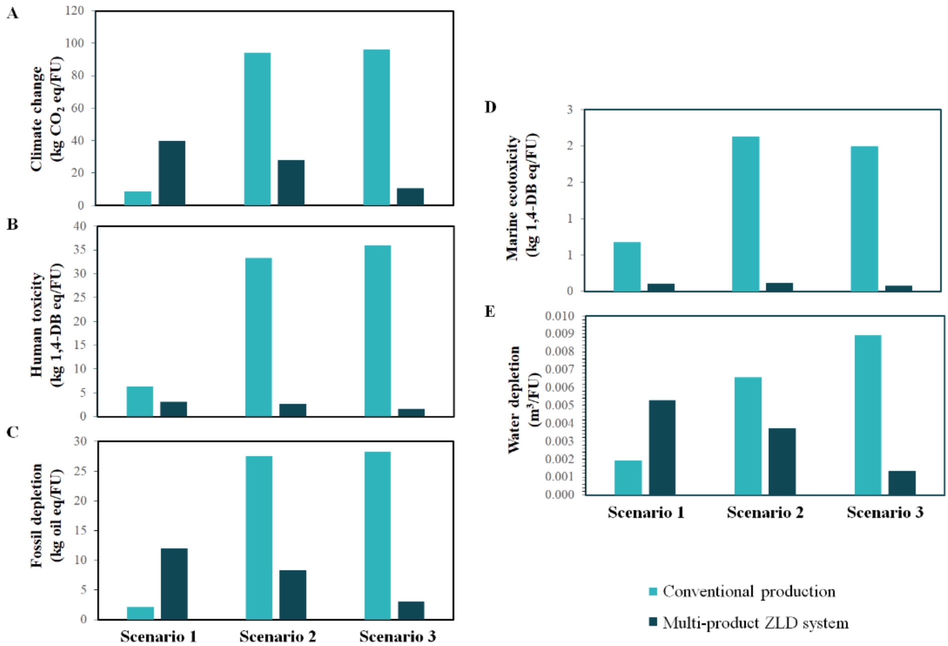


Figure 6. 4. Comparative analysis of the five environmental impact categories between the three resource recovery desalination scenarios with respect to the conventional production systems. Subfigures illustrate the comparison for (A) Climate change (kg CO_2 eq/FU), (B) Human toxicity (kg 1,4-DB eq/FU), (C) Fossil depletion (kg oil eq/FU), (D) Marine ecotoxicity (kg 1,4-DB eq/FU), (E) Water depletion (m^3/FU). FU: $1m^3$ seawater fed.

A comparative analysis of water production using a conventional SWRO and a multi-product ZLD system (with economic allocation) highlights the environmental advantages and disadvantages of each approach. Conventional desalination in Scenario 1 has significantly lower environmental impacts across most of the five selected impact categories compared to the multi-product ZLD systems, with marine ecotoxicity being the exception. Specifically, the impact on climate change and fossil depletion is approximately five to six times higher for the multi-product ZLD systems due to their high energy requirements and the absence of co-products other than water. This leads to most environmental impacts being allocated to water based on economic revenues. The significantly higher climate change and fossil depletion impacts observed for thermal-based ZLD systems (like Scenario 1) that focus only on maximizing water recovery highlight the critical need for improving energy efficiency.

In contrast, water production within a multi-product ZLD system like Scenario 2 has significantly lower environmental impacts across the impact categories (79%-97%) compared to conventional desalination. This demonstrates the potential environmental benefits of multi-product ZLD systems when additional co-products are recovered, making the multi-product ZLD systems, like Scenario 2, a viable option for future designs (desalination systems).

Details of this comparison can be found in **Figure S.7** in Supplementary Information II. A similar analysis for Magnesium can be found in Supplementary Information II (Section 6.5.2 S1, **Figure S.8**).

6.3.2. Contribution analysis: Identification of hotspots

Figure 6. 5 shows the contribution of each process unit to the impact categories, using Scenario 2 as an example to demonstrate the analysis and identify hotspots. Scenario 2 is selected here for simplicity, but similar analyses could be conducted for the other scenarios to provide a comprehensive understanding across all cases. The MED, MF-PFR, and EDBM units collectively contribute approximately 82% to the four impact categories and 73% to water depletion. These hotspots can be attributed to the substantial energy demands of the MED and EDBM units, coupled with chemical requirements (NaOH, HCl) for MF-PFR. Identifying these hotspots reveals a map that guides the designers and decision-makers to make changes and improvements. For instance, environmental benefits are expected if all the chemical requirements can be produced internally (less dependent on external sources). Moreover, transitioning to more renewable energy sources, especially for the energy-intensive MED and EDBM units, holds promise for significant environmental benefits.

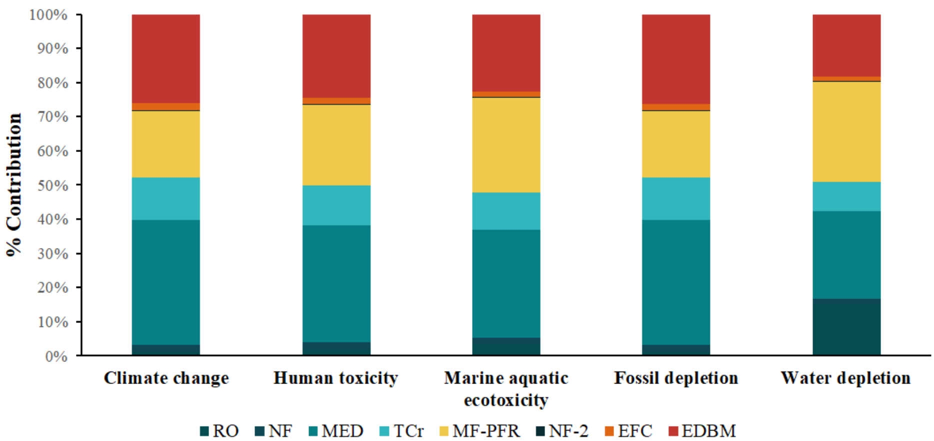


Figure 6. 5. Contribution analysis of the process stages, to the five environmental impact categories, for Scenario 2 with 1m^3 seawater fed as functional unit. ED: Electrodialysis; EDBM: Electrodialysis with bipolar membranes; EFC: Eutectic freeze crystallization; MED: Multi-effect distillation; MFPR: Plug-flow reactor; NF: Nanofiltration; RO: Reverse Osmosis, ThCryst: Thermal crystallizer.

Building on the contribution analysis, the contribution of energy supply (thermal and electrical) and chemicals consumption to the five impact categories reveals that chemicals consumption accounts for 21% of climate change impact, highlighting the need for a reduction in chemicals usage. Within each impact category, thermal energy use accounts for 49%, indicating the need to decrease the thermal energy demand and also to shift towards more renewable energy sources for both electrical and thermal energy. Chemicals consumption contributes 43% to water depletion, emphasizing the importance of addressing the supply of chemical requirements internally, minimizing the external costs, and optimizing the EDBM unit to reduce water needs, which contributes to 18.3% of water depletion in Scenario 2. This analysis not only identifies critical areas demanding attention but also illuminates pathways for a more ecologically friendly design. Results for the contribution of energy supply (thermal and electrical) and chemicals consumption are available in Section 6.5.2, S1 (see **Figure S.5**).

6.3.3. Effect of key methodological choices

Evaluating key methodological decisions is a crucial step in this LCA study to understand their influence on outcomes. This evaluation, divided into conceptual and numerical levels, provides valuable insights into the methodological adjustments necessary for assessing novel systems, particularly those focused on resource recovery. The numerical analysis, on the other hand, offers significant information for the design of process chains.

6.3.3.1. Methodological option A: Effect of functional unit

The first and crucial methodological decision is the selection of a functional unit. **Figure 6. 6** compares LCA results for two functional units: 1m^3 seawater fed *versus* 1m^3 desalinated water output, focusing on climate change (**Figure 6. 6 A**) and marine eco-toxicity **(Figure 6. 6 B**). This analysis uses economic allocation to address multifunctionality. Results for the five environmental impact categories for both functional units are available in Section 6.5.2 S2 (see **Table S.18**). **Figure 6. 6** shows that the choice of functional units significantly impacts Scenario 3. This is due to the lower quantitative difference between the volume of seawater fed and the volume of desalinated water recovered in scenarios 1 and 2 compared to Scenario 3. Scenario 1 aims to maximize water recovery, Scenario 2 aims at maximum water and

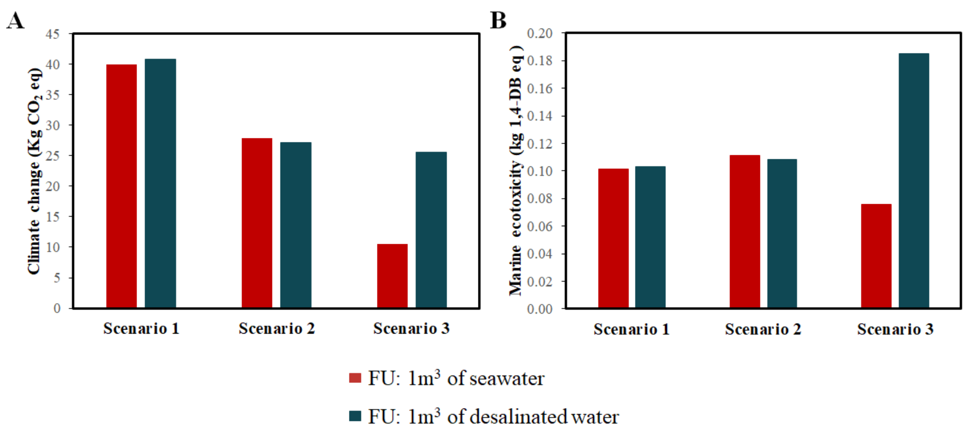


Figure 6. 6. Comparison of LCA results for 1m^3 seawater fed *vs.* 1m^3 desalinated water output as functional units for (A) climate change and (B) marine eco-toxicity impact categories.

resource recovery, while Scenario 3 targets the recovery of valuable materials (like Mg) and chemicals. Consequently, choosing 1m^3 desalinated water output as the functional unit results in lower water recovery and, therefore, in higher energy and chemicals intensity for Scenario 3, which in turn leads to higher impacts.

Similarly, higher environmental impacts by scenario 3 are observed across the other impact categories when 1m^3 desalinated water output is used as functional unit instead of 1m^3 seawater fed (see Section 6.5.2 S2, **Table S.18**). This underscores the complexity of the decision-making process. The selection of a functional unit forms a critical factor in LCA methodologies and should be based on the objective of the project. If the objective is to maximize water recovery, the functional unit should be set as 1m^3 desalinated water output. In that case, the decision becomes more intricate, as Scenario 3 demonstrates a higher impact on marine eco-toxicity and water depletion than Scenarios 1 and 2. Additionally, the differences between Scenarios 2 and 3 are less significant when using 1m^3 of desalinated water as functional unit, making Scenario 2 more attractive compared to using 1m^3 of seawater fed. In particular, for the climate change impact category, the difference between Scenario 2 and Scenario 3 decreases significantly when comparing the two functional units: from 62% with a functional unit of 1m^3 of seawater fed to 12% with a functional unit of 1m^3 of desalinated water. Similarly, for fossil depletion, the difference between the two scenarios drops from 63% to 14%. For human toxicity, marine eco-toxicity, and water depletion, Scenario 2 results in lower impacts than Scenario 3 by 31%, 39%, and 94%, respectively, when the functional unit of 1m^3 desalinated water is used.

6.3.3.2. Methodological option B: Effect of multifunctionality approaches

After selecting the functional unit, the question is how to handle multi-functionality in systems with multiple products. Two multifunctionality approaches (substitution and economic allocation) are compared when applied to three resource recovery desalination systems for the five selected impact categories at the midpoint level (see **Figure 6. 7**). Supplementary Information II contains the relative impact scores and absolute values for both choices of functional units (see Section S2). The comparison between economic and mass allocation is conducted separately to simplify the analysis. Supplementary Information II contains the detailed results (see Section S2).

When the substitution approach is used, Scenarios 2 and 3 have significant credits from avoided products' production elsewhere (see **Figure 6. 7**). In Scenario 2, the substitution approach resulted in a 54% lower impact for Climate change, 53% in Fossil depletion and over 86% in the other impact categories compared to the economic allocation approach. Scenario 3 results in around 90 % or more lower impacts in the evaluated impact categories.

Note that the water production itself, and thus its impact on the water depletion category, is not considered for the resource recovery scenarios because of simulation constraints (see

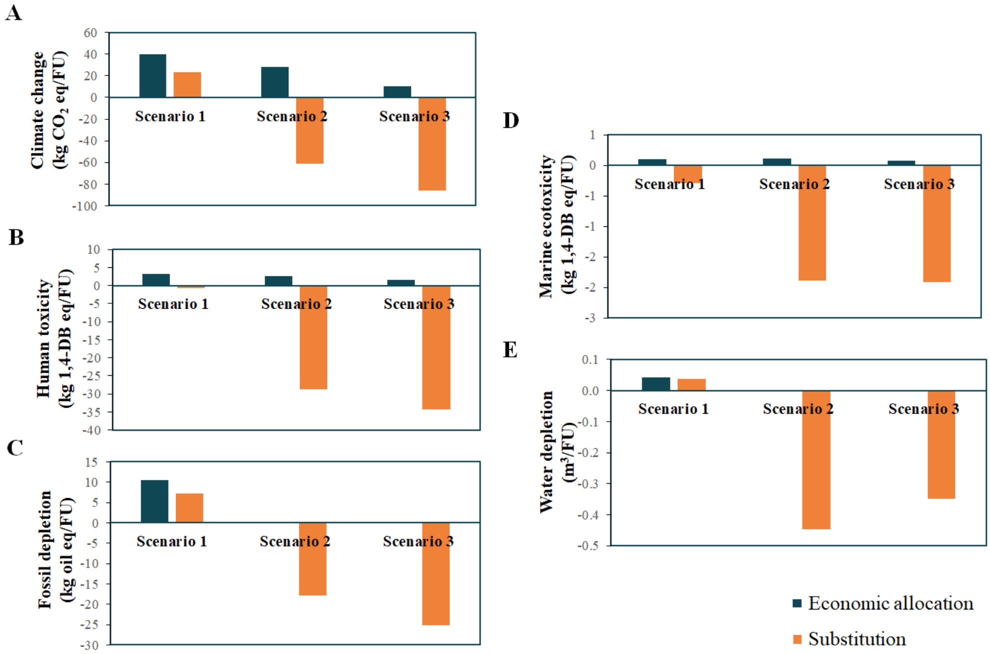


Figure 6. 7. Comparison of three resource recovery desalination systems using multifunctionality approaches (economic allocation, and substitution) for the five selected impact categories at the midpoint level. Subfigures illustrate the comparison for (A) Climate change (kg CO_2 eq/FU), (B) Human toxicity (kg 1,4-DB eq/FU), (C) Fossil depletion (kg oil eq/FU), (D) Marine ecotoxicity (kg 1,4-DB eq/FU), (E) Water depletion (m^3/FU). FU: $1m^3$ seawater fed.

Section 6.3.1.1). Scenario 1 focuses on water production and not on the recovery of multiple products, hence the deducted credits for product recovery are limited. Results for Scenario 1 suggest that focusing solely on water production may limit the environmental benefits of resource recovery systems, as shown in Section 6.3.1.2. Incorporating multiple product recovery, as in Scenarios 2 and 3, results in more sustainable economy positive outcomes.

When comparing multi-product ZLD systems with conventional systems, substitution can provide more useful information. Decision-makers can use the results, with the substitution approach applied, to inform their choice of desalination technologies based on their potential for resource recovery. One limitation of the analysis regarding substitution is the requirement of accurate data on the environmental impacts of substituted products, which may be difficult to obtain. Specifically, in this analysis, inventory modeled in global (GLO) and inventory for the regional markets for Europe (REW) were used for conventional production, and the credits from the avoided products (see Supplementary Information I, Section S4, **Table S.15**). Those choices can influence the results and lead to uncertainty.

Comparing the mass and economic allocation on a process level shows that the economic allocation results in lower environmental impacts across all the impact categories, ranging from a 33% reduction for climate change to a 54% reduction for water depletion. Economic allocation distributes the environmental impacts based on the economic value of the co-products, which often results in lower impacts for the main product when high-value co-products are present. This approach is useful for systems where economic revenue plays a significant role in design, such as resource recovery systems. When the overall system results are compared with the two allocation approaches, there is no difference in the environmental impacts (see Supplementary Information II, **Figure S.7, Figure S.8**).

6.3.3.3. Methodological option C: Effect of allocation in alternative energy sources

Figure 6. 8 presents the comparison of the LCA results for three different methodological options related to waste heat inclusion in the calculation: 1) Economic allocation, 2) Energy allocation, and 3) Non-allocation (zero environmental impacts). An effect analysis of the allocation methods (and related factors, or non-allocation with zero environmental impacts to waste heat recovery) is conducted, focusing on climate change (**Figure 6. 8 A**), fossil depletion (**Figure 6. 8 B**), and water depletion (**Figure 6. 8 C**). The impact categories are

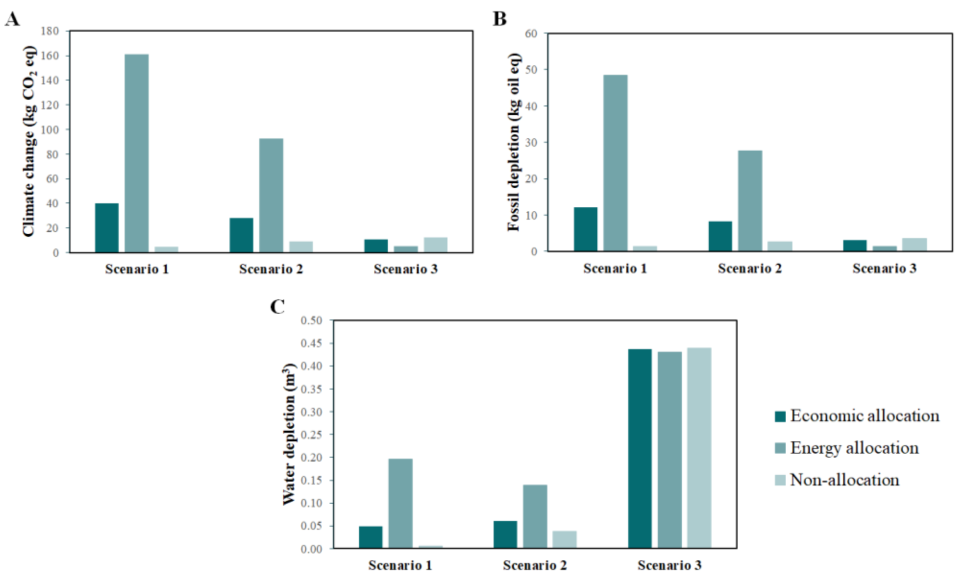


Figure 6. 8. Comparison of LCA results for waste heat inclusion by Economic allocation, Energy allocation and non-allocation (no environmental burdens), for three impact categories: (A) Climate change, (B) Fossil depletion and (C) Water depletion. FU: $1m^3$ seawater fed.

selected based on the relevance to the methodological decision. Additionally, all impact category results for $1m^3$ seawater-fed FU are available in Section 6.5.2, S2.

The three allocation methods significantly affect environmental impact performance and, consequently, the decision-making process. In the case of the energy allocation method, Scenario 1's environmental impacts increase by 75% across all categories, Scenario 2 increases by 56-70% across all categories, and Scenario 3 decreases by a wide range (2%-114%) compared to the economic allocation. This decrease in Scenario 3 is attributed to the absence of waste heat utilization. Despite not utilizing waste heat, Scenario 3 still allocates the environmental impacts of electricity consumption based on the energy value of both streams (electricity and waste heat). Notably, economic allocation assigns a 4.4 times higher environmental burden to electricity consumption than energy allocation. Consequently, even in the absence of waste heat utilization in Scenario 3, the choice of allocation methodology results in significant variations in assessed environmental impacts.

The analysis demonstrates that the consideration of waste heat significantly influences the environmental performance of the scenarios and, consequently, the decisions based on the numerical results. The Non-allocation approach results in an 88-89% lower value than the economic allocation approach across impact categories for Scenario 1 and 38-68% for Scenario 2, highlighting the potential for misleading decisions when waste heat is excluded from the analysis.

Figure 6. 9 shows the contribution from electricity, thermal energy, and chemicals for the LCA results of the comparative analysis for waste heat inclusion by the three allocations approached (economic*,* energy and no environmental burdens) across three impact categories (Climate change, Fossil depletion and Water depletion). Scenario 2, with *$1m^3$ seawater fed* as FU, serves as an example of the impact of the results. Results for all impact categories using the three allocation approaches are available in Section 6.5.2 S2. The contribution analysis aids in discussing design improvements to address the primary sources of impact and reduce the environmental impacts. The analysis shows that using the different allocation approaches, the contribution of the three components varies largely.
This variation highlights the importance of the methodological decision. For instance, in the case of economic allocation, electricity emerges as the primary contributor across impact categories (51%-71%), directing attention towards energy optimization, reducing electricity consumption, and increasing renewable energy sources. Conversely, when energy allocation is used, the results underscore the importance of measures like replacing waste heat, identifying alternative waste heat sources (e.g., solar energy), and utilizing renewable energy sources.

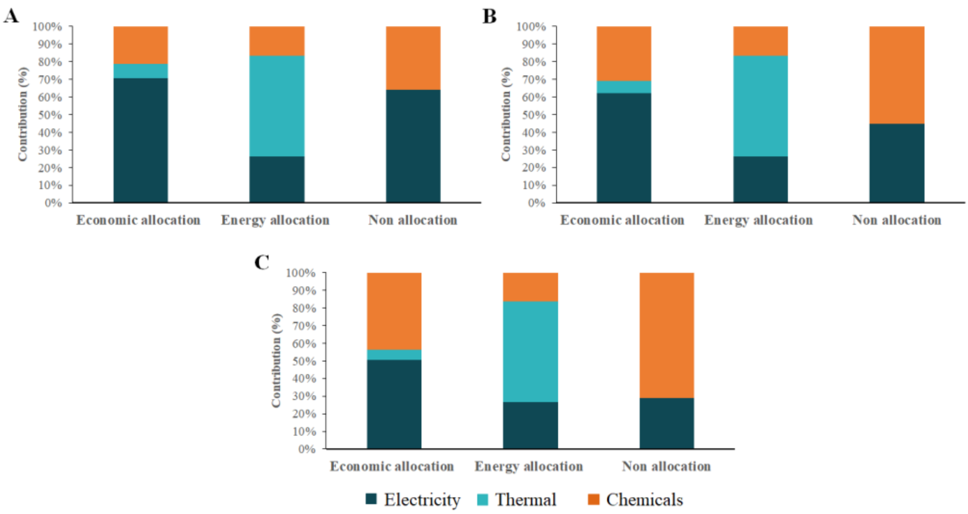


Figure 6. 9. Comparison of LCA's contributions (from chemicals and energy sources) for waste heat inclusion for Scenario 2 by considering: Economic allocation, Energy allocation and non-allocation (no environmental burdens); for three impact categories: (A) Climate change, (B) Fossil depletion and (C) Water depletion.

Finally, there is a notable variation in the contribution from chemicals consumption to the impact categories when different allocation approaches are applied: 21%-44% for economic allocation, 17% for energy allocation, and 36%-71% for the non-allocation approach. This means that chemicals consumption can play an important role in design improvement. In the case of non-allocation, internal chemicals production and the utilization of renewable energy sources could substantially reduce the system's environmental impacts. The choice of allocation method evidently influences potential design improvements and the priorities of the decision-makers. This analysis demonstrates that the selection of key methodological approaches in complex multi-product systems has profound consequences on the final results.

6.3.4. Sensitivity analysis: Effect of the energy mix on environmental impact

A sensitivity analysis has been conducted regarding energy policy, following the European Green Deal guidelines [33] as explained in Section 6.2.2.5. The sensitivity of climate change impacts to changes in the energy mix was assessed by comparing the differences across various scenarios. As expected, transitioning to more renewable energy sources led to significant reductions in climate change impacts. For instance, in Scenario 1, transitioning to a case where 55% of electrical and thermal energy comes from renewable energy sources (RES) resulted in a reduction in the impact of climate change by 54%. Similarly, in Scenario 2, this transition led to a reduction of approx. 53% in the climate change impact, while in Scenario 3, the reduction was approx. 45%. Furthermore, when considering a scenario where

100% of electrical and thermal energy comes from RES, the reductions on the climate change impact were even more significant, with reductions of approx. 99% for Scenario 1, 96% for Scenario 2, and 82% for Scenario 3.

The linear reduction observed specifically for Scenario 1 is due to the assumption that 0% RES is used in the baseline energy mix (see Section 6.2.2.3). Scenario 1 is a very energy-intensive scenario, utilizing both electricity and waste heat, with negligible use of chemicals and other sources of environmental impacts. Therefore, the impacts from energy consumption are dominant in this scenario, and they are reduced proportionally to the percentage of RES integrated into the energy mix.

Overall, Scenario 3 consistently exhibited the lowest reductions in the impact of climate change compared to Scenarios 1 and 2 under similar energy mix uses. This suggests that Scenario 3's environmental performance is less sensitive to changes in energy mixes or related policies compared to the other two scenarios because it uses only electrical-based technologies, compared to Scenarios 1 and 2, where the thermal requirements are higher.

The impact of water depletion due to changes in the energy mix was analyzed by comparing water depletion impacts across different scenarios. When transitioning to cases with higher shares from renewable energy sources (RES), there is a variation in water depletion impacts across technical Scenarios 1 and 2. For example, in Scenario 1, transitioning to the eCSP-55 case where 55% of electrical and thermal energy comes from RES led to a decrease in water depletion impact of 47%. Similarly, in Scenario 2, this transition resulted in a decrease of 18% in water depletion impact, while in Scenario 3, the increase is 1% compared to the baseline. Furthermore, for the eCSP-100 case, the decrease in water depletion impacts is 85% in Scenario 1 and 33% in Scenario 2, while in Scenario 3, there is an increase of 1% compared to the baseline. Therefore, a neglectable increase of 1% is observed for the e-55 case for Scenarios 1 and 2 for water depletion and an exponential decrease in the other two cases, eCSP-55 and eCSP-100. The analysis underscores the influence of transitioning to renewable energy sources on water depletion, with Scenario 3 showing marginal increases compared to Scenarios 1 and 2. However, experts' assessment is crucial to determine the significance of these marginal differences in absolute numbers in decision-making processes. Detailed results can be found in Supplementary Information II (see Section S2.6).

After examining the sensitivity analysis results across various energy mix cases, **Figure 6. 10A** zooms in on Scenario 2, revealing significant potential reductions in climate change, human toxicity, and fossil depletion impacts with the transition to renewable energy sources. Notably, a reduction of 95.5% on climate change was observed for the eCSP-100 case, highlighting the effectiveness of renewable energy integration in mitigating climate change impacts. Similar to climate change, human toxicity and fossil depletion impacts decrease with the implementation of renewable energy sources. In particular, human toxicity decreased only by 1% in e-55, 34% in the eCSP-55 case and 62% in the eCSP-100 case compared to the baseline, while fossil depletion follows the same trends as climate change. Transitioning to renewable energy sources led to increases in marine ecotoxicity in Scenario 2 (of 23%-48%), suggesting potential trade-offs between renewable energy use and environmental sustainability in Scenario 2.

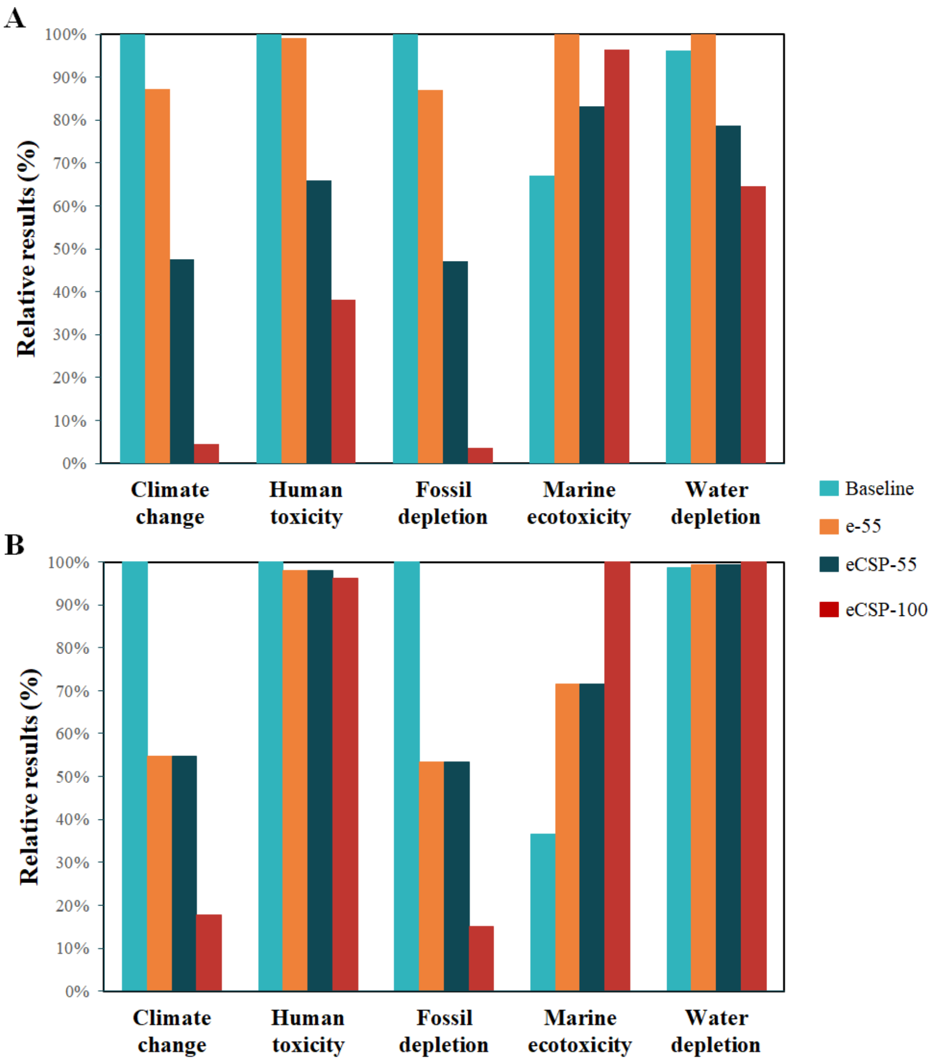


Figure 6. 10. Sensitivity analysis of energy mixes on the five environmental impact categories for (A) Scenario 2 and (B) Scenario 3.

Figure 6. 10B zooms in on Scenario 3, which has different trends compared to Scenarios 1 and 2. For the impact of energy mix on climate change and fossil depletion in Scenario 3, the

impacts decreased by 45-82% and 47-84%, respectively, compared with Scenario 2, where the decreases in those two categories are 55-96% and 55-96%, respectively. The effect of energy mix on human toxicity for Scenario 3 is limited to 2% for e-55 and eCSP-55 and 4% for eCSP-100. Contrary to climate change, human toxicity and fossil depletion, transitioning to renewable energy sources led to increases in marine ecotoxicity by 95-173% and water depletion impacts by 1% for all energy mixes in Scenario 3. Note that for Scenario 3, there is no use of thermal energy, and therefore, there is no CSP, meaning that the effect is related to the use of PVs.

Overall, the results underscore the importance of considering the broader environmental implications of the used energy mix and the potential policy decisions. While renewable energy integration yields substantial reductions in climate change and fossil depletion impacts, it also introduces challenges such as heightened marine ecotoxicity and water depletion.

6.3.5. Discussion and future work

This study highlights the critical role of LCA in designing and evaluating multi-product ZLD systems for desalination and brine treatment. It is the first comprehensive LCA study to address methodological challenges specific to integrated desalination and resource recovery systems, including the impact of functional unit selection, allocation methods, and waste heat inclusion—factors that have not been fully explored in previous studies on desalination LCA.

Functional unit selection: This study uniquely compares two functional units (1 m^3 of desalinated water and 1 m^3 of seawater) to capture the diverse objectives of ZLD systems, which include both water and resource recovery. Selecting 1 m^3 of seawater as the functional unit proves more appropriate for maximizing resource recovery, while 1 m^3 of desalinated water aligns with minimizing brine discharge, similar to findings in wastewater treatment where functional unit choice affects outcomes due to differences in influent and effluent volumes [5]. This insight extends beyond previous desalination studies, which typically focus on water output alone [12], underscoring the need for flexible, functional units in multi-objective systems.

Allocation methods and co-product credits: This study compares economic allocation and substitution, demonstrating that substitution provides a more comprehensive assessment by capturing the avoided impacts of conventional production for recovered products. Previous studies, such as [16], often rely solely on economic allocation, potentially overlooking the environmental credits from material recovery. Our findings show that Scenarios 2 and 3, which integrate multi-product recovery, achieve significant environmental credits, especially in climate change and fossil depletion impacts, unlike Scenario 1, which focuses solely on water recovery. This demonstrates the environmental benefits of adopting multi-product ZLD systems and highlights the importance of careful allocation choice. Detailed results can be found in Section 6.5.2 S2.

Waste heat inclusion: This study examined the critical impact of waste heat inclusion on LCA outcomes, challenging the common assumption of zero environmental burden for waste heat [6,28] By contrasting economic and energy allocation of waste heat, we demonstrate substantial differences in environmental impact values, particularly for climate change and fossil depletion categories. Excluding waste heat significantly underestimates impacts, potentially leading to misleading conclusions. Even if waste heat is not directly utilized, as in Scenario 3, the allocation method impacts environmental assessments. This finding suggests that waste heat should be incorporated in environmental evaluations of energy-intensive processes, offering new insights for LCA studies on desalination and resource recovery.

Membrane replacement scenario: In addition to the core analysis, a scenario was evaluated to assess the potential environmental impacts of membrane replacement as consumables. The results indicated that the inclusion of membrane replacement did not significantly alter the environmental performance across the key impact categories. This suggests that, for this specific system configuration, membrane replacement has a relatively minor environmental impact compared to other factors, such as energy consumption and chemical use. Their disposal might affect the environmental impact of the system [36], but it is out of the system boundaries of this analysis. Detailed figures comparing the scenarios with and without membrane replacement are provided in see Section 6.5.2 S2.

Renewable energy integration and environmental trade-offs: This study provides a comprehensive analysis of the impact of renewable energy implementation on desalination and brine treatment. The results underscore the significant influence of the local energy mix on assessment outcomes, with substantial reductions in climate change impact (up to 99% in Scenario 1) and fossil depletion impact (up to 96% in Scenario 2) when transitioning to renewable energy sources. However, renewable energy integration also introduces challenges such as increased marine ecotoxicity (up to 173% in Scenario 3) or water depletion impacts. This pattern has been similarly observed in LCA studies for solar MED systems [13]. By quantifying the impact of different energy scenarios on key environmental indicators, this analysis offers insights into the trade-offs and synergies between energy choices and environmental sustainability.

Environmental benefits: Beyond the methodological focus, this study provides actionable insights into the environmental impacts of integrated desalination and brine treatment systems. Compared to conventional seawater desalination (SWRO), multi-product ZLD systems have higher environmental impacts across all categories due to their complexity. However, resource recovery scenarios (Scenario 2 and 3) outperformed Scenario 1, which aimed solely at water recovery and minimized brine discharge. This highlights the environmental benefits of adopting resource recovery strategies in desalination. Compared to conventional production of the recovered products, Scenarios 2 and 3 present significant environmental benefits associated with the recovery of salts and chemicals, paving the way for more sustainable water treatment. This aligns with studies emphasizing the advantages of material recovery [4,37] but extends these findings by demonstrating that multi-product systems can match or exceed conventional water production's environmental performance.

Future directions: While this study provides valuable insights, future research should deepen our understanding and refine the proposed methodology. Although the data sources and assumptions are consistent across all scenarios, future work should incorporate a detailed uncertainty analysis to account for variability in input data and assess how this impacts the robustness of the findings. Additionally, expanding the system boundaries to include the full life cycle will provide a more comprehensive environmental evaluation. Addressing these aspects will refine the LCA approach for desalination and resource recovery systems, offering a framework for more sustainable seawater treatment.

6.4. Conclusion

This study underscores the importance of methodological choices in Life Cycle Assessment (LCA) for resource recovery systems in desalination, offering novel insights into how key methodological choices affect environmental outcomes. By comparing conventional and multi-product Zero Liquid discharge systems, it becomes evident that methodological decisions, such as the selection of multifunctionality handling approaches (e.g., economic allocation and substitution), play a pivotal role in shaping environmental assessments. The choice of a functional unit is crucial and aligns with the assessment objectives and the needs of decision-makers. This study demonstrates that the environmental impact can vary significantly depending on the chosen functional unit for desalination, especially when there are major differences in volumetric flows. This reveals a novel consideration for assessing resource recovery systems. Selecting an appropriate multifunctionality approach is essential, with economic allocation and substitution offering complementary perspectives. Substitution, in particular, provides a clearer picture of the environmental benefits of resource recovery systems. Excluding waste heat from the inventory in current methods can lead to significantly misleading conclusions, as demonstrated by the substantial differences in impact values when waste heat is neglected. These findings emphasize the necessity of incorporating waste heat into assessments for accurate and reliable environmental performance evaluations.

Overall, this paper contributes to improving LCA methodologies for integrated desalination and resource recovery systems, providing a more robust framework for decision-analysis and offering valuable insights for optimizing sustainable solutions. Future work should build on these findings by incorporating uncertainty analysis and considering full life cycle assessments, which will lead to more reliable environmental evaluations and better system designs.

6.5. Supplementary information

6.5.1. Supplementary Information I

See documentation.

6.5.2. Supplementary Information II

See documentation.

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7

Criteria interdependency in multi-criteria decision-making on sustainability: Desalination for resource recovery case study

ABSTRACT

In real-world sustainability assessments, decision criteria often influence each other, but traditional multi-criteria decision-making methods assume independence, potentially overlooking critical cross-criteria influences. This work addresses this limitation by integrating the Best-Worst Method with Decision-Making Trial and Evaluation Laboratory (DEMATEL) techniques to account for interdependencies in the weighting process and explores their effects on decision-making outcomes. The methodology was applied to assess technological alternatives for integrated desalination and brine treatment plants, aiming at recovering resources like water, salts, and chemicals. Hierarchical clustering and PROMETHEE were employed to rank the sustainability performance of the alternatives. The analysis identified operating expense as the most dominant cause factor and water production as the strongest effect factor, highlighting key system drivers. Incorporating interdependencies slightly adjusted weight distributions, notably in social and environmental dimensions, without altering final rankings. Stakeholder clustering revealed three distinct preference groups, and interdependencies reduced variability in weight judgments, enhancing alignment within clusters. Clustering preferences exert a more pronounced influence on rankings than interdependencies alone. While interdependencies had minimal numerical impact on rankings, they provided valuable conceptual insights into the complexity of criteria interactions. This study highlights the trade-offs of incorporating interdependencies and the importance of stakeholder clustering in participatory sustainability assessments and decision-making.

Keywords: *BWM; DEMATEL; MCDM; Interdependency; Desalination; Resource recovery.*

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7.1. Introduction

Multi-criteria decision-making (MCDM) is a well-established field that offers a variety of tools, methods and techniques for addressing the trade-offs inherent in sustainability assessments [1–3]. It enables decision-makers to evaluate and prioritize alternatives based on multiple criteria, encompassing economic, environmental, social, and technological dimensions [4]. MCDM methods provide a structured and transparent approach, making diverse data (qualitative and quantitative) more manageable and comparable [5]. Qualitative approaches and evaluations have become the rule rather than the exception in evaluating problems concerning socio-economic and physical planning [6] and are essential to include the best available information in the assessment process [7,8].

According to [9,10], effective multi-criteria methods should 1) prioritize simplicity to ensure transparency, 2) adopt a non-compensatory structure to prevent high scores in some criteria from offsetting bad performances in other criteria, and 3) use weights strictly as importance coefficients. Although there is no “best” MCDM method [11], the selection of MCDM methods depends on the characteristics of the problem, such as the data, the scope of the study, and the number of indicators [11–13]. Weighting criteria is a critical step in MCDM as it assigns relative importance to indicators, reflecting their significance in sustainability assessments [14].

In real-world sustainability assessments, decision criteria are rarely independent [15,16]. Interdependence occurs when criteria mutually influence one another, affecting their relative importance. However, many traditional MCDM methods assume independence between criteria. This simplification can lead to solutions that fail to reflect real-world complexities [17]. In sustainability contexts, criteria often support or conflict with one another. Ignoring these interdependencies can lead to less practical insights [16]. Integrating methods that account for these interrelationships could be crucial for more accurate and robust decision-making in sustainability assessments [1,18].

The Analytic Hierarchy Process (AHP) [19] and Best-Worst Method (BWM) [20] are widely used MCDM techniques for defining criterion weights through pairwise comparisons. AHP structures the decision problem hierarchically, with the objective at the top and alternatives at the bottom, requiring $n(n-1)/2$ comparisons for n criteria. BWM enhances this process by reducing the pairwise comparisons and employing an optimization model that minimizes inconsistencies arising from multiple pairwise comparisons. However, both methods typically assume that criteria are independent, whereas criteria are often interdependent in real-world contexts, potentially influencing outcome robustness.

To address interdependencies, methods like the decision-making trial and evaluation laboratory (DEMATEL) are frequently used to determine the influence matrix that reflects the degree of impact one criterion has on another [21]. The analytic network process (ANP), an extension of the AHP, handles dependence within and among different sets of criteria [22,23]. Integrated approaches like DEMATEL-ANP (DANP) have been widely used to address dependent relationships among criteria and obtain the relative importance/weighting preferences for each criterion [24–26]. However, these approaches can be procedurally complex, requiring a large number of pairwise comparisons. This complexity not only increases subjectivity but also makes communication with stakeholders challenging, especially when expertise is needed to assess the relationships between criteria accurately or when there is a time constraint. Incorporating BWM into this framework can mitigate these challenges by significantly reducing the number of pairwise comparisons required.

Few studies have explored the integration of BWM and DEMATEL to account for interdependencies among criteria in decision-making processes. For instance, [27] and [28] applied BWM to determine the relative weights of criteria, followed by DEMATEL to analyze interrelationships among them. While effective in highlighting critical factors, these approaches stop short of fully integrating interdependencies into a unified decision-making framework. Other studies, like [29], have proposed hybrid models, but they either rely heavily on expert judgment or fail to provide a robust, objective assessment of the interdependencies' impact on decision outcomes.

Despite these advances, there remains a critical gap in understanding how interdependencies influence both the numerical and conceptual aspects of decision outcomes, particularly in sustainability assessments where interactions among economic, environmental, and social dimensions are essential. Existing studies often prioritize identifying relationships among criteria but do not assess how interdependencies influence final rankings or decision robustness.

The study aims to evaluate the impact of interdependencies among criteria in an MCDM process for sustainability assessment. We propose a novel integration of BWM and DEMATEL, developing a composite weighting system that balances methodological rigor with practical feasibility by reducing the number of pairwise comparisons required. The potential benefits and limitations of incorporating interdependencies are also evaluated, highlighting the value of this integrated approach in addressing decision-making scenarios. The framework is applied to the sustainability assessment of desalination and brine treatment systems, a domain characterized by interdependencies among environmental, economic, and social criteria, making it an ideal case for evaluating the effectiveness of the proposed methodology.

7.2. Development of methodology

Weight determination in multi-criteria decision-making aims to reflect the relative importance of each criterion while accounting for their interdependencies. However, depending on the multicriteria aggregation method, the meaning of the weights can be different [30]. Weights in linear aggregation methods have the meaning of trade-offs, allowing full compensation among criteria. In outranking methods, weights have the meaning of importance coefficients, reflecting the relative importance among criteria and requiring non-compensatory aggregation procedures. In the proposed model, the initial weights are derived using the BWM and then refined through DEMATEL, which quantifies the interdependencies among criteria. This integrated approach ensures that the final weights more accurately represent real-world relationships, providing a more realistic foundation for sustainability assessments.

The weighting process follows three stages: (1) DEMATEL is used to calculate the indirect influence of criteria on the goal by analysing interdependencies; (2) BWM determines the direct importance of each criterion through pairwise comparisons; and (3) the composite weight is calculated by combining the results from both methods, providing a more comprehensive set of weights for ranking and prioritizing alternative scenarios. **Figure 7. 1** presents an overview of the proposed three-stage weighting.

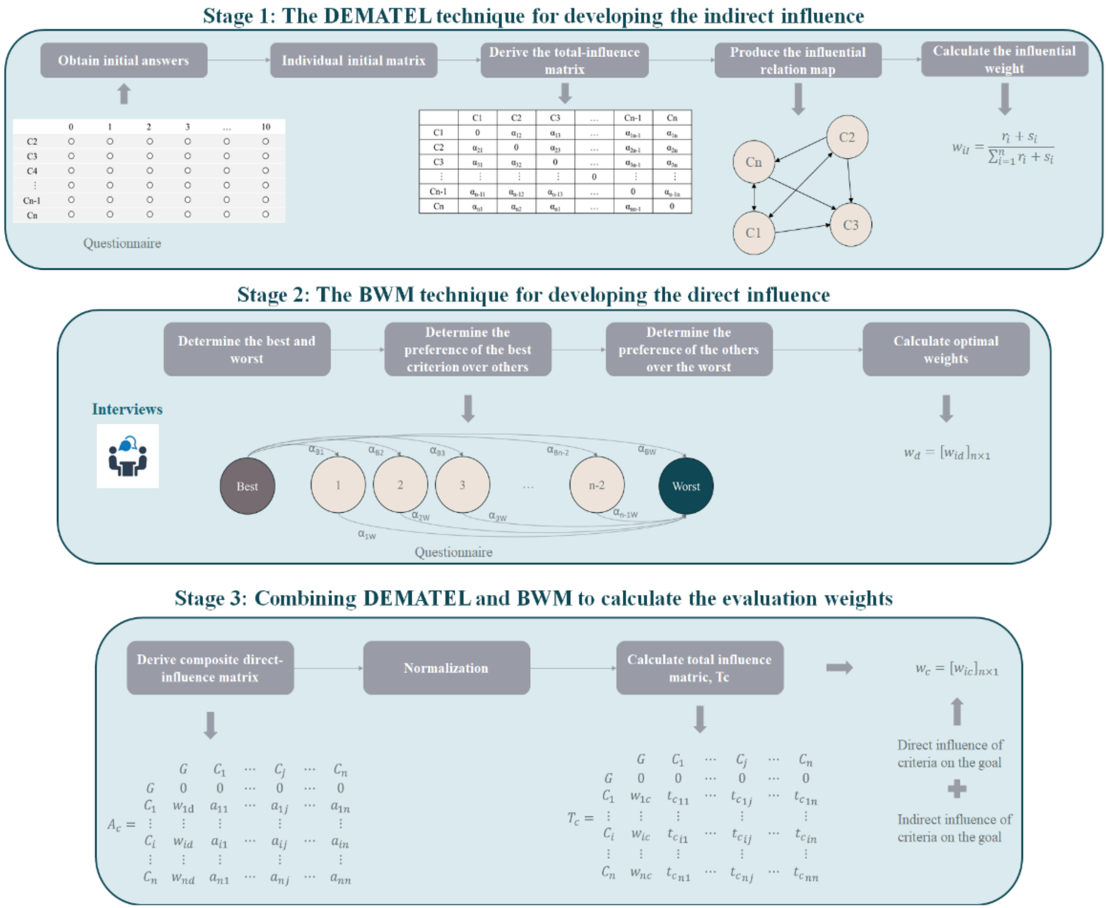

Figure 7. 1. Overview of the proposed three-stage weighting process integrating BWM and DEMATEL to calculate composite weights with interdependencies.

7.2.1. Stage 1: The DEMATEL technique for developing the indirect influence

In this stage, the degree of interdependence among the criteria is obtained, and the relative influence-intensity weights of the criteria according to the interdependencies are derived. Following the work from [23], the DEMATEL method can be summarised in the four key steps.

Step 1: Obtain the indirect-influence matrix.

In this step, the answers of respondents indicate the degree of influence each criteria i exerts on each criterion j. The influence degree is expressed by a_{ij}, using an integer scale ranging from 0 to 10 (see **Table 7. 1**).

Table 7. 1. Influence-intensity scales for the correlations among criteria.

Verbal phrase	Relative influence-intensity score
No influence	0
Somewhat between no and low	1
Low influence	2
Somewhat between low and medium	3
Medium influence	4
Somewhat between medium and high	5
High influence	6
Somewhat between high and very high	7
Very high influence	8
Somewhat between very high and dominated	9
Dominated influence	10

Then, an indirect-influence matrix $A = [a_{ij}]_{n\times n}$ is derived, within which all principal diagonal elements are equal to zero. The direct-influence matrix is presented as shown in eq. 1:

$$\mathrm{A} = \begin{bmatrix} a_{11} & \cdots & a_{1j} & \cdots & a_{1n} \\ \vdots & & \vdots & & \vdots \\ a_{i1} & \cdots & a_{ij} & \cdots & a_{in} \\ \vdots & & \vdots & & \vdots \\ a_{n1} & \cdots & a_{nj} & \cdots & a_{nn} \end{bmatrix} \qquad \text{eq.1}$$

Calculate the normalized direct-influence matrix. The normalized direct-influence matrix $X = [x_{ij}]_{n\times n}$ can be achieved by using eq. 2 and 3, in which all principal diagonal elements are equal to zero.

$$X = A \times z$$ eq.2

$$z = \min\left\{\frac{1}{\max\limits_{1\le i\le n}\sum_{j=1}^{n} a_{ij}}, \frac{1}{\max\limits_{1\le i\le n}\sum_{i=1}^{n} a_{ij}}\right\}$$ eq.3

All elements in the matrix X are complying with $0 \le x_{ij} < 1$, and $0 \le \sum_i x_{ij} \le 1$ or $0 \le \sum_j x_{ij} \le 1$, and at least one column or one row of summation, but all, equals to one.

Step 2: Derive the total-influence matrix T.

A continuous decrease of the indirect effects of problems can be determined along the powers of X, e.g., $X^2, X^3, \ldots, X^h$ and $\lim_{h\to\infty} X^h = [0]_{n\times n}$. The total-influence matrix $T = [t_{ij}]_{n\times n}$ is then computed by summing the direct effects and all of the indirect effects by eq. 4, in which I denotes the identity matrix.

$$T = X + X^2 + X^3 + \cdots + X^h = X(I-X)^{-1} \quad \text{when } h \to \infty$$ eq.4

Explanation

$$T = X + X^2 + X^3 + \cdots + X^h = X(I + X + X^2 + \cdots + X^{h-1})(I-X)(I-X)^{-1}$$
$$= X(I - X^h)(I-X)^{-1}$$

Then,

$$T = X(I-X)^{-1}, \qquad \text{when } h \to \infty$$

Step 3: Produce the influential relation map (IRM)

The sum of rows and columns from the total-influence matrix T are defined as vector R and S:

$$R = [r_i]_{n\times 1} = \left[\sum_{j=1}^{n} t_{ij}\right]_{n\times 1}$$ eq.5

$$S = [s_j]_{n\times 1} = \left[\sum_{i=1}^{n} t_{ij}\right]_{1\times n}^{T} \quad \text{eq.6}$$

r_i is the i^{th} row sum in the matrix T and shows the sum of direct and indirect effects of criteria i on the other criteria. Similarly, s_j is the j^{th} column sum in the matrix T and shows the sum of direct and indirect effects that criteria j is receiving from the other criteria. When $i = j$, the horizontal axis vector $(R + S)$ named "Prominence" illustrates the strength of influences that are given and received by the criteria. It stands for the degree of the central role that the criteria play in the system. In addition, the vertical axis vector $(R - S)$ called "Relation" shows the net effect that the criterion contributes to the system. If $r_i - s_i$ is positive, then the criterion i is influencing other criteria in the system and can be grouped into cause group; if $r_i - s_i$ is negative, then criterion i is being influenced by other criteria and should be grouped into effect group. Finally, an IRM can be created by mapping the dataset of $(R + S, R - S)$, which provides valuable insights into the interdependence of criteria in the system.

Step 4: Calculate the influential weight of the criteria.

Utilizing the prominence $(R + S)$ obtained in previous steps, the weights of criteria can be calculated in DEMATEL. It is important to note that the weights calculated through this method represent the relative strength of influence of the criteria on the entire system rather than the relative importance of criteria with respect to the goal of decision-making. The influence weight of criteria $w_I = [w_{iI}]_{n\times 1}$ is calculated through a normalization of prominence $(R + S)$ as follow:

$$w_{iI} = \frac{r_i + s_i}{\sum_{i=1}^{n} r_i + s_i} \quad , i = 1, 2, \dots, n \quad \text{eq.7}$$

7.2.2. Stage 2: The BWM technique for developing the direct influence

In this stage, the relative importance of each criterion to the decision-making goal is obtained and the direct weights $w_d = [w_{id}]_{n\times 1}$ are calculated using the Linear Best Worst Method (LBWM). This involves soliciting expert opinions on the best and worst criteria concerning the goal and using pairwise comparison to determine the preference of the best criterion over other criteria and the preference of other criteria over the worst criterion. A numerical scale ranging from 1 to 9 is utilized to express the degree of preference (see **Table 7. 2**). Following the work from [20,31], the implementation of the Linear BWM method can be summarised in the four key steps.

Table 7. 2. Relative importance scale.

Verbal phrase	Relative importance score
Extremely important	9
Very strongly to extremely important	8
Very strongly important	7
Strongly to very strongly important	6
Strongly important	5
Moderately to strongly important	4
Moderately important	3
Equally to moderately important	2
Equally important	1

Step 1: Determine the best (e.g., the most important) and the worst (e.g., the least important) criteria.

In this step, the decision-maker identifies the best and the worst criteria. No comparison is made at this stage.

Step 2: Determine the preference of the best criterion over all the other criteria using a number between 1 and 9.

Determine the preference of the best criterion over all the other criteria using a number between 1 and 9. The resulting Best-to-Others (BO) vector would be $A_B = (a_{B1}, a_{B2}, \dots, a_{Bn})$, where a_{Bj} indicates the preference of the best criterion B over criterion j. It is clear that $a_{BB} = 1$.

Step 3: Determine the preference of all the criteria over the worst criterion using a number between 1 and 9.

The resulting Others-to-Worst (OW) vector would be $A_w = (a_{1W}, a_{2W}, \dots, a_{nW})^T$, where a_{jW} indicates the preference of the criterion j over the worst criterion W. It is clear that $a_{WW} = 1$.

Step 4: Find the direct weights.

The direct weight is the one with minimum inconsistency, where $\frac{w_B}{w_j} = a_{Bj}$ and $\frac{w_j}{w_W} = a_{jW}$ can be satisfied. To satisfy these conditions for all j, the solution should minimize the maximum absolute differences $|w_B - a_{Bj}w_j|$ and $|w_j - a_{jW}w_W|$ for all j. A linear optimization model is applied as a solution to obtain the direct weights $w_d = [w_{id}]_{n\times 1}$:

$$\begin{aligned} &\text{Min } \varepsilon \\ &s.t. \\ &|w_B - a_{Bj}w_j| \le \varepsilon, \quad \text{for all } j \\ &|w_j - a_{jW}w_w| \le \varepsilon, \quad \text{for all } j \\ &\textstyle\sum_J w_j = 1 \\ &w_j \ge 0 \qquad\qquad \text{for all } j \end{aligned} \qquad \text{eq.8}$$

7.2.3. Stage 3: Combining DEMATEL and BWM to calculate the evaluation weights

In this stage, the composite weights that reflect the relative importance of each criterion while accounting for their interdependencies are calculated. To obtain the composite weights, the direct weights $w_d = [w_{id}]_{n\times 1}$ from stage 2 and the direct-influence matrix $A = [a_{ij}]_{n\times n}$ from stage 1 are combined into a composite direct-influence matrix A_c as shown in eq. 9:

$$A_c = \begin{array}{c|cccccc} & G & C_1 & \cdots & C_j & \cdots & C_n \\ G & 0 & 0 & \cdots & 0 & \cdots & 0 \\ C_1 & w_{1d} & a_{11} & \cdots & a_{1j} & \cdots & a_{1n} \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ C_i & w_{id} & a_{i1} & \cdots & a_{ij} & \cdots & a_{in} \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ C_n & w_{nd} & a_{n1} & \cdots & a_{nj} & \cdots & a_{nn} \end{array} \qquad \text{eq.9}$$

In accordance with the normalization approach outlined in stage 1, the direct-influence matrix A_c is normalized to produce the normalized direct-influence matrix X_c using eq. 10 and eq. 11.

$$X'_C = \begin{array}{c|cccccc} & G & C_1 & \cdots & C_j & \cdots & C_n \\ G & 0 & 0 & \cdots & 0 & \cdots & 0 \\ C_1 & w_{1d} & a_{11}/d_1 & \cdots & a_{1j}/d_j & \cdots & a_{1n}/d_n \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ C_i & w_{id} & a_{i1}/d_1 & \cdots & a_{ij}/d_j & \cdots & a_{in}/d_n \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ C_n & w_{nd} & a_{n1}/d_1 & \cdots & a_{nj}/d_j & \cdots & a_{nn}/d_n \end{array} \qquad \text{eq.10}$$

Where $d_j = \sum_{i=1}^{n} \alpha_{ij}$

$$X_c = X_c' \times \frac{1}{n+1} \tag{11}$$

The composite total-influence matrix T_c is then calculated using Eq. (4) and presented in Eq. (12).

$$T_c = \begin{matrix} & G & C_1 & \cdots & C_j & \cdots & C_n \\ G & 0 & 0 & \cdots & 0 & \cdots & 0 \\ C_1 & w_{1c} & t_{c_{11}} & \cdots & t_{c_{1j}} & \cdots & t_{c_{1n}} \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ C_i & w_{ic} & t_{c_{i1}} & \cdots & t_{c_{ij}} & \cdots & t_{c_{in}} \\ \vdots & \vdots & \vdots & & \vdots & & \vdots \\ C_n & w_{nc} & t_{c_{n1}} & \cdots & t_{c_{nj}} & \cdots & t_{c_{nn}} \end{matrix} \tag{12}$$

where the composite weights of criteria are represented by $w_c = [w_{ic}]_{n\times 1}$.

7.3. Application of the model to empirical case

The methodological approach described in Section 7.2 has been applied to the case of integrated desalination and brine treatment plants, which aim to recover valuable resources such as water, salts, and chemicals (see **Figure 7. 2**). Various technological alternatives exist for integrating desalination with the recovery of different products, and selecting the most sustainable option is a challenge for stakeholders and decision-makers [13]. An MCDM framework is essential for evaluating these alternatives, as it helps assess the sustainability of each design, considering multiple objectives, such as environmental impact, economic

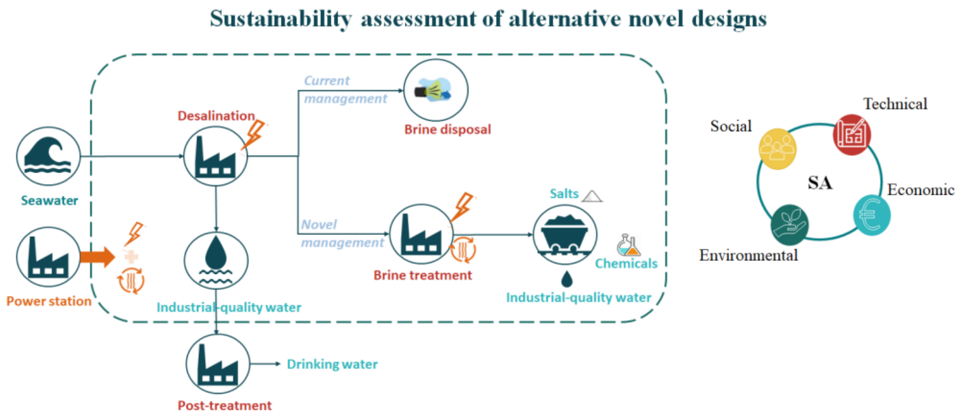

Figure 7. 2. Schematic description of integrated desalination and brine treatment plants aiming to resource recovery (Adjusted from [32]).

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feasibility, and social acceptability. The multi-objective nature of desalination for resource recovery adds complexity to the system, leading to greater interdependence among the influencing factors. This makes the analysis of conflicting criteria in sustainability assessments particularly challenging, further underscoring the need for a robust MCDM approach that can capture both the direct importance of criteria and their interdependencies.

7.3.1. Definition of scenarios

Three technical scenarios are evaluated and ranked regarding their sustainability performances. Although all scenarios aim to increase water recovery and reduce brine discharge compared to typical seawater desalination, they differ in their specific objectives [32]. These technical scenarios aim to recover water, salts (NaCl, $Mg(OH)_2$, Na_2SO_4), and chemicals (HCl, NaOH) from seawater. Each scenario corresponds to distinct real-world recovery objectives, ranging from simple water recovery to advanced chemical extraction:

- **Scenario 1** focuses on maximizing water recovery while minimizing brine discharge without the recovery of additional products.
- **Scenario 2** integrates the RO plant with the brine treatment plant to optimize both water and salt recovery.
- **Scenario 3** prioritizes the recovery of specific chemicals, such as HCl and NaOH, using only electricity-based technologies.

A detailed overview of the technical scenarios, including their objectives, the technologies, and the recovered products, is reported in **Table 7. 3**. Additionally, visualizations of the scenarios are available in Section 7.7.1, S3. The feed flow rate is the same for all the scenarios, and it is set equal to 3000 m^3/d. Further details on the design and simulations of these scenarios can be found in [32].

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Table 7. 3. Overview of technical scenarios for integrated desalination and resource recovery from seawater.

Scenario	Objective	Technologies	Recovered products
1	Maximize water recovery and minimize brine discharge	NF, MED, ThCryst	Water, Mixed salts
2	Integrated RO plant with brine treatment for recovery of water and valuable products and minimizing brine discharge	RO, NF, MED, ThCryst, MFPPR, EFC, EDBM	Ca(OH)2, HCl, Ice, Mg(OH)2, NaCl, NaOH, Na2SO4, Water
3	Integrated RO plant with brine treatment focusing on chemical recovery, using only electricity-based desalination	RO, NF, ED, MFPR, EDBM	$Ca(OH)_2$, HCl, $Mg(OH)_2$, NaOH, Water

ED: Electrodialysis; EDBM: Electrodialysis with bipolar membranes; EFC: Eutectic freeze crystallization; MED: Multi-effect distillation; MFPR: Plug-flow reactor; NF: Nanofiltration; RO: Reverse Osmosis, ThCryst: Thermal crystallizer.

7.3.2. Define assessment indicators

Table 7. 4 gives an overview of the selected indicators used for the sustainability assessment. The detailed definitions and mathematical formulations of the indicators are given in Section 7.7.1, S1.

Table 7. 4. The indicators used to operationalize the objectives in view of sustainability assessment.

	Objective	Indicator	Units	Code
Technological	Energy performance	Energy consumption	GWh	T1
	Increase water recovery	Quantity of water produced	1000 m^3/year	T2
	Increase efficiency	Resource efficiency	%	T3
	Minimize brine production	Brine production	Ton/year	T4
Economic	Product value	Levelized cost	€/amount of product	F1
	Economic viability of the plant	CAPEX	M€	F2
		OPEX	M€/year	F3
	Profitability	Production efficiency	€/€	F4
Environmental	Climate change impact	Carbon dioxide emission	MTon CO_2-Equ	E1
	Resource utilization	Water footprint	1000 m^3/year	E2
	Use of chemicals	Human toxicity	MTon1,4-DB eq	E3
Social	Improve working conditions	Operational complexity	-	S1
		Safe and healthy conditions	-	S2
	Impact on employment created by local employers	Local employment	-	S3
	Social acceptance	Level of aesthetic acceptability	-	S4

7.3.3. Indicator score determination

Technological, economic, environmental and social indicators are determined by techno-economic models and Life cycle assessment (LCA). In particular, technical process models developed using the open-source software explained in Chapter 3, are employed to generate the inventory for data on mass and energy flows. The software, available at the GitHub repository (https://github.com/rodoulak/desalsim), facilitated the creation and implementation of these models. Additionally, results from Chapter 5 were employed for the Levelized cost of water (with economic allocation) and results from Chapter 6 were employed for the environmental indicators. **Table S.3** in Supplementary Information I presents the inventory data for scenarios 1-3.

7.3.4. Measuring relationships among dimensions and among indicators by DEMATEL

The questionnaire for calculating interrelationships between indicators is designed based on the DEMATEL technique and adapted from [23]. Due to the large number of indicators in the case study, the DEMATEL questionnaire contains an excessive number of questions, and thereby, it is time-consuming to complete. Due to time constraints, one expert with deep knowledge of the project was selected to respond, ensuring that experienced decision-makers evaluated the interrelationships. The responses are used to construct an average direct influence matrix in the preliminary analysis.

7.3.5. Weighting of each dimension and indicator by BWM

In this step, diverse stakeholders were asked to assign criterion weights through the BWM. Stakeholders were identified based on their roles in the technological, economic, environmental, and social dimensions of the project, ensuring that all key areas were covered, including both beneficiaries and those potentially affected by the outcomes [13].

The stakeholders were selected according to their expertise and potential impact on the project. For example, researchers and academic institutions bring valuable expertise in desalination technologies and sustainability assessments, ensuring that scientific advancements and environmental impacts are considered when assigning weights to indicators. Policymakers play a crucial role in ensuring that regulatory, environmental, and public safety standards are properly reflected in the decision-making process, helping align project outcomes with national and international policies. Local communities and industrial users are directly impacted by the environmental and economic outcomes of desalination and resource recovery projects, making their input essential to ensure that social equity and economic viability are adequately weighted. The analysis, which includes the identification of technological experts, advisors, policymakers, and community representatives, is available in Section 7.7.1, S1.

The questionnaire for calculating direct weights follows the official BWM template (https://bestworstmethod.com/). Stakeholders first evaluate the four dimensions—technological, economic, environmental, and social—before assessing the specific indicators within each dimension. Expert evaluations are completed individually and then integrated at the end. The optimal weights for each criterion are calculated by solving the BWM optimization model for all respondents.

7.3.6. Combining DEMATEL and BWM to calculate the evaluation weights

To calculate the composite weights, the influence matrix (DEMATEL matrix) is combined with the direct weights (BWM) to form composite direct influence matrices, reflecting input from each stakeholder. To efficiently integrate these matrices with the weights obtained from the BWM optimization model, as explained in Section 7.2.3, a Python script was developed to automate the calculation of the composite weights.

7.3.7. Group weighting: Hierarchical clustering

Following [33], hierarchical clustering is applied in the group weighting stage to establish group priorities, minimize information loss, and include unpopular opinions. This method aggregates stakeholder opinions without forcing consensus in the MCDM process [33]. It acknowledges differing views and ensures less common perspectives are considered, offering decision-makers insight into the distribution of opinions. Note that the average weights (aggregation method) within each stakeholder cluster were computed using the arithmetic mean. Given that the stakeholder groups were formed based on similar weight patterns and the BWM outputs are normalized importance coefficients, the arithmetic mean was considered a suitable approach for aggregating the individual weights.

Each stakeholder j is represented as a point $W_c^j = (w_{1c}^j, w_{2c}^j, \dots, w_{nc}^j)$ in an n-dimensional weight space, where n is the number of criteria, w_{ic}^j is the evaluation weight of criteria i evaluated by stakeholder j. Initially, each point is treated as a cluster. Using Ward's method [34], clusters are iteratively merged to minimize intra-cluster variance. This is achieved by calculating the squared Euclidean distance between cluster pairs and merging the closest ones. This process repeats until all clusters are merged into a single cluster. Eq. (13) presents the distance measure between the composite weights w_c from two clusters.

Ward's method minimizes information loss at each step by selecting the pair of clusters that increase variance the least. It's crucial to determine an appropriate number of clusters, as fewer clusters increase within-cluster variance. This decision is often based on statistical tests and the researcher's expertise. Once the clusters are formed, each group's preferences are represented by an average set of composite weights [33].

$$d_{ij} = d(\{W_c^p\}, \{W_c^q\}) = \|W_c^p - W_c^q\|^2 = \sum_{i=1}^{n}(W_{ic}^p - W_{ic}^q)^2 \quad \text{eq. 13}$$

For further details and access to the code, see Supplementary Information I (Section 7.7.1, S5).

7.3.8. Performance score calculation: Alternative ranking by PROMETHEE II

Performance scores indicate the relative preference across alternatives by ranking them. PROMETHEE II is applied according to [35] and [36] to aggregate information and provide a full ranking of desalination and brine treatment alternatives based on sustainability performance. PROMETHEE constructs an outranking relation, comparing alternatives based on their performance across criteria to highlight contribution differences between them [37].

PROMETHEE was selected for its simplicity and ability to handle data uncertainty with fewer parameters. It supports partially or non-compensatory decision-making, essential for sustainability assessments where trade-offs between criteria are undesirable [38].

The ranking process aggregates the performance of alternatives across all criteria using pairwise comparisons. The selection of a preference function depends on the scale of the underlying criteria [39]. Considering the criteria selected for the case study, the preference functions selected are provided in Section 7.7.1, S6. To apply the model and obtain the ranking of alternatives, indifference and preference thresholds must be defined. The indifference threshold q represents the maximum difference between two alternatives where no preference is given, while the preference threshold p represents the minimum difference that makes one alternative preferable to the other under a given criterion [38]. Following [40], thresholds of 5% for q and 10% for p of the lower criterion score were used, with adjustments for increased uncertainty.

These thresholds, combined with the criterion weights and preference functions, form the basis for ranking the alternatives. Once all the parameters are defined, PROMETHEE II is implemented using the Python pyrepo-mcda package [41,42] to automate calculations and allow sensitivity analysis.

7.4. Results

7.4.1. Relationships among indicators

Following the procedure described in Section 7.2.1, the relationships among the indicators were calculated using the average values derived from two expert evaluations. The initial evaluation matrix is available in Supplementary Information II (Section 7.7.2). **Figure 7. 3** shows the influential relation map (IRM) for assessment indicators, which provides valuable insights into how different criteria interact and influence each other within the desalination and brine treatment systems.

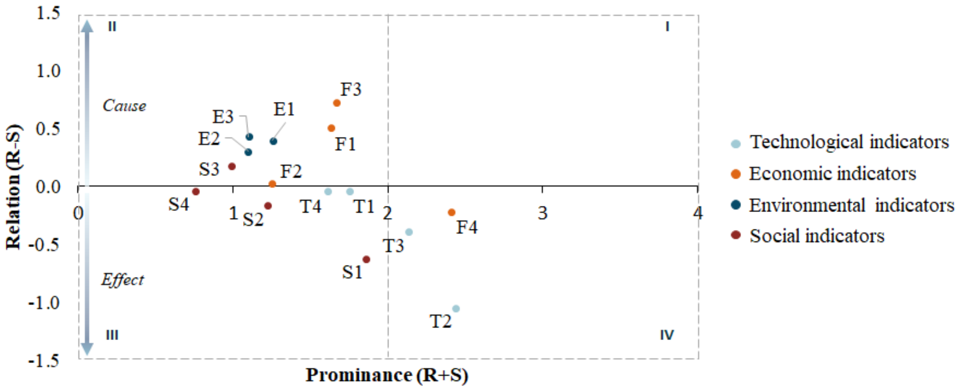

Figure 7. 3. Influential relation map (IRM) at indicators level. T1: Energy consumption; T2: Quantity of water produced; T3: Resource efficiency; T4: Brine production; F1: Levelized cost; F2: CAPEX; F3: OPEX; F4: Production efficiency; E1: Carbon dioxide emissions; E2: Water footprint; E3: Human toxicity; S1: Operational complexity; S2: Safe and healthy conditions; S3: Local employment; S4: Level of aesthetic acceptability.

The IRM categorizes the indicators into four quadrants based on their prominence (R+S) and relation (R-S). Indicators in quadrant I (top-right) are strong cause factors, exerting significant influence over other criteria, while indicators in quadrant III (bottom-left) are strong effect factors, heavily influenced by other indicators [21]. This differentiation helps identify which criteria drive system performance and which are more responsive to external factors.

The OPEX (F3) emerges as the most dominant cause factor, with the highest influence on other indicators. This implies that controlling operational costs is crucial for improving the overall performance of the system. On the other hand, the quantity of water produced (T2) is the strongest effect factor and can be largely affected by other criteria. Indicators like production efficiency (F4) and resource efficiency (T3) exhibit high prominence but low direct influence, implying that while these factors are important for the sustainability of the system, they depend on improvements in other areas.

Based on the IRM at the dimension level (see Section 7.7.2, S1), the economic and environmental dimensions are the key drivers in desalination sustainability, exerting the most influence on overall system performance. Improvements in these areas are crucial for driving positive outcomes across other dimensions. In contrast, the technological and social dimensions are more dependent, indicating that advancements in these areas rely on progress made in the economic and environmental factors.

7.4.2. Individual weights

At the individual level, stakeholders provided direct weights (BWM method) for the dimensions and the selected indicators. The results of this prioritisation exercise are available in Supplementary Information II (see Section 7.7.2, S2). Following the developed methodology described in Sections 7.2 and 7.3, the composite weights are calculated at the individual level. **Figure 7. 4** shows the dispersion of individual composite weights assigned to the various criteria by each stakeholder. The spread of points reveals the variability in stakeholders' preferences, emphasizing differences in how certain criteria are valued. For example, criteria E1 (carbon dioxide emissions) and S2 (safe and healthy conditions) show a wide range of assigned weights, indicating a high degree of disagreement among stakeholders about their importance. In contrast, criteria F2 (CAPEX) and F3 (OPEX) show more concentrated opinions, reflecting a stronger agreement among stakeholders on their importance.

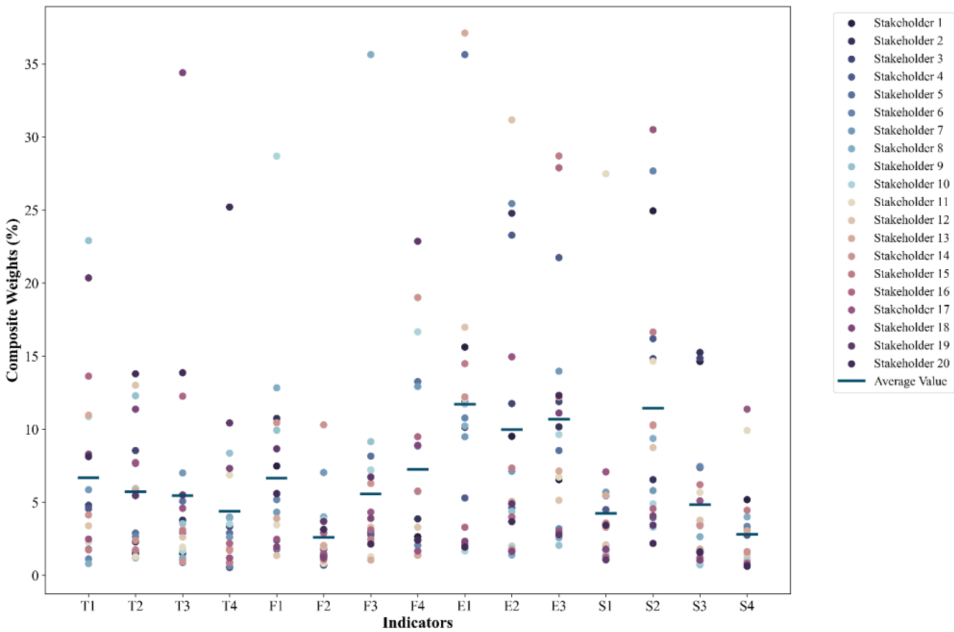

Figure 7. 4. Dispersion of individual stakeholder composite weights assigned to various indicators (T1 to S4). Each point represents the weight assigned by a specific stakeholder to a particular indicator, with the horizontal lines indicating the average value across all stakeholders. T1: Energy consumption; T2: Quantity of water produced; T3: Resource efficiency; T4: Brine production; F1: Levelized cost; F2: CAPEX; F3: OPEX; F4: Production efficiency; E1: Carbon dioxide emissions; E2: Water footprint; E3: Human toxicity; S1: Operational complexity; S2: Safe and healthy conditions; S3: Local employment; S4: Level of aesthetic acceptability.

Descriptive statistics of the weights assigned to each criterion are provided in **Table 7. 5**. E1 (carbon dioxide emissions) shows the highest variability (S.D 9.90%), followed by E2 (water footprint), reflecting diverse stakeholder opinions on its importance and indicating differing

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views on the environmental impact of integrated desalination and brine treatment projects. Overall, the analysis reveals that environmental indicators generate the most disagreement. In contrast, F2 and S4 exhibit the lowest variability.

Extreme opinions (see criteria T3, T4, F1, F3) or a number of stakeholders with different opinions (see criteria S2, S3) on the importance of the indicators are visible. These divergences are often overlooked when averaging opinions, as explained in Section 7.3.7. To better capture this diversity, hierarchical clustering was applied to group individual weights and highlighted diverse preferences rather than achieving a forced consensus. This approach allows for more tailored decision-making, recognizing the complexity of stakeholder preferences. The detailed results of the individual composite weights are given in Supplementary Information II (see Section 7.7.2, **Table S.9**).

Table 7. 5. Descriptive statistics according to individual direct and composite weights.

	Direct weights				Composite weights			
	Average(%)	**Min(%)**	**Max(%)**	**SD(%)**	**Average(%)**	**Min(%)**	**Max(%)**	**SD(%)**
T1	6.68	0.51	24.08	6.72	6.63	0.80	22.91	6.30
T2	5.72	0.83	14.26	4.51	5.75	1.19	13.79	4.23
T3	5.46	0.46	36.34	8.18	5.55	0.88	34.41	7.65
T4	4.37	0.20	26.49	5.98	4.50	0.54	25.20	5.61
F1	6.65	0.92	30.18	6.62	6.71	1.36	28.70	6.20
F2	2.59	0.29	10.65	2.49	2.82	0.69	10.30	2.30
F3	5.56	0.54	37.55	7.94	5.78	1.05	35.65	7.42
F4	7.25	0.95	23.84	6.95	7.31	1.37	22.86	6.52
E1	11.71	1.30	39.26	10.61	11.35	1.67	37.11	9.90
E2	9.99	1.17	33.05	9.90	9.64	1.38	31.18	9.24
E3	10.67	1.82	30.25	8.37	10.36	2.05	28.71	7.81
S1	4.24	0.75	28.92	6.08	4.38	1.06	27.48	5.70
S2	11.43	1.91	32.27	9.07	11.14	2.19	30.51	8.48
S3	4.85	0.39	15.79	5.06	5.02	0.72	15.25	4.76
S4	2.80	0.30	11.73	3.13	3.06	0.62	11.37	2.94

7.4.3. Group weighting: determination of group priorities

The dendrogram in **Figure 7. 5** shows the sequence by which stakeholders and groups are merged according to the similarities of their priorities (**Figure 7. 5A** direct weights and **Figure 7. 5B** composite weights). At each step, the number of clusters decreases and the within-cluster variance (the difference of opinions within the cluster) increases. The cutting line results in three distinct clusters based on the potential similarities and discrepancies in individual weights.

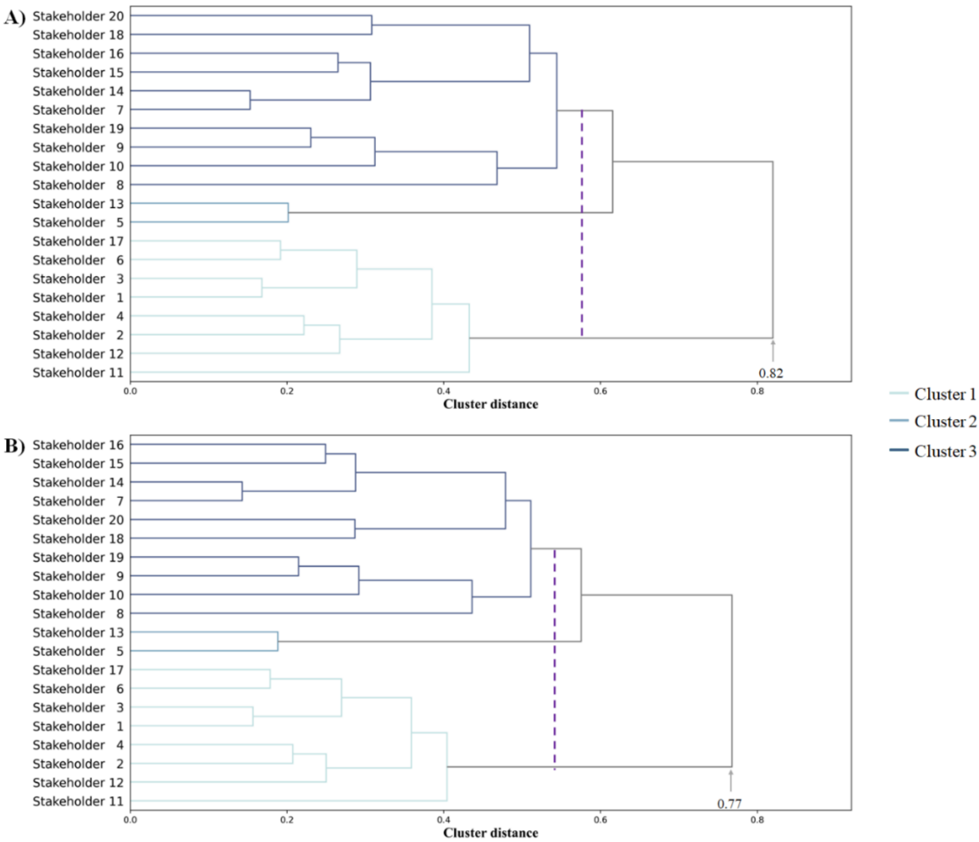

Figure 7. 5. Comparison of stakeholder clustering based on direct weights (A) and composite weights (B). The vertical dashed lines indicate the distances at which key separations between clusters occur.

The clustering results for both direct and composite weights are similar, as expected. This is because a single influence matrix is consistently applied across all stakeholders for the indirect influence weights (derived from DEMATEL), whereas direct weights (from BWM) are individualized. The uniformity in the influence matrix stabilizes the clustering outcomes. Although interdependencies do not change the final cluster assignments, they affect hierarchical clustering by reducing the maximum clustering distance. The maximum distance for composite weights (0.77) is slightly smaller than for direct weights (0.82), indicating that considering interdependencies in desalination criteria reduces the variability of the weights, which represents the stakeholder judgments.

Clusters show clear priorities across stakeholder groups:

- **Cluster 1: social and environmental advocates** represents stakeholders with a strong focus on both social and environmental dimensions. This group assigns significantly higher importance to these two dimensions than to economic and technological factors in both the direct and composite weightings. The stakeholders in this cluster likely prioritize environmental protection and social concerns.

- **Cluster 2: environmentally focused stakeholders with balanced priorities** shows a clear preference for ecological considerations, with the environmental dimension receiving three times higher weight than the other dimensions. The other dimensions—technological, economic, and social—are of relatively similar importance to those of stakeholders in this cluster.
- **Cluster 3: technology-driven stakeholders** are primarily focused on the technological dimension, assigning it the highest importance, followed closely by the economic and environmental dimensions. This group places little emphasis on the social dimension, suggesting that these stakeholders are likely driven by the need for technological advancements and economic viability to achieve sustainability goals.

These distinct priorities highlight the need for tailored strategies in decision-making to address the specific sustainability concerns of each group. The detailed results of the cluster analysis are given in Supplementary Information II (see Section 7.7.2, S3).

7.4.4. Group weights: direct and composite weights

The group weights are calculated by averaging the individual weights in each cluster. **Figure 7. 6-Figure 7. 8** present the direct and composite weights for the four dimensions and the individual indicators for the three clusters. The analysis reveals that integrating interdependency among criteria into weight determination affects the final relative importance of each criterion.

In Cluster 3 (cluster with majority opinions), the relative ranking of the dimensions remains consistent, with the technological and economic dimensions retaining the highest importance. However, the actual weight percentages shift once interdependencies are accounted for, as shown in **Figure 7. 6A**. The composite weights reflect a slight increase in the social dimension (18%) and a slight decrease in the environmental dimension (3%) compared to their direct weights. These results align with insights from the influential relation map (see **Figure 7. 3** and **Figure S.4** in Section 7.7.2, S1), where the social dimension, acting as an effect factor, is more reactive and influenced by other dimensions. This dependency contributes to its increase in composite weight, indicating its responsiveness within the system. In contrast, the environmental dimension, identified as a cause factor, influences other dimensions more than it is influenced, leading to a slight reduction in its composite weight. These shifts emphasize that interdependencies affect dimensions differently based on their roles as either dependent or influencing factors, highlighting the need for careful consideration of these roles in the decision-making process.

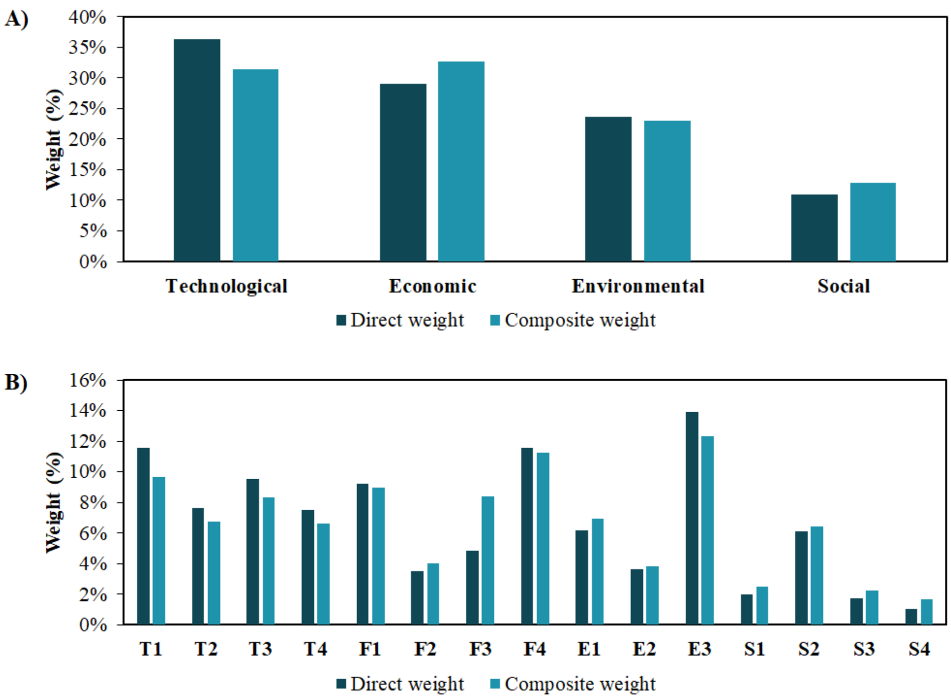

Figure 7. 6. Direct and composite weights in cluster 3 for (A) the four dimensions and (B) the assessment indicators.

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Regarding individual indicators, F3 (OPEX) and S4 (level of aesthetic acceptability) present the highest variation (73% and 58%, respectively), followed by S3 (local employment) and S1 (operational complexity, while most other indicators show limited variation 2%-17%. This greater variation in the social dimension reflects their inherent interconnectedness with other dimensions.

The Wilcoxon non-parametric test, together with other descriptive statistics, were applied to assess the significance of the differences between direct and composite weights [43,44]. The test resulted in a *p-value* of 0.8, indicating no significant difference between the two sets of weights, supporting the conclusion that while interdependencies reduce variability, they do not significantly alter the relative importance of the criteria. This lack of significant difference suggests that stakeholder preferences remain stable even after considering interdependencies, which helps maintain consistency in decision-making priorities.

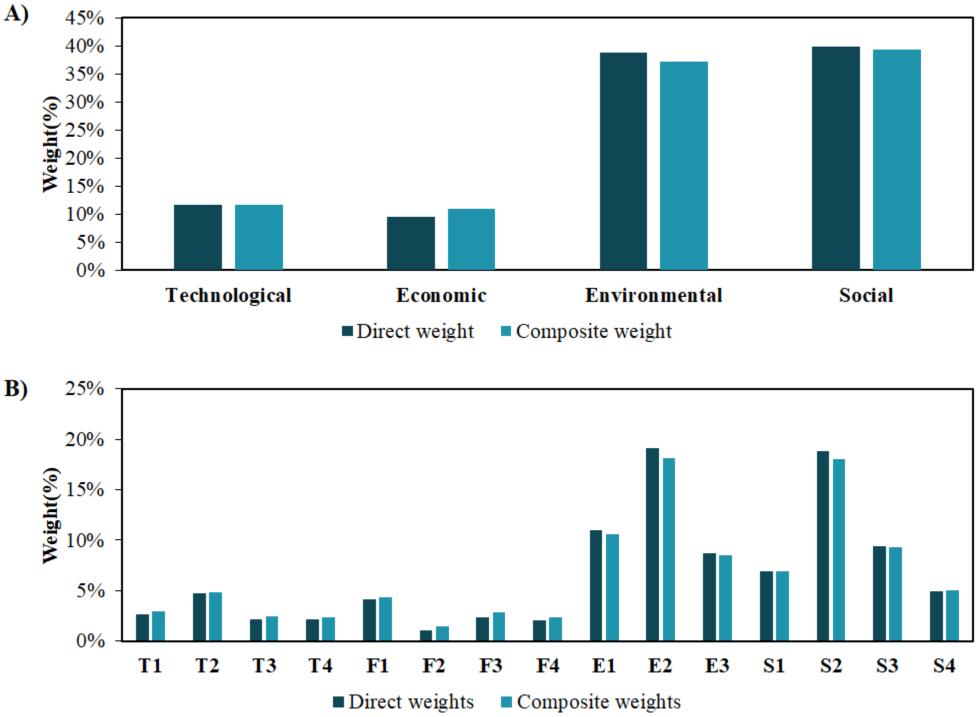

Figure 7. 7. Direct and composite weights in cluster 1 for (A) the four dimensions and (B) the assessment indicators.

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Regarding the dispersion of individual weights, the integration of interdependencies resulted in a decrease in S.D. across all four dimensions in Cluster 3 (2%-7% decrease), as well as in cluster 1 and cluster 2 (cluster 1: -9%-7% variation, cluster 2: 0%-41% decrease). This reduction in weight variability suggests a more consistent representation of stakeholder preferences when interdependencies are considered, which can streamline the prioritization process and enhance the alignment of decision-making outcomes.

The impact of integrating interdependencies varies across clusters, depending on the strength of the interdependencies and the original direct weights assigned. This highlights the importance of considering both direct priorities and the interconnected nature of criteria when forming sustainability strategies. Note that due to the use of the same influence matrix in the calculations of the composite weights, the difference between the two sets of weights is primarily due to the interdependency of the weights. Overall, the results suggest that while interdependencies refine the weight distribution, direct weights are the dominant factors, with interdependencies playing a secondary role. It is important to highlight that in this context, clustering preferences among stakeholders exerts a more substantial effect on outcomes than interdependencies alone. Detailed results for the three clusters, including the statistical analysis, are available in Section 7.7.2 (see Section S3).

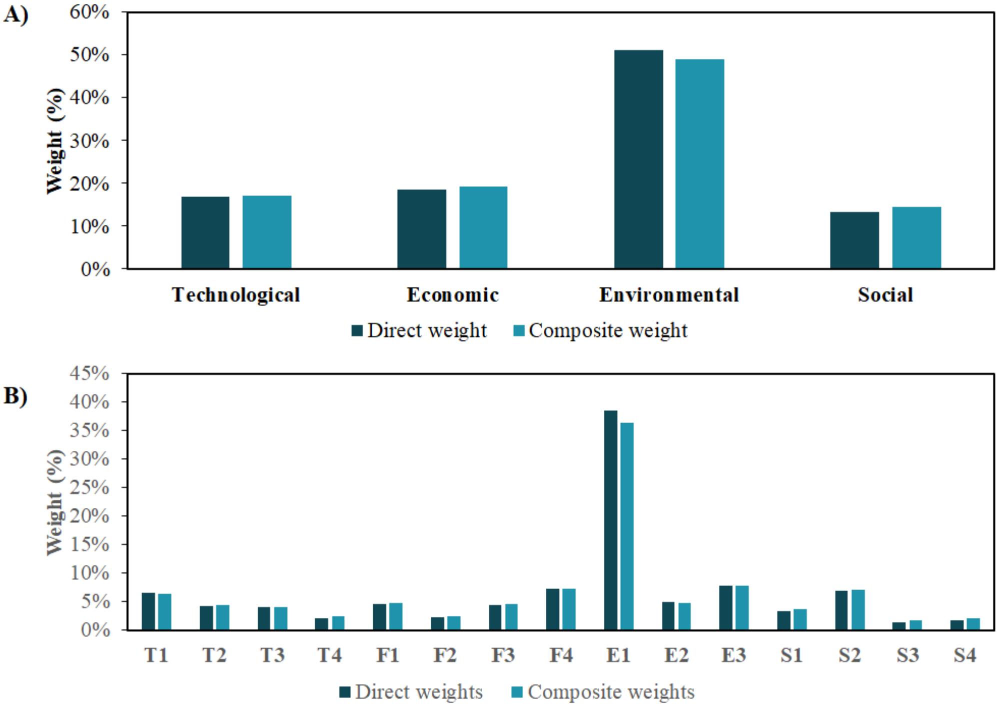

Figure 7. 8. Direct and composite weights in cluster 2 for (A) the four dimensions and (B) the assessment indicators.

7.4.5. Performance scores: ranking of alternative scenarios

Figure 7. 9 presents the rankings of alternatives with their φ *scores* according to the priorities of each group (cluster). The comparison of scenario rankings across clusters using direct weights (**Figure 7. 9A**) and composite weights (**Figure 7. 9B**) reveals how preferences shift based on the stakeholder priorities and the performance of each scenario in relation to the sustainability dimensions.

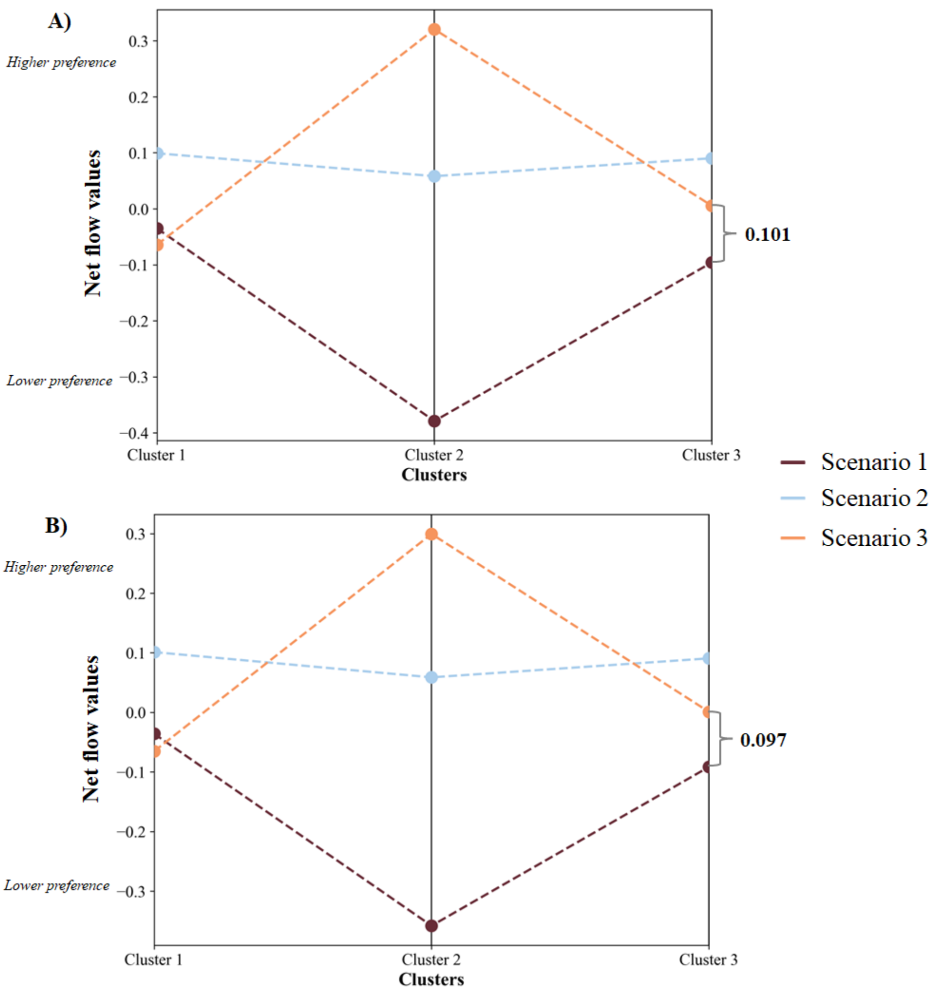

Figure 7. 9. Comparison of scenario rankings across clusters using direct weights (A) and composite weights (B). The dashed points represent the net flow values of three scenarios (scenario 1, scenario 2, scenario 3) across three clusters. Each dashed line how the rankings of three scenarios change across the clusters. Higher net flow values indicate a stronger preference.

For cluster 1 (social and environmental advocates), scenario 2 is the most preferred, followed by scenario 1, with scenario 3 being the least preferred. While scenario 1 performs better in one of the social indicators (operational complexity) compared to scenario 2, its higher environmental impact (carbon dioxide emissions and human toxicity) explains why it ranks below scenario 2. Note that scenarios 2 and 3 perform similarly in terms of social indicators.

For cluster 2, scenario 3 is the most preferred, followed by scenario 2, with scenario 1 ranked last. Scenario 3 presents the lowest environmental impact in two out of three indicators (carbon dioxide emissions and human toxicity), which aligns perfectly with the sustainability priorities of this cluster. Scenario 2 ranks second due to its balanced performance in the technological and environmental dimensions. Scenario 1 performs the worst in 2 out of 3 environmental indicators (with the highest emissions and poor water footprint), explaining why it is the least preferable for this environmentally driven group.

For cluster 3, scenario 2 is the most preferred, followed by Scenario 3, with Scenario 1 ranked last. Scenario 2 is preferred because of its technological performance, maximizing water production with the lowest OPEX and levelized cost of water. These factors align well with the priorities of technology-driven stakeholders, who focus on achieving high operational efficiency and cost-effectiveness. Scenario 3 ranks closely behind due to its better environmental performance and moderate economic performance, which explains why it is not as highly rated as scenario 2. Scenario 1, despite having lower CAPEX, ranks last because it underperforms in terms of profitability, making it less attractive to this cluster. Detailed results for the performance scores across three clusters are available in Section 7.7.2 (see Section S4).

These results highlight the importance of considering clusters when analysing sustainability preferences. The variations in preferences across the clusters reflect how different groups prioritize social, environmental, technological, and economic factors, which should be integrated into decision-making to ensure that solutions align with diverse stakeholder concerns.

When comparing the rankings using direct and composite weights (**Figure 7. 9A** and **9B**), the overall ranking order of the scenarios remains unchanged across the clusters, indicating that the ranking order of scenarios is stable despite the incorporation of interdependencies. However, negligible shifts in the net flow values (φ scores) are observed when interdependencies are considered. In cluster 1 and cluster 2, there is no change in the preference rankings between direct and composite weights. This suggests that in these clusters, the interdependencies among criteria have a minimal effect on altering the relative importance of the scenarios. In cluster 3, however, the gap between scenario 1 and scenario 3 narrows by 8% when composite weights are applied, indicating that interdependencies influence the results more strongly in this cluster. While the ranking order remains the same, this reduction in the gap shows that the interdependencies make scenario 1 more competitive with Scenario 3 in terms of preference.

Although, in this case study, the variation due to interdependencies does not significantly alter the final rankings, it demonstrates that interdependencies can influence the decision-making process, particularly when the criteria weights are sensitive or when scenarios have close net flow values.

7.4.6. Sensitivity analysis

Sensitivity analysis was conducted to investigate the extent to which variations in the criteria's composite weights impact the ranking results of the evaluated scenarios. Specifically, the analysis focused on perturbing the interdependency weights between the criteria, as derived from the DEMATEL method, to examine whether these changes would lead to different ranking outcomes.

The sensitivity analysis involved systematically altering the interdependency weights while keeping the BWM weights fixed, as listed in **Table S6** of Supplementary Information II. For each criterion, the interdependency weights were perturbed individually within a discrete range of integer values from 0 to 10, aligning with the influence scale defined by the DEMATEL method. This process ensured that the sensitivity analysis isolated the effect of interdependency weights on the composite weights while maintaining the integrity of the BWM weights. The modified PROMETHEE II method was then applied to each perturbed weight set to compute new rankings for the evaluated scenarios. This structured approach allowed for a comprehensive evaluation of how the interdependencies between criteria influence the decision-making process.

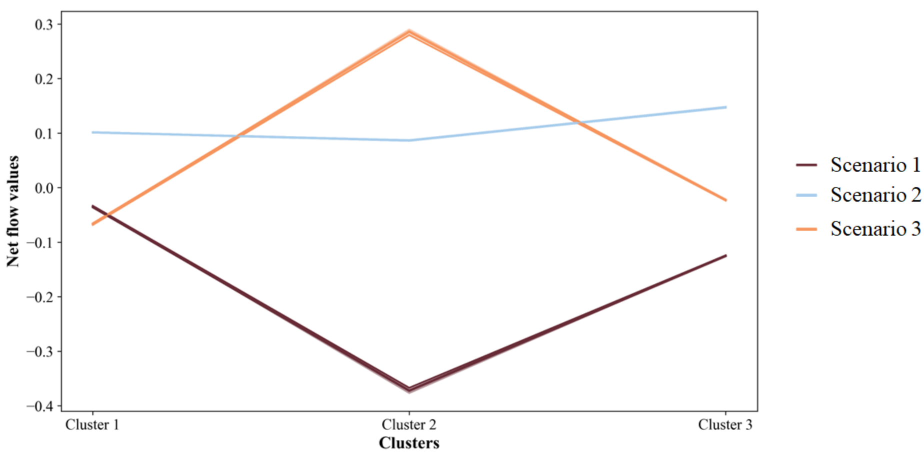

Figure 7. 10. Sensitivity analysis of interdependency weights across clusters.

The sensitivity analysis demonstrates that despite variations in the interdependency weights, there is no significant change in the final net flow values across the three clusters for the different scenarios (see **Figure 7. 10**). This indicates that, while the interdependencies do contribute to the composite weight calculation, their influence is not strong enough to alter the rankings or shift the net flow outcomes between scenarios. The stability of the results highlights that the direct weights, derived from the BWM method, are the primary determinant of the composite weight. The interdependency weights have a more moderate effect and do not override the influence of the direct weights and other key factors in the decision-making process.

Additional parameters that could impact scenario rankings were assessed to evaluate sensitivity further. This supplementary analysis (detailed results in Section 7.7.2, S4) applied thresholds of 10% for preference parameter *q* and 15% for preference threshold *p* based on the lower criterion scores. In Cluster 1, there was a slight change in net flow values for both composite and direct weights, though not substantial enough to alter the final ranking of scenarios. In Clusters 2 and 3, no variation in net flow values was observed. Overall, the results indicate that performance scores remain stable and are not sensitive to these threshold adjustments.

7.5. Discussion

This study introduces a novel integration of BWM and DEMATEL to incorporate the interdependence among decision criteria in sustainability assessments. The application of this combined methodology allows for a better understanding of the interrelationships between criteria, leading to more informed decision-making. By reflecting both the direct importance of each criterion and their interdependencies, this approach adds an extra layer of depth to traditional MCDM processes, offering more robust insights into how criteria mutually influence one another.

The interdependencies revealed through DEMATEL provide valuable insights into how different criteria impact each other, which traditional models often overlook. These relationships were reflected in slight shifts in weight distribution, particularly in the social and environmental dimensions, when interdependencies were considered. However, the numerical impact on final rankings was limited, demonstrating that interdependencies can refine weights but may not significantly alter decision outcomes in cases where rankings are less sensitive to such changes.

The results indicate that changes in weights due to differing stakeholder priorities had a more significant impact on rankings than interdependencies. This underscores the importance of considering stakeholder clustering in participatory evaluations. Aggregating all stakeholder inputs into a single analysis may oversimplify diverse perspectives, potentially leading to less nuanced decision-making insights. Group weighting through hierarchical clustering enhances inclusivity by aligning the final ranking more closely with distinct stakeholder priorities. In participatory settings, interdependencies may be more valuable for raising awareness about complex relationships between criteria than for directly influencing ranking outcomes. Conversely, in single-stakeholder or limited-participant settings, interdependencies may play a more substantial role in shaping weights and decision outcomes. This distinction highlights the need to carefully consider the context when deciding whether to incorporate interdependencies into the decision-making process, a critical insight for participatory multicriteria evaluations.

While BWM-DEMATEL enriches the analysis by integrating interdependencies, its application has practical limitations [45]. For instance, DEMATEL requires $n(n-1)$ comparisons (e.g., 210 pairwise comparisons for 15 indicators) [45], compared to BMW's simpler structure ($2n-3$ comparisons) [15], makes it time-intensive and may discourage broad stakeholder participation under tight time constraints. Compared to DEMATEL-ANP, DEMATEL-BWM simplifies the process by requiring fewer pairwise comparisons, making it more practical for participatory contexts (non-expert stakeholders). However, this simplicity comes at the cost of capturing feedback loops, which ANP handles more comprehensively [23]. While DEMATEL-ANP may offer deeper insights, its complexity and high demands make it less real-world applicability.

Due to the complexity of the method (high number of pairwise comparisons needed) and time constraints, only one decision-maker completed the DEMATEL survey. This reliance on a single expert raises concerns about potential biases, as the perception of interdependencies can vary significantly across stakeholders. Defining the degree of interdependencies accurately is challenging and can lead to subjectivity in the results, as expert judgments may introduce biases or oversimplifications. In an ideal situation, each stakeholder should make judgments on the direct weights and the interdependencies in criteria and combine them to indicate the composite weights. This simplification could explain the relatively small differences in the criteria weights observed.

The timing of conducting the DEMATEL survey can play a critical role in capturing accurate interdependencies among criteria. Subjective reasons such as limited knowledge can decrease the quality of judgment information in the DEMATEL [45]. Stakeholders' understanding of interdependencies often deepens as they engage with the project, which can refine their judgments over time [33,46,47]. Typically, the weighting process is conducted mid-project, with findings presented toward the end. In this study, the survey was repeated with an expert after significant project engagement, aiming to assess potential differences that might arise as stakeholder knowledge matures. The proposed BWM-DEMATEL process, hierarchical clustering and the ranking of the alternative scenarios were repeated, and all the results are available in Section 7.7.2 (see Section S5). It is observed a significant difference in the relationships among indicators, and the composite weights changed from 0% to 43%. However, the final ranking of the alternative scenarios across the different clusters remained the same. This analysis confirmed the hypothesis that understanding interdependencies changes during the project, and this can refine judgments. Future applications could benefit from strategically timing interdependency assessments or conducting iterative rounds to capture evolving stakeholder knowledge more accurately.

The outcomes of the interdependency analysis are influenced by the chosen set of indicators and their placement within the cause-effect groups (e.g., quadrants in the influential relation map, **Figure 7. 3**). Indicators in quadrants I (cause group) and II (effect group) typically exhibit stronger direct relationships and feedback loops. If more indicators had been positioned in these quadrants, the changes in weights due to interdependencies might have been more pronounced, further refining the evaluation process.

Future research should explore alternative methods or algorithms that can incorporate interdependencies while reducing the complexity of pairwise comparisons. Hybrid approaches combining the simplicity of DEMATEL-BWM with iterative feedback mechanisms from ANP could balance practicality and accuracy. Workshops could be used to both raise awareness about interdependencies and enhance data quality by fostering collaborative discussions among stakeholders. Furthermore, system dynamics modeling could offer a more objective way to assess interdependencies, addressing current limitations related to reliance on expert judgment. Models addressing the directionality of influence between criteria could offer more precise insights into how changes in one criterion affect others (positive or negative) [48]. Moreover, conducting analyses under uncertain conditions—such as using fuzzy logic or stochastic models—may further enhance the robustness of this approach in handling real-world complexities [49].

7.6. Conclusions

This study addresses limitations in traditional multi-criteria decision-making methods, which often assume independence between evaluation criteria, leading to less representative decision-making. By integrating the Best-Worst Model and the Decision-Making Trial and Evaluation Laboratory technique, we propose a novel weighting method that considers both the direct importance of each criterion and the interdependencies between them. This weighting method was applied to the sustainability assessment of desalination and brine treatment systems. The results revealed that while interdependencies provide valuable insights into the relationships between criteria, their numerical impact on the final rankings is limited in cases where decision outcomes are less sensitive to weight variations. Conceptually, however, incorporating interdependencies offers a deeper understanding of the decision problem and establishes a more comprehensive evaluation framework.

The findings indicate that interdependencies between evaluation criteria hold a moderate effect in multi-stakeholder contexts (participatory approaches), where clustering stakeholder preferences has a more pronounced impact on rankings than interdependencies alone. Instead, in single-stakeholder or limited-participant settings, accounting for interdependencies may have a more significant impact. Future research should explore methods to simplify pairwise comparisons while incorporating directional influences among criteria, with applications in both collaborative and single-stakeholder decision-making environments.

7.7. Supplementary information

7.7.1. Supplementary Information I

See documentation.

7.7.2. Supplementary Information II

See documentation.

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8

Conclusions and Outlook

The thesis started in **Chapter 1** by setting the stage for the transition from traditional, linear desalination to resource recovery systems, positioning this shift as a critical example of sustainable development in practice. While technological innovation is a key driver of this transition, it also brings significant economic, environmental, and social challenges. These challenges demand a holistic approach that incorporates non-technical aspects early in the process design stage. Questions such as how to effectively combine innovative technologies, how to tailor solutions to local needs, and how to evaluate these solutions for sustainability within specific contexts are central to this work.

From **Chapter 1**, the importance of interdisciplinary perspectives, collaborative methods, and stakeholder participation were highlighted. Stakeholders from diverse backgrounds—including policymakers, industry representatives, and community members—must work together to clearly define problems, co-design solutions, and evaluate their sustainability in ways that align with both local priorities and global sustainability goals.

To support these practices, a tailored sustainability assessment (SA) framework for integrated desalination and brine treatment systems is provided, designed to address the specific challenges of multi-objective systems. By combining value-sensitive design (VSD), life cycle analysis, levelized cost analysis, and multi-criteria decision-making methods, the framework operationalizes participatory and context-sensitive assessment. This integration bridges disciplinary boundaries and operationalizes stakeholder inclusion in both data-rich and data-scarce contexts.

This chapter reflects on the key scientific insights from the thesis and their relevance to the field of resource recovery. It also discusses the main limitations of this work and outlines future directions for advancing methodologies in the sustainability assessment of resource recovery systems.

8.1. Main learnings

The extensive review in **Chapter 2** revealed significant gaps in existing sustainability frameworks for integrated systems, particularly in the context of desalination and brine treatment. Current assessment tools lack the transparency needed for replicable and accountable decision-making, fail to adopt a comprehensive approach, and often overlook critical social dimensions, including stakeholder involvement. These gaps limit their effectiveness in evaluating complex systems like those integrating resource recovery.

To address these gaps, the key learnings from this thesis are framed around four critical characteristics essential for robust and meaningful sustainability assessments:

comprehensiveness, transparency, stakeholder participation, and interdisciplinarity and transdisciplinarity.

Comprehensiveness ensures that assessments account for the full spectrum of impacts, from technical feasibility to societal relevance. Transparency is crucial for establishing trust, ensuring accountability, and promoting reproducibility in methodological choices and decision-making processes. Stakeholder participation incorporates diverse perspectives, fostering inclusivity and aligning decisions with real-world needs and concerns. Finally, transdisciplinary approaches integrate knowledge across disciplines, bridging the gap between technical solutions and societal priorities.

These four characteristics emerged as fundamental for improving the relevance and effectiveness of sustainability assessments in the context of integrated resource recovery systems. The following sections delve into each of these pillars, reflecting on the insights gained throughout this thesis and their broader implications for advancing sustainability practices.

8.1.1. Stakeholder Participation

In an era of rapid technological progress and growing awareness of sustainability challenges, the idea of participatory design and assessment feels like a natural fit for some. The simple idea of involving more people in the design and evaluation process can lead to solutions that are more inclusive, tailored, and responsive to real-world needs [1,2]. These approaches align with principles of fairness, inclusivity, and usability, holding the promise of more equitable and impactful technological advancements [1].

However, while participatory approaches sound like a democratic approach to shaping our future, their implementation is far from straightforward. They raise questions about justice, accessibility, and power dynamics, particularly in relation to skills, education, and time. The saying *"time is money"* fits perfectly here. Participation requires individuals to invest their time, often without financial compensation. For some, this investment can come at a significant cost, as the hours spent contributing to a participatory project in unpaid involvement take time away from paid work. Another critical factor is the privilege of time itself. Not everyone has the luxury of setting aside hours for participatory processes, even relevant professionals. Additionally, individuals with higher education or strong communication skills may need less preparation time and often exert greater influence during discussions. This creates a selection bias, as those who can afford to contribute are not necessarily representative of the broader community, undermining the inclusivity that participatory design seeks to achieve.

As discussed in **Chapter 2**, the level of stakeholder participation in a project can vary widely depending on factors such as power, capacity, interest, and ability to engage. Effective participation ranges from simply informing stakeholders to full collaboration, where they take an active role in defining problems, analysing options, and co-creating solutions. There is no optimal level of participation. The ideal level of engagement depends on the specific project [3], but early and continuous involvement is vital to fostering trust, transparency, and democratization. Participation that begins at the problem-definition stage helps ensure that solutions reflect community needs and values, promoting more relevant and accepted outcomes.

Chapter 7 illustrates the complexities and benefits of participatory approaches, particularly when incorporating advanced methods like interdependency analysis. Knowledge, time, and skills proved to be pivotal factors in ensuring the success of these approaches. Specifically, the complexity of the DEMATEL method and the time constraints limited stakeholder participation to a single decision-maker. This reliance on a single expert highlighted potential biases, as perceptions of interdependencies often vary among stakeholders.

Additionally, the time spent participating significantly impacts the quality of the outcomes. Stakeholders often gain a deeper understanding of interdependencies as they engage with the project, which can enhance their judgments over time [4–6]. This was evident in the repeated survey conducted during the later stages of the project, which demonstrated how growing knowledge can improve the accuracy of assessments.

This underscores a crucial benefit of participatory processes: their ability to enhance stakeholders' understanding of the problem and proposed solutions. This enables more informed feedback and promotes more robust evaluations. At the same time, these findings underscore the importance of carefully structuring participatory approaches. Allowing sufficient time for stakeholder learning, using iterative rounds to refine inputs, and employing strategies to manage complexity are crucial for achieving meaningful engagement.

Participation is far from a simple or universal solution. It demands thoughtful implementation, creativity, and a genuine commitment to making design processes more inclusive and representative. Building trust among stakeholders, reducing conflicts, and clearly communicating the benefits of participation are vital for fostering collaboration. By balancing ambition and practicality, participatory approaches can create more inclusive, representative, and impactful outcomes, ultimately contributing to sustainable solutions that align with diverse needs and priorities.

This thesis shows that meaningful participation is possible even when direct engagement is limited by embedding stakeholder values through VSD and structured preference modelling. These pragmatic strategies offer a path toward more inclusive and value-sensitive decision-making in resource recovery systems.

8.1.2. Comprehensiveness

The success of desalination and resource recovery projects depends not only on evaluating technical, economic, and environmental dimensions but also on accounting for the broader context in which these systems operate. This thesis advances a more comprehensive approach to sustainability assessment, one that considers regional priorities, local market conditions, institutional constraints, and the diversity of stakeholder values and capabilities.

Chapter 4 is an example of this shift by applying VSD to structure decision-making scenarios that reflect local trade-offs and priorities. Instead of relying on static optimization, the analysis revealed how system performance varies significantly depending on contextual variables like waste heat availability and societal goals.

Analysing these trade-offs in dialogue with stakeholders fosters informed decision-making and context-specific solutions that balance competing priorities. A key challenge lies in aligning global sustainability principles with region-specific needs shaped by factors such as climate, economy, and cultural norms. Tailoring systems via VSD to these local contexts promotes solutions that are not only effective but also embraced by the communities they serve.

Understanding trade-offs extends beyond immediate feasibility. It is fundamental for ensuring long-term viability and adaptability, enabling systems to remain resilient in the face of evolving challenges. A good example is the use of waste heat to cover the thermal requirements of desalination and resource recovery plants, as illustrated by the technical scenarios in **Chapters 4-7**. While utilizing waste heat may be a viable solution today, it may not align with the carbon-free energy systems of the future. Building on such principles while seeking truly sustainable, long-term alternatives is essential for lasting success.

Chapter 7 further underscores the importance of comprehensive evaluation frameworks. While incorporating interdependencies among criteria provides a deeper understanding of decision problems, their numerical impact on final rankings is often limited in multi-stakeholder contexts, such as participatory approaches, where clustering stakeholder preferences plays a more decisive role. By grouping stakeholder perspectives, decision-makers gain valuable insight into the distribution of opinions and priorities, enabling more nuanced and representative analyses. These findings from **Chapter 7** underscore the importance of incorporating stakeholder clustering into participatory evaluations to achieve a comprehensive understanding of complex decision-making problems.

The thesis redefines comprehensiveness in sustainability assessment by integrating social, economic, environmental, and contextual dimensions into one coherent framework, enabling solutions that are resilient, context-specific, and stakeholder-aligned.

8.1.3. Transparency

Transparency is not a static concept in sustainability assessments. It shifts in meaning and importance at different stages of the process. By openly addressing the *"how"* and *"why"* of methodological and participatory decisions, sustainability assessments can ensure their results are both credible and actionable. Without clear communication about who is included, why, and how their input is used, participatory processes risk disruptive stakeholders and undermining their legitimacy.

Methodologically, transparency is key to avoiding misinterpretation and ensuring that studies can be reliably replicated. As highlighted in **Chapter 2**, the desalination literature often prioritizes the development of new assessment methodologies, overlooking the importance of documenting key decisions, such as indicator selection or multi-criteria decision-making methods. This gap not only limits the reproducibility of studies but also risks producing results that are incomplete or misleading [7].

This thesis tackled these challenges by embedding transparency into every stage of the assessment process (**Chapters 3-7**), explicitly documenting all methodological steps, assumptions, and rationales. It shows how methodological choices, such as functional unit definition or assumptions about waste heat (see **Chapter 6**), can substantially alter results, reinforcing the need for full transparency in modelling decisions to avoid misleading conclusions. This emphasis on transparency supports not only credibility but also reproducibility and future improvement, particularly relevant given the open-source nature of the software developed in this thesis (**Chapters 3**).

8.1.4. Interdisciplinarity and Trans-disciplinarity

This thesis is an example of an interdisciplinary effort, integrating tools and methods from engineering, economics, environmental sciences, and social sciences to assess complex desalination and resource recovery systems: value-sensitive design (**Chapter 4**), economic evaluation with levelized cost analysis (**Chapter 5**), and environmental assessment with life cycle analysis (**Chapter 6**). Their integration into a multi-criteria decision-making process in **Chapter 7** enabled a more holistic evaluation than any single-discipline approach could achieve. Together, these methods provide a robust analytical foundation for addressing sustainability challenges.

However, the work goes beyond interdisciplinary integration. It embraces a transdisciplinary orientation, recognizing that sustainability problems cannot be solved by disciplinary knowledge alone. In particular, trans-disciplinarity here involved identifying shared values, navigating trade-offs, and proposing context-specific, socially robust solutions. This was operationalized through the participatory framework outlined in **Chapter 2** and applied in decision-making in **Chapter 7**, even though stakeholder input was simulated or drawn from existing studies. In addition, this thesis is among the first to operationalize VSD for desalination and brine treatment systems in **Chapter 4**, offering a replicable method to align technical system design with societal values, co-producing knowledge.

A key insight is that no single framework can be universally applied—sustainability assessments must evolve with the context, stakeholders, and system complexity. The work highlights that methodologies from other sectors are useful starting points, but must be reconfigured through engagement with real-world stakeholders. This confirms the thesis's core message: sustainability challenges demand both integrated use of interdisciplinary methods and participatory, inclusive design logic.

Finally, a key principle emerges from these findings: tools are advisors, not decision-makers. In resource recovery, where uncertainty is high and methods are assumption-sensitive, outcomes can be misleading if tools are used without critical interpretation. Blindly following tool-generated rankings or metrics is risky. Decision-makers must critically assess results, understand trade-offs, and engage in collaborative dialogue to ensure solutions are not only technically sound but also socially just and contextually relevant. This thesis demonstrates that robust, fair, and forward-looking decisions require both interdisciplinary rigor and transdisciplinary inclusion.

By bridging engineering, economics, social sciences, and environmental modelling, the thesis delivers a rare example of operationalizing transdisciplinary logic in sustainability assessments, demonstrating that robust, context-aware outcomes demand methodological integration and social engagement.

8.2. Insights and impacts of this research

8.2.1. Bridging policy, society, and technology for sustainable progress

The findings of this thesis underline the critical role of societal values and policy in shaping the adoption of sustainable desalination and resource recovery systems. Technological advancements alone are insufficient if they fail to address societal priorities such as equitable access to resources, affordability, and environmental protection.

Policies play a pivotal role in bridging these gaps by integrating stakeholder perspectives, ensuring that solutions are not only technically and economically viable but also socially and ethically aligned. For instance, engaging diverse stakeholders can help policy-makers identify context-specific needs and barriers, fostering more inclusive and democratic decision-making. Moreover, targeted policies, such as subsidies for recovered materials, can address economic challenges and promote market development. By balancing technological innovation with societal and ethical considerations, this work offers a roadmap for policy frameworks that support sustainable, equitable, and contextually relevant solutions.

8.2.2. Implementation of resource recovery systems in desalination: How close are we?

Desalination has made important steps toward the full-scale implementation of resource recovery systems, with advancements over the past two decades driven by pilot plants [8–10] and EU-funded projects aimed at developing and optimizing technologies for brine treatment and the recovery of valuable products (see Water Mining project, Searcular Mine). These projects have offered valuable knowledge on managing materials, water, energy, products, and components to preserve their maximum intrinsic value [11]. This thesis builds on these foundations, using such projects as case studies to evaluate systems and develop comprehensive methodologies for sustainability assessments.

Furthermore, these initiatives have actively engaged relevant stakeholders, fostering a dialogue about practical social, environmental, and economic challenges. By involving industry leaders, policymakers, and local communities, these projects have laid the groundwork for scaling up resource recovery in desalination. While foundational work and dialogue are underway, significant technical, regulatory, and market challenges still hinder full-scale adoption.

The most significant limitation lies in aligning the recovered products with market adoption and demand. Are industries prepared to embrace these new materials? It's still unclear! Uncertainty surrounds the integration of resource recovery systems into existing value chains. For example, feedstock supply uncertainty, the lack of established markets for emerging materials, and limited coordination across industries and policymakers are critical barriers to scaling these systems.

Another major hurdle is the policy landscape. While progress has been made in raising awareness and initiating dialogue, the regulatory frameworks required to support resource recovery systems are still in development. Clear policies and incentives are needed to bridge the gap between innovation and widespread adoption.

The scenario analysis showed that no single configuration dominates across the sustainability dimensions. For instance, water-prioritizing systems performed best when waste heat was available, while other configurations were more suited to chemical recovery or economic feasibility under specific regional conditions. These findings underscore the need to align system design with local priorities—what works in one context may be ineffective or undesirable in another.

Economic feasibility plays a central role in determining whether resource recovery systems can be successfully implemented. However, decisions about material recovery should not be reduced to purely economic considerations. Society's willingness to pay for recovery efforts, driven by values like environmental protection and resource efficiency, is equally crucial. Recovery systems must strike a balance between economic efficiency and broader societal priorities, including sustainability and equity.

In addition to these challenges, environmental performance must also guide implementation decisions. LCA results (**Chapter 6**) show that integrated resource recovery systems can outperform conventional desalination and salt production in key environmental metrics, particularly when multi-product recovery is included. This highlights that their adoption is not only technically and economically promising but also environmentally justified.

Addressing these socio-technical and environmental barriers is essential for accelerating the uptake of resource recovery systems in desalination. While this thesis primarily focused on assessing technical configurations and methodologies, external factors such as market dynamics and policy readiness are also critical considerations for specific business cases.

8.2.3. Breaking boundaries: applying insights beyond desalination

This study goes beyond desalination, offering methodologies and frameworks that can be applied across various resource recovery systems, regardless of the feedstock or end products. While integrated sustainability assessment frameworks exist in fields like biorefineries, this thesis shows that their direct transferability is often limited. These existing approaches offer valuable methodological starting points and insights; however, they must be carefully adapted to account for the unique characteristics of water systems, particularly the public service role of desalination and region-specific societal values.

The methods developed in this thesis, such as integrated VSD and sustainability assessments (**Chapters 2&4**), the novel economic cost allocation methods (**Chapter 5**), and the revised life cycle assessment methodologies (**Chapter 6**), were designed with these contextual requirements in mind. For example, **Chapter 6** provides a robust approach for evaluating the environmental performance of multi-product systems, making them applicable to other contexts. Similarly, **Chapter 5** presents a structured and flexible framework for calculating fair selling prices and assessing the financial viability of systems recovering multiple products or utilizing waste as feedstock (e.g., brine, wastewater sludge), with a focus on determining a fair selling water price.

While desalination served as the primary case study, the contributions of this thesis provide a broader roadmap for adapting existing frameworks to new contexts. By demonstrating how to tailor generic methodologies to the specific challenges of integrated resource recovery systems, this research contributes both practical tools and a transferable assessment logic for sustainability across diverse domains.

8.2.4. A tool for advancing resource recovery research and practice

The software developed in this thesis addresses a critical gap in the field of desalination and resource recovery by offering an open-access, integrated platform for modelling and analysis (see **Chapter 3)**. By providing a freely accessible, modular platform, it fosters transparency, reproducibility, and collaborative development, key principles for advancing sustainability research. The tool is designed not only for researchers but also for practitioners, enabling users without specialized expertise to explore system performance and assess early-stage design options. Its flexibility and user-friendliness make it suitable for diverse applications, from scenario screening to system integration planning. Importantly, its open structure invites future adaptation and improvement, allowing others to refine models, incorporate new technologies, and tailor analyses to evolving regional and technical needs. In this way, the software serves as both a practical tool and a foundation for continued innovation in the field.

8.3. Limitations

While this study advances methodologies for assessing sustainability in desalination and resource recovery systems, several limitations should be noted:

- *Specific socio-economic context:* The methodologies developed in this study are not tailored to a specific socio-economic context. The problem statements and values analysed were derived from prior literature. The problem statements used in developed methodologies were inspired by real-world scenarios and built upon previous experience; however, they may limit their direct applicability.
- *Stakeholder engagement:* The stakeholder values used in this thesis were based on previous research rather than direct engagement methods, such as interviews,

surveys, or workshops. While these values are robust in the context of prior studies, direct interaction with stakeholders would enable the capture of a broader range of perspectives and the validation of these values for specific applications. Incorporating participatory workshops and focus groups could significantly enhance the robustness of analyses.

- *Validation of technical scenario design:* The technical scenarios in **Chapter 4** were designed based on stakeholder values, but further rounds of empirical validation with stakeholders are necessary to assess the practical implications and feasibility of the proposed designs. Future work could involve multiple validation rounds, including stakeholder workshops and feedback sessions, to refine these scenarios.
- *Software:* The integrated software tool developed in this thesis served as the primary source of technical and economic performance data used throughout the assessment. While the software was validated through comparisons with literature (e.g., specific energy consumption) and further reviewed by technology experts and suppliers (e.g., specific energy consumption, recovery rates, product quality), discrepancies remain for some technologies, particularly where data is scarce, or model simplifications were required. These deviations in energy use or system behaviour may affect the accuracy of the assessments. These limitations are especially relevant for less mature processes or those that rely on estimated input values. Although the tool is suitable for scenario exploration and comparative evaluations, its predictive precision is constrained by these assumptions. Nevertheless, we believe that these limitations do not compromise the overall conclusions of this thesis, as the comparative and methodological insights remain valid across a range of potential values.
- *Assumptions in methodologies:* Many aspects of this research rely on assumptions, such as the stability of market conditions, market prices, technological performance under ideal conditions etc. These assumptions, while necessary for modelling, introduce uncertainties that need to be critically evaluated in real-world implementations.

8.4. Future work: what is important for the future

Integrating system dynamics for enhanced problem definition

A key limitation of this thesis is the reliance on problem statements derived from existing literature rather than specific socio-economic contexts. Future work could address this by incorporating system dynamics modelling, which excels at capturing long-term system behaviour, feedback loops, and the evolution of systems under varying conditions, such as policy shifts, market changes, and environmental dynamics.

This approach could enhance the methodologies developed in this thesis by modelling how resource recovery systems evolve in response to factors such as policy changes, market dynamics, and environmental conditions. For example, system dynamics could help identify trade-offs and unintended consequences by simulating feedback loops and long-term system behaviour. It could also improve early-stage decision-making by structuring problem statements in a way that captures interdependencies and interactions among technical, economic, and societal factors. Furthermore, its application in participatory modelling can enhance stakeholder understanding of system complexity, fostering trust in model outcomes and supporting collaborative decision-making [12]. By integrating system dynamics, future work could provide more robust and predictive insights, supporting more informed and adaptive strategies for implementing resource recovery.

Additionally, integrating system dynamics with decision-making methods could provide a more objective approach to assess interdependencies in **Chapter 7**, addressing current limitations related to reliance on expert judgment.

Integration of data envelopment analysis for scenario evaluation

Future work could extend the assessment of technical scenarios by integrating data envelopment analysis (DEA) with the MCDM methods applied in this thesis. While MCDM methods help structure preferences and rank alternatives based on stakeholder preferences, DEA offers a complementary way to assess the scenarios (system performance). DEA could evaluate how well each scenario transforms multiple inputs (e.g., energy, capital, emissions) into outputs (e.g., recovered resources, water), assigning a relative efficiency score from 0 to 1 [13]. This enables the identification of the most efficient scenarios and highlights the degree and direction of improvement for others. Future research should investigate whether combining MCDM with DEA can enhance the robustness of scenario selection. MCDM filters and prioritizes options based on value alignment, while DEA benchmarks their operational performance and effectiveness.

Extending the open-source platform

As an open-source platform, the software developed in this thesis also offers a transparent and adaptable foundation for future work. Researchers can build upon and refine the existing models by incorporating additional process units, expanding validation metrics, or adapting the tool to new contexts and technologies. This openness encourages collaborative improvement, supports reproducibility, and fosters broader application of the sustainability assessment methodologies developed here.

Validating the framework through diverse case studies

Conducting case studies in diverse socio-economic contexts is essential to validate the methodologies developed in this thesis. These studies could address specific challenges such as environmental trade-offs, the economic feasibility of recovery systems, and stakeholder engagement processes. For example, applying the frameworks in industrialized regions could explore their scalability and integration into established supply chains, while case studies in low-resource settings could highlight barriers to adoption and the need for tailored solutions.

A critical aspect for future validation is the role and quality of stakeholder participation. While this thesis proposed stakeholder participation in different stages in the SA (see **Chapter 2**) and integrates stakeholder values indirectly, real-world applications must assess how participatory approaches affect outcomes. Future research should explore how to operationalize the participatory steps outlined in **Chapter 2:** how to structure effective stakeholder groups, determine who should be involved, and assess whether participation leads to broadly accepted and socially relevant solutions. Key challenges include managing diverse interests, maintaining engagement over time, and ensuring the group remains representative and capable of co-producing knowledge, a core requirement for achieving the transdisciplinary goals of sustainability assessment.

By validating the framework across different settings and through richer forms of participation, future research can strengthen the framework's adaptability, legitimacy, and overall impact.

Supply chain transformation

Future work must focus on transforming supply chains to support the adoption of resource recovery systems. While the development of value chains is primarily the responsibility of the economic sector, science plays a crucial role in informing this process. Early assessments of the marketability and value chain development potential of recoverable resources are vital for ensuring that these systems are not only economically viable but also determine whether recovered resources can serve as viable commodities. Key factors, such as demand, logistics, consumer acceptance, regulatory frameworks, market supply potential, and application possibilities—often overlooked in scientific studies—must be systematically analysed to enable informed decisions and effective value chain integration.

Additionally, future research should analyse the ability to supply recovered resources in sufficient quantities to compete with conventional suppliers. Identifying which resources are more favourable for recovery requires understanding both existing market demand and the potential for creating new applications or markets for recovered products. Alongside optimizing recovery processes, research should also explore innovative uses for these materials. This effort would help prioritize resources that can be integrated effectively into existing value chains and support the broader adoption of resource recovery systems.

Addressing policy needs through research

Future research must bridge the gap between technological advancements and policy frameworks to accelerate the adoption of resource recovery systems. As technical innovations advance, they must be complemented by a deeper focus on marketization, regulatory alignment, and policy formulation. A critical bottleneck for implementation lies in ensuring competitiveness and creating dedicated markets for recovered resources supported by clear and enforceable legal frameworks.

Research should aim to identify how policies can foster market development, mitigate risks, and incentivize industries to adopt resource recovery technologies [14]. This includes examining mechanisms like subsidies, tax incentives, or penalties for non-compliance with circular economy principles. Moreover, collaborative efforts among researchers, policymakers, and industry stakeholders will be essential to create adaptable and context-specific policies that strike a balance between economic feasibility and environmental and societal goals. By aligning policy needs with technological capabilities, future work can ensure resource recovery systems become both practical and impactful.

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Nomenclature

AHP	Analytic Hierarchy Process
ANP	Analytic Network Process
BC	Brine concentrator
CAPEX	Capital Expenditure
CSP	Concentrate Solar Power
DCMD	Direct Contact Membrane Distillation
DEMATEL	Decision-Making Trial and Evaluation Laboratory
ED	Electrodialysis
EDBM	Electrodialysis With Bipolar Membranes
EFC	Eutectic Freeze Crystallization
EIA	Environmental impact assessment
ESM	Early-stage methodologies
ESS	Energy Self-Sufficiency
FD	Freeze desalination
FO	Forward Osmosis
FU	Functional Unit
GHG	Greenhouse gas
GOR	Gain Output Ratio
GRA	Grey relational analysis
HPRO	High-pressure Reverse Osmosis
IX	Ion Exchange
LCA	Life Cycle Assessment
MAUT	Multi-Attribute Utility Theory
MCDA	Multi-criteria decision analysis
MCDM	Multi-criteria decision making
MCr	Membrane Crystallizer
MD	Membrane Distillation
MED	Multi-Effect Distillation
MF-PFR	Multiple Feed Plug Flow Reactor
MLD	Minimal Liquid Discharge
MSF	Multistage flash
MVC	Mechanical Vapor Compression

NF	Nanofiltration
OARO	Osmotically Assisted Reverse Osmosis
OD	Osmotic Distillation
OPEX	Operating Expenditure
PROMETHEE	Preference Ranking Organization Method for Enrichment of Evaluations
PV	Photovoltaic
RES	Renewable Energy Sources
RO	Reverse Osmosis
SA	Sustainability Assessment
SAW	Simple Additive Weighting
Sc	Scenario
SDGs	Sustainable Development Goals
SEC	Specific energy consumption
SWRO	Seawater Reverse Osmosis
TCr	Thermal Crystallizer
TEA	Techno-economic analysis/assessment
TLR	Technology Readiness Level
TOPSIS	Technique for Order Preference by Similarity to an Ideal Solution
UF	Ultrafiltration
VSD	Value Sensitive Design
WH	Waste heat
ZLD	Zero Liquid discharge

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Φωτεινή και **Pelle** ήσασταν μια ευχάριστη προσθήκη στην ζωή μας στην Ολλανδία όχι μονο επειδή κάνατε και τον **Μιχάλη** να έρθει τόσες φορές. Φωτεινή είσαι ο άνθρωπος που με καταλαβαίνει φουλ. Άνοιξες την αγκαλιά σου από την πρώτη στιγμή. Σε ευχαριστώ. Άντε και στα δικά σου.

Το **αυτοκολλητάκι** μου. Ήσουν, είσαι και θα είσαι το αυτοκολλητάκι μου, ακόμα και αν δεν μιλάμε κάθε μερα. Είμαι πολύ περήφανη για εσένα, CEO της καρδιάς μου. Ευχαριστώ για όλη την στήριξη, που άκουγες με υπομονή το «δράμα» μου αλλά και την πρατκική βοήθεια (μου έδωσε μέχρι και τιμές για χημικά). Που ξέρεις μπορεί να ξανα-συνεργαστούμε στο μέλλον. **Ορφίκο** μου, ξέρω ότι κάθε φορά που ερχόσουν στο χωρίο μας ήταν με μισή καρδιά αλλά περνούσαμε υπέροχα. Ψαράκι, μπύρα και ινδικό, Ροδίκο και Αγγελούκος. What not to like? Ήταν το ψυχολογικό boost που χρειαζόμουν. Το υπόλοιπο μάχιμο team Θεσσαλονίκης, **Βιβή, Ίκαρος, Μαρια, Μιχάλης, Οδυσσέας**, ευχαριστώ που ξεσηκώνεστε για το ετήσιο εορταστικό σκ (χρόνια πολλά Ροδούλα), ακολουθείτε την τρέλα μου και δεν λείπετε από εκεί. Για όλες τις πρωτοχρονιές μας και όλες τις στιγμές που ζήσαμε όλα αυτά τα χρόνια.

Τις πελλές κυπραίες φίλες μου, **Αναστασία, Ελένη, Κική, Νάγια, Χριστιάνα**. Οι φάκτορες της απαφαλάτωσης. Όλα ξεκίνησαν μετά την διπλωματική μου στο μάστερ, σας τράβηξε αμέσως το θέμα περισσότερα και από εμένα. Έμαθα τόσα πολλά από εσάς. Πέρα από την πλάκα, ευχαριστώ για όλες τις μοναδικές στιγμές που περάσαμε και θα περάσουμε, εντός και εκτός του νησιού. Πάντα βοηθούσατε πολύ στο να παίρνω απόσταση από τα «προβλήματα» του διδακτορικού. Ευχαριστώ που τραγουδούσατε Pedro, Pedro, Pedro στο αεροπλάνο και το Κατερινάκι στους γκρεμούς στο Madeira.

Ευχαριστώ όλη την οικογένεια **Κτωρή&Κούννου** για την στήριξη. Στηριξατε τον τρελό επιστήμονα της οικογένειας με κάθε τρόπο. **Μάμα, παπά** ευχαριστώ για την υπομονή και την στήριξη όλα αυτά τα χρόνια σε οτι επιλογή και να έκανα. Που με κάνατε αυτό που είμαι σήμερα. **Κορίνα** και **Ελίνα** τα βίντεο σας βοήθησαν πολύ σε δύσκολες στιγμές ακόμα και αν δεν το ξερατε. Ανυπομονώ για το real bonding μας. **Άννα** για τη θετική σου ενέργεια και **Μιχάλη** για την στήριξη (σε όλα τα επίπεδα) με τον δικό σου τρόπο και που ανάλαβες την θέση recruiter, real estate κ.α.. Είσαι πρότυπο. **Georgia**, cheese and charm, είσαι η αδερφή που όλοι θα ήθελα. Όποτε χρειάζομαι κάτι είσαι εκει, ευχαριστώ. Είμαι πολύ περήφανη για αυτό που εξελίσσεσαι. Διάλεξε προορισμό για του χρόνου. Ευχαριστώ και την νέα μου οικογένεια, την οικογένεια **Γιάννη**, η φροντίδα σας είναι μοναδική.

Last but not least, που λένε και στο χωριό μου, μετά από τα παράπονα σου για το master thesis μου, ήρθε επιτέλους η στιγμή να σε ευχαριστήσω δημόσια, **Αγγελούκο** μου. Η αντοχή σου, η υπομονή σου, η αδιανόητη κατανόηση και η ανιδιοτελής στήριξη σου είναι αξιοθαύαμστα. Σου ανήκει μισό από το πτυχίο δικαιωματικά. Ήσουν βράχος δίπλα μου όλα αυτά τα χρόνια και σε ετοιμότητα να φύγουμε εκδρομή για να ξεσκάσω. Είσαι μοναδικος και είμαι πολυ τυχερή που σε έχω δίπλα μου. Σε θαυμάζω για όλα αυτά και για πολλά άλλα. Σε ευχαριστώ για όλα και σου υπόσχομαι ότι τα καλύτερα έρχονται. Μόνο fun Ροδούλα από εδώ και πέρα. Σ’αγαπώ.

Curriculum vitae

Rodoula Ktori

Rodoula was born in Nicosia, Cyprus, on July 1st 1994. In 2012, she moved to Greece to begin her academic journey, studying Chemical Engineering at Aristotle University of Thessaloniki, where she completed an Integrated Master's degree. Her thesis explored the valorisation of spent coffee grounds through pyrolysis, contributing to circular economy strategies for energy and material recovery. Driven by a strong desire to deepen her understanding of sustainability, she pursued an MSc in Industrial Ecology at TU Delft and Leiden University. Her MSc thesis introduced her to the field of brine treatment systems for resource recovery, laying the groundwork for her future research.

In 2020, she began her PhD at TU Delft in the Environmental Biotechnology group under the supervision of Prof. Dr. Ir. Mark van Loosdrecht and Dr. Dimitris Xevgenos, as part of the EU-funded WATER MINING project. Her research focuses on the sustainability assessment of desalination technologies, with an emphasis on resource recovery, proposing novel methodologies for techno-economic and environmental evaluation. The results of her research are presented in this thesis.

Most recently, she joined the E-Protein project as a postdoc, where she is conducting a techno-economic and environmental assessment of single-cell protein production from various substrates to support greenhouse gas emission reductions and sustainable protein alternatives.

Scientific contribution

Publications included in this thesis:

R. Ktori, M.P. Parada, M. Rodriguez-Pascual, M.C.M. Van Loosdrecht, D. Xevgenos, Sustainability assessment framework for integrated seawater desalination and resource recovery : A participatory approach, Resour. , Conserv. Recycl. 212 (2025).

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R. Ktori, F. Vassallo, G. Virruso, C. Morgante, A. Culcasi, D. Diamantidou, N. Van Linden, A. Trezzi, A. Krishnan, A. Cipollina, G. Micale, M. C.M. van Loosdrecht, D. Xevgenos, Desalination and brine treatment systems integrated modeling framework: simulation and evaluation of water and resource recovery. The Journal of Open Source Software (2024).

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R. Ktori, C.Li, M.C.M. Van Loosdrecht, Gonzalo Gamboa, D. Xevgenos, Criteria interdependency in Multi-criteria Decision-making on sustainability: Desalination for resource recovery case study. *(submitted)*

Other publications:

A. Culcasi, **R. Ktori**, A. Pellegrino, M. Rodriguez-Pascual, M.C.M. van Loosdrecht, A. Tamburini, A. Cipollina, D. Xevgenos, G. Micale, Towards sustainable production of minerals and chemicals through seawater brine treatment using Eutectic freeze crystallization and Electrodialysis with bipolar membranes, J. Clean. Prod. 368 (2022) 133143.

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G. Micale, D. Xevgenos, Pioneering minimum liquid discharge desalination : A pilot study in Lampedusa Island, Desalination. 581 (2024).

G. Gamboa, P. Palenzuela, **R. Ktori**, D.C. Alarcón-Padilla, G. Zaragoza, S. Fayad, D. Xevgenos, M. Palmeros Parada, Thermal seawater desalination for irrigation purposes in a water-stressed region: Emerging value tensions in full-scale implementation, Desalination. 593 (2025).

Tool/software:

desalsim: Desalination and Brine Treatment simulation model

- Webpage with tutorials: https://desalsim-web.readthedocs.io/en/latest/index.html
- GitHub repository: https://github.com/rodoulak/desalsim
- Python package: https://pypi.org/project/desalsim/

Conference Contributions:

R. Ktori, M. Palmeros Parada, M. Rodriguez-Pascual, M. C.M. van Loosdrecht, D. Xevgenos Sustainability assessment framework of integrated desalination and resource recovery: a participatory approach, **Watermatex**, Quebec City, Canada, September 2023, Oral presentation.

R. Ktori, M. Palmeros Parada, M. van Loosdrecht, D. Xevgenos. Designing for the future: a value-sensitive approach to integrated desalination and brine treatment, **Desalination for the Environment: Clean Water and Energy**, Limassol, Cyprus, May 2023, Oral presentation.

R. Ktori, A. Krishnan, M. Rodriguez-Pascual, M. van Loosdrecht, D. Xevgenos. Implementation of circular economy and energy efficiency in seawater desalination by integrating brine treatment technologies, **17th IWA Leading Edge Conference on Water and Wastewater Technologies**. Reno, Nevada, United States of America, March 2022, Oral presentation.

A. Culcasi, **R. Ktori**, A. Pellegrino, M. Rodriguez-Pascual, M.C.M. van Loosdrecht, A. Tamburini, A. Cipollina, D. Xevgenos, G. Micale. Valorization of seawater desalination brines through the integration of Eutectic Freeze Crystallization and Electrodialysis with Bipolar Membranes innovative technologies. **16th SDEWES conference**, Dubrovnik, Croatia, October 2021, Oral presentation.

The presenting author is underlined.