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

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A B S T R A C T

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

1. Introduction

Water scarcity is an increasing concern across the world due to a geographic mismatch of fresh water demand and availability [1,2]. Business-as-usual scenarios predict that by 2030 the demand for fresh water will exceed supply by 40% [3]. The finite amount of accessible and available fresh water is further impacted by over-withdrawal, changes to the hydrological cycle, and contamination [2,4,5]. The most common form of contamination is salinization which is primarily caused by either salt water intrusion or waste water discharge [6]. Salinization ranges from brackish (1000–35,000 mg L⁻¹) to seawater (35,000+ mg L⁻¹) [5].

Desalination is the process of removing salts from saline water and is one of the most popular methods for addressing water scarcity [7]. Desalination produces around 95 million m³ d⁻¹ of fresh water and its installed capacity is rapidly increasing [7,8]. There are four main desalination technology types: membrane, thermal, electro/chemical, and emerging [9–11]. The most common form of desalination is reverse osmosis (RO) which accounts for 69% of all desalination plants globally [7]. However, no single technology or technology type is best for all situations since technology selection depends on several factors [12,13]. These factors include feed water quality, product water requirements, operating conditions, technology parameters, and local information.

To date, desalination optimization research has primarily focused on reducing the impacts of individual technologies [9,14]. This includes reducing energy demand, lowering costs through optimal configurations, and other technological advancements [9,14]. As many of these optimization paths have been exhausted, research has now turned towards improving performance through combining technologies (i.e. treatment trains) [15,16]. Treatment trains are defined as a sequence of treatment technologies used to desalinate a saline water source [17].

Treatment trains have the potential to both achieve produced water quality standards while also reducing the associated impacts [18]. However, research and application of desalination has been primarily focused on high-salinity sources [19]. Fortunately, technological improvements coupled with treatment train benefits make it possible to widen the input salinity eligibility [20]. By increasing the range of eligible feed salinities, the number of viable sources also increases thus creating more options to meet fresh water demand.

Determining which treatment trains are worth pursuing is complicated due to the variety of available technologies, the range in their
operations, the variance in their performance under different operating conditions, and the needs of the user [21]. Modelling is a potential method to analyze and compare the expected performance of different treatment trains. A treatment train model, however, must include multiple aspects and take into account a myriad of considerations in order to accurately predict treatment train performance and reflect the operating conditions.

1.1. Research objective

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

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

This paper begins by determining the guidelines of treatment train modelling through a review of the existing treatment train models (Section 2). The DESALT modelling framework design is then presented in Section 3 and the model results are illustrated in Section 4. To conclude, a summarization of the paper and crucial findings are presented in Section 5. Supplementary information regarding additional calculations are presented in the appendices.

2. Model guidelines

2.1. Existing hybrid treatment train models

Existing treatment train models tend to fall into one of three categories: detailed, general, or hybrid [22]. Detailed evaluation models focus primarily on mimicking the exact performance of a specific treatment train and are not meant to assess how different combinations perform [9,23–26]. General assessment models are more commonly focused on estimating performance, costs, or environmental impacts [27,28]. However, general assessment models typically do not include technological limitations and neglect crucial interactions between operating conditions and performance.

Hybrid-modelling has the potential to integrate detailed evaluation and general assessment models in order to provide a comprehensive systems level analyses [12,21–23,29–33]. An example of this is the MINLP method developed by Skiborowski [23]. This method uses a hybrid-modelling approach for evaluating treatment trains that breaks down the components of each individual technology and optimizes based on the specific technology. The evaluation then uses a step-wise optimization strategy for achieving a set economical objective [23]. This approach results in both an accurate evaluation and a manageable optimization process, however, does not include a comprehensive decision support tool [23].

In incorporating a decision support tool it is important to focus on impacts outside of technical performance such as economic and environmental decision-criteria [23]. Al-Nory and Graves present one of the most comprehensive and thorough approaches to desalination decision support including both environmental and economic impacts as well as long term performance [12,29]. Additionally, Al-Nory and Graves address the complexities of decision support by providing an interactive visualization of the modelling outputs. The user can select two decision parameters which are then plotted on a Pareto Optimal graph depicting the trade-offs [12]. Though very thorough, the approach presented in Al-Nory and Graves does not account for the impact of the operating conditions on treatment train performance.

Operating conditions are important for assessing treatment train performance as they can directly link to the technical, economical, and environmental decision-criteria. Technology specific evaluations, therefore, are crucial to accurately assessing treatment train performance and impact. Some models address this by using secondary technology-specific software that is operated separately from the model [21,30]. However, requiring multiple models makes the evaluation process much more complex and can sometimes result in accessibility issues [21,30,34]. Gassemi and Danesh addressed this by developing their own technology specific evaluations within their model making the model reflective of the operating conditions and simpler to use [33]. However, Gassemi and Danesh did not incorporate customization as a feature in their model, instead focusing on pre-set scenarios.

Customization capabilities for both the input criteria and technology evaluation methods are necessary since the former allows for the model to be case specific and the latter allows for the model to remain up to date. The input criteria should include multiple data points including feed water quality, local conditions, and user preferences as exemplified by the EVALEAU model [21]. The EVALEAU model monitors 168 water quality criteria for producing high-quality drinking water. The customization capabilities of these input criteria allow for the model to be reflective of the given scenario. However, EVALEAU does not include customization of the technology evaluation or internal generation of treatment train combinations. Instead, EVALEAU uses an existing database of pre-determined treatment trains. Limiting the treatment train length [12,23] and/or combination possibilities [21,30] limits the discovery of unconventional combinations that could be effective. Additionally, relying on a database for treatment train evaluations can limit the applicability to a given situation, especially if a specific technology needs to be considered. Therefore, it is recommended that in addition to the input criteria being customizable, the technology evaluations and treatment train composition should be customizable as well.

2.2. Desalination treatment train modelling guidelines

While each model reviewed can reach its own target, no single model was able to meet the full objective for the DESALT model. From the literature review, five desalination treatment train modelling guidelines were compiled (Table 1). These guidelines were referred to during the development of the DESALT model to assure that this research both builds upon existing knowledge and expands the accuracy and potential of treatment train modelling.

3. Model design

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

3.1. Treatment train evaluation process

The treatment train evaluation in the DESALT model follows four major steps (Fig. 1). First, the input criteria are applied which include the feed water quality, treatment train combination, operating condition combination, and technology specific parameters. This information is used to set up the treatment train steps and apply the appropriate evaluation method and operating conditions.

Second, the treatment train evaluation begins by applying the feed water to the first technology (e.g. Tech A). The evaluation output from Tech A is determined using the technology specific evaluation method, parameters, and operating conditions. The product water from Tech A is then passed to Tech B and so on until the treatment train is complete. Third, the modelling output is broken into three aspects: product, brine, and impacts. The product is the desalinated water coming out of the final technology in the treatment train. The associated brine water and impacts, on the other hand, are accumulated over the course of the total treatment train evaluation. Finally, the modelling outputs are filtered based on the product water and user requirements. It should be noted that the DESALT method presented in this paper uses a feed forward approach. This makes it possible for a variety of treatment trains to be more simply evaluated as the incorporation of a brine treatment step or recirculation poses a larger and more complex evaluation process. While it is possible for the model to be expanded to incorporate brine treatment, the scope of this research is limited to treatment trains with consecutive, feed forward treatment to illustrate the models design. Since brine treatment

![Fig. 1. Overview of how data is handled in the DESALT treatment train evaluation process.](image_url)
is a valuable addition to the model, it is planned to include this feature in future versions of the DESALT model.

3.2. DESALT model framework

The DESALT model framework (Fig. 2) was developed to support the treatment train evaluation discussed in Section 3.1 while also following the modelling guidelines outlined in Table 1. The framework uses a systematic evaluation approach where each treatment train combination is evaluated under all discrete-based operating condition combinations. This approach was selected since, in the initial development of the DESALT model, it was found that the impact of the operating conditions and complexity of technology interactions resulted in a non-linear optimization problem. Therefore, a full evaluation for each treatment train configuration was necessary before narrowing down to the most preferable options.

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

The input criteria, detailed in Section 3.2.1, is organized in a controllable Excel workbook which allows for simple review of all input criteria without needing to dissect the model. This format is also customizable so that the input criteria can be reflective of the actual scenario and technology parameters.

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

3.2.1. Input criteria and data import

The first step of the DESALT model is to import and organize all the input criteria. This is done separately to facilitate processing speed and data reliability.

The input criteria for the DESALT model includes multiple data points which break down into four categories: feed water quality, product water requirements, technology parameters, and user information (Table 2). For both the feed water quality and product water requirements, 11 criteria were selected based on expert interviews and literature reviews. Water quality criteria were selected based on their impact on fouling, corrosion, or scaling. Water condition criteria were selected based on their impact on technology performance [10]. In addition, an osmotic pressure conversion factor is needed as the osmotic pressure is dependent on the feed water composition. Osmotic pressure is the amount of force needed to prevent a solvent from passing from one solution to another by osmosis. It is dictated based on the water composition, therefore an osmotic pressure calculator provided by Dow was used and a correction factor was determined which converted the water composition to an osmotic pressure value. This value has a particular impact on membrane processes such as reverse osmosis (RO).

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

The technology parameters are the most extensive aspect of the input criteria. This includes the driving force and operating condition variable range, both of which directly effect a technologies performance. Meanwhile, technology limitations prevent the technology evaluation from operating out of scope and the technology parameters provide information for the technology specific evaluation. Examples of technology parameters can be found in Appendices A.1 and B.1.

3.2.2. Combinations

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

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

3.2.3. Treatment train evaluation

The accuracy of the model is entirely reliant on the accuracy of the technology evaluation, therefore, guidelines were developed to guide the development of these evaluations (Table 3). It was determined that the most effective evaluation method is one based on systems level physical equations [35–37]. The level of physical modelling must reflect the effects of the operating conditions but must also be capable of using the same set of common input criteria as the other technology evaluations.

Almost any technology can be included that is able to adhere to these guidelines and is also accurate. As the model does not include feedback loops or recirculation schemes, it is possible for any
Table 2: Input criteria necessary for the DESALT model.

| Feed water specifications | Product water requirements | User information | Technology parameters | Test conditions |
|---------------------------|---------------------------|------------------|-----------------------|-----------------|
| **Quality**               | **Quality**               | **Information**  | **Technology parameters** | **Test conditions** |
| Bicarbonate [mg L⁻¹]      | Bicarbonate [mg L⁻¹]      | CO₂-eq conversion for energy [kg kWh⁻¹] | General Technology: name, type | Feed salinity (NaCl) [mg L⁻¹] |
| Calcium [mg L⁻¹]          | Calcium [mg L⁻¹]          | Local energy cost [$US kWh⁻¹] | Driving force: type, min, max | Flow rate [m³ h⁻¹] |
| Chloride [mg L⁻¹]         | Chloride [mg L⁻¹]         | Working hours per day [hours] | Variable A: type, min, max | Pressure [Pa] |
| Iron [mg L⁻¹]             | Iron [mg L⁻¹]             | Preferences First priority [UPC, energy use, ...] | Variable B: type, min, max | Product salinity (NaCl) [mg L⁻¹] |
| Magnesium [mg L⁻¹]        | Magnesium [mg L⁻¹]        | Second priority [UPC, energy use, ...] | General performance Recovery ratio [%] | Recovery ratio [%] |
| Salinity (NaCl) [mg L⁻¹]  | Salinity (NaCl) [mg L⁻¹]  | Train length [1, 2, 3, ...] | Availability [%] | TDS removal rate [%] |
| Total organic carbon [mg L⁻¹] | Total organic carbon [mg L⁻¹] | Evaluation period (years) | Technology lifetime [years] | Temperature [°C] |
| **Condition**             | **Condition**             | **Requirements**  | **Feed limits**        | **Impact factors** |
| Flow rate [m³ h⁻¹]        | Flow rate [m³ h⁻¹]        | Maximum investment cost [$US] | Bicarbonate: min, max [mg L⁻¹] | Capital: UPC coefficient b [−] |
| Pressure [Pa]             | Pressure [Pa]             | Unit production cost [$US m⁻³] | Calcium: min, max [mg L⁻¹] | Capital: UPC coefficient m [−] |
| Temperature [°C]          | Temperature [°C]          | | Chloride: min, max [mg L⁻¹] | CO₂ conversion factor [kg m⁻³] |
| **Other**                 |                           | | Flow rate: min, max [m³ h⁻¹] | O&M: UPC coefficient b [−] |
| Osmotic pressure conversion [Pa mg L⁻¹] |                           | | Iron: min, max [mg L⁻¹] | O&M: UPC coefficient m [−] |
|                           |                           | | Magnesium: min, max [mg L⁻¹] | O&M: share general [%] |
|                           |                           | | Pressure: min, max [Pa] | **Technology specific parameters** |
|                           |                           | | Salinity (NaCl): min, max [mg L⁻¹] | |
Pareto front analyses. In a Pareto front analyses, eligible options are applied to a multi-criteria analyses. Once these filters are applied, the filtered set of options are then reduced through a reduce step, the filtered set of options are reduced through a reduce step, the filtered set of options are reduced through a reduce step. The decision support consists of 3 steps: filter, reduce, and refine. In the filter step, a treatment train configuration is only considered to be verifiable if it only contains one technology to be included that can be applied to brackish-water for the purposes of a feed-forward analyses.

To illustrate the capabilities of the DESALT model, two evaluation methods were developed for two different technology types: brackish-water reverse osmosis ((BW)RO) and electrodialysis (ED). (BW)RO is a pressure driven technology that has been extensively researched and modelled. The extensive amounts of available data and modelling approaches allows for the technology evaluation to be easily validated against existing data. ED was selected to test the capability of the model to incorporate a different technology type with a different level of available data. ED is an energy driven technology with limited available data, especially on a systems level and commercial scale. The evaluation method for (BW)RO is presented in Appendix A while the evaluation method for ED is presented in Appendix B. While these are the only evaluation models presented in this paper, other technologies were tested as well (e.g. nano-filtration). It is expected that the technology evaluations will grow with further modifications of the model.

3.2.4. Decision support and modelling output data

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

The decision support consists of 3 steps: filter, reduce, and refine. In the filter step, a treatment train configuration is only considered to be an option after it passes several constraints. If at any point in the evaluation the limits of a technology are exceed (i.e. exceeds maximum feed TDS), the treatment train configuration is discarded. Configurations are also omitted if they are not able to meet the produced water quality and quantity requirements or if the modelling outputs are outside the user specified limits (i.e. exceeds the maximum cost). Once these filters are applied, the filtered set of options are then applied to a multi-criteria analyses.

In the reduce step, the filtered set of options are reduced through a Pareto front analyses. In a Pareto front analyses, eligible options are reduced to only those that are considered Pareto-efficient. Pareto-efficient is defined as options where one objective cannot be improved without worsening at least one other [47]. An objective, in this case, is to either maximize or minimize a given decision-criteria, as outlined in Table 4 [43,44]. For each decision-criteria, a single-objective problem is defined and these single-objective problems are then optimized so that only options which behave well for all objectives are considered. This removes poor performers and results in a Pareto front which is a set of options that are globally beneficial for all decision-criteria [65].

In the refine step, the set of filtered and reduced options are further narrowed through use of data envelopment analysis (DEA). DEA is a non-parametric multi-criteria decision technique that calculates the relative efficiency of each decision-criteria as compared with the set of

### Table 3
Evaluation method guidelines for use in the DESALT model and their explanations.

| Guideline                        | Explanation                                                                 |
|----------------------------------|-----------------------------------------------------------------------------|
| Common inputs and evaluation outputs | • Must be able to use the same common input criteria regarding feed water specifications, product water requirements, and user information (presented in Table 2).  
  • Must be able to produce the same set of information as presented in the feed water specification in Table 2 so that the next technology evaluation can continue the treatment train evaluation. |
| Attainable technology parameters | • Needed technology parameters must be found on a common datasheet.  
  • If data points are not easily found, a standard value must be used |
| Reasonable complexity            | • Must reflect changes in feed water quality and operating conditions.  
  • Include technology limitations and parameters  
  • Mindful of computation time |
| Verifiable                        | • Verifiable through comparison to existing literature or empirical results |

### Table 4
Decision-criteria used in the multi-criteria analysis in the DESALT model.

| Decision metric                  | Symbol | Unit          | Objective      |
|----------------------------------|--------|---------------|----------------|
| Recovery ratio                   | $\delta$ | %            | Maximize       |
| Removal rate                     | R      | %            | Maximize       |
| Unit production cost             | UPC    | $\text{SUS m}^{-3}$ | Minimize      |
| Specific energy                  | $E_{\text{spec}}$ | kWh m$^{-3}$ | Minimize       |
| CO$_2$-equivalent                | CO$_2$-eq | CO$_2$-kg m$^{-3}$ | Minimize       |

![Fig. 3.](https://example.com/fig3.png) **Fig. 3.** The decision-criteria performance of all possible treatment train configurations of (BW)RO and ED are plotted for both high and low feed salinities. Figures a, b, and c represent the model being run with a low feed salinity (1500 mg L$^{-1}$), while Figure d, e, and f use a moderate feed salinity (15,000 mg L$^{-1}$).
decision-criteria [44]. In the DESALT model the classic Charnes, Cooper, and Rhodes multiplier model with constant returns to scale was used with equal weight constraints given to each decision-criteria [55]. This mathematical approach normalizes and compares the decision-criteria associated with each option, referred to in decision science as a decision making unit (DMU) [66]. The result is an efficiency score for each option between zero and one, where a score of one means the option is considered efficient. The output of the “refine step” is a set of final options to be used as an intelligent starting point for further discussion on the appropriate desalination approach for a given scenario. While this list is useful to review, a best performing options for all five decision-criteria is included to visualize the trade-offs between options [67].

4. Model results

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

4.1. Effect of feed salinity

The model was run for both mildly brackish (1500 mg L\(^{-1}\)) and moderately brackish (15,000 mg L\(^{-1}\)) feed water concentrations. Highly brackish feed water was not tested as this concentration exceeded the limitations of the included technologies and the scope of the DESALT model. To demonstrate the number of evaluations, all modeling outputs before the decision support filter were plotted in Fig. 3. This large amount of data depicts the full range of treatment train configurations and, as a result, some basic correlations can be seen. With a lower feed salinity, the treatment trains can achieve lower product salinity and lower specific energy values. With a higher feed salinity, the lowest possible product salinity increases. Additionally, the UPC also increases with the product salinity as compared to the lower feed salinity scenario.

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

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

This large amount of data highlights the need for a systematic facilitation towards decision support so that the best performing options can be identified. Further, there are some options completely unnecessary for a user to consider. For example, in Fig. 3b and Fig. 3e the upper right corner of the (BW)RO + (BW)RO data represents the highest recovery ratio and the highest applied pressure. This is a non-preferred option since it is more energy intensive and less effective.

4.2. Effect of recovery ratio

The effect of the recovery ratio was reviewed by setting a recovery ratio minimum (\(\delta_{\text{min}}\)) and then reviewing the effects of the product salinity on the specific energy. This was done again for both mildly and moderately brackish feed water scenarios (Fig. 4).

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

Low recovery ratios are associated with low specific energy requirements. This is due to lower operating condition requirements because of: i) the inverse relation of salt removal and recovery ratio for (BW)RO (Appendix A.2: Eq. (A2)); and ii) the direct relation between the quantity of salt being removed from a smaller stream for ED (Appendix B.3: Eq. (B15)). Further, it can also be seen that ED performs worse at higher recovery ratios because higher recovery ratios result in higher velocities which are inversely related to salt removal (Appendix B.4: Eq. (B18)).

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

4.3. Effect of product salinity requirements

The product salinity requirement is one of the most limiting factors for treatment train feasibility. As presented in Fig. 5, the combination of product salinities and feed water salinities dictate which treatment trains are even possible.

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

While ED + (BW)RO and (BW)RO + ED are very similar to each other, a difference is seen at the higher required removal rates. When ED is first, it shoulders more of the burden for removing salts. Since it operates at a lower cost and reduces the need for (BW)RO to operate at a higher level, it becomes the cheaper option. However, once the product salinity is at a much higher level, the difference in cost becomes negligible.

4.4. Case study

The DESALT model was applied to the case study of Dow Benelux [10]. In this case study, the feed water is cooling tower blow down with produced water requirements based on their internal demi water requirement (Table 5) [10].

The DESALT model was run and 22,650 evaluations were completed. Applying the product water requirements, the number of results was immediately decreased to 4120. Next, the Pareto front analyses was run with equal weight given to each decision metric (see Table 4). The resulting Pareto frontier reduced the total options to 365 final results. This translates to a 99.9% reduction from the total initial options. The visualization of the filter and Pareto front analyses as compared to all original options can be seen in Fig. 6.

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

The recovery ratio has a further effect on the graph as the UPC (good = center of radar), specific CO2-eq (good = center of radar), and specific energy (good = center of radar) are in terms of the product flow rate. Therefore, if the recovery ratio decreases, the product flow rate decreases, and the other impacts increase.

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

5. Conclusion

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

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

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

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

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

| Treatment train | Operating cond. 1 | Operating cond. 2 |
|-----------------|------------------|------------------|
| (BW)RO + (BW)RO | \( P_{\text{app}} = 500 \text{ kPa} \) \( \delta = 90\% \) | \( P_{\text{app}} = 500 \text{ kPa} \) \( \delta = 90\% \) |
| (BW)RO + ED    | \( P_{\text{app}} = 500 \text{ kPa} \) \( V_{\text{p}} = 0.15 \text{ V} \) \( \delta = 90\% \) \( N_{\text{f}} = 350,000 \) |
| ED + (BW)RO    | \( V_{\text{p}} = 0.10 \text{ V} \) \( P_{\text{app}} = 500 \text{ kPa} \) \( \delta = 90\% \) \( N_{\text{f}} = 250,000 \) |

Fig. 7. Radar chart of best option per treatment train configuration using a balanced DEA and including changes in operating conditions, as presented in the accompanied table. These options are based on a feed flow rate of 190.26 m³ h⁻¹ with a NaCl salinity of 2564.1 mg L⁻¹ that is treated to meet a product water requirement flow rate of 20 m³ h⁻¹ and salinity of 9.62 mg L⁻¹.
Nomenclature

\( \eta \) & Channel width, m \\
\( b_{\text{cap}} \) & Capital cost coefficient, – \\
\( i_{\text{c}, y} \) & Current density, A m\(^{-2}\) \\
\( m_{\text{cap}} \) & Capital cost coefficient, – \\
\( n_{\text{subcell}} \) & Number of sub-cells, – \\
\( q_{\text{osm}, x} \) & Electroosmotic flux at point x, m\(^3\) m\(^{-2}\) s\(^{-1}\) \\
\( q_{\text{osm}, \text{CEM}} \) & Osmotic flux across the CEM, m\(^3\) m\(^{-2}\) s\(^{-1}\) \\
\( q_{\text{osm}, \text{AEM}} \) & Osmotic flux across the AEM, m\(^3\) m\(^{-2}\) s\(^{-1}\) \\
\( q_{\text{total}, x} \) & Total volumetric flux at point x, m\(^3\) m\(^{-2}\) s\(^{-1}\) \\
\( \delta_{\text{min}} \) & Minimum recovery ratio, % \\
\( \pi_{\text{feed}} \) & Osmotic pressure of the feed, kPa \\
\( J \) & Average permeate flux, m\(^3\) m\(^{-2}\) h\(^{-1}\) \\
\( \text{NDP} \) & Net driving pressure, kPa \\
\( P \) & Pressure, kPa \\
\( S \) & Surface area of the membrane subsection, m\(^2\) \\
\( TCF \) & Temperature correction factor, – \\
\( \text{UPC} \) & Unit production cost, $US m\(^{-3}\) \\
\( a \) & Availability, % \\
\( l \) & Expected lifetime, year \\
\( \delta \) & Recovery ratio, %

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Brackish water reverse osmosis evaluation method

A.1. Technology parameters

Table A1

| BW30XFR-400/34i technology parameters | Min | Max | Impact factors |
|---------------------------------------|-----|-----|----------------|
| Driving force: \( P_{\text{app}} \)   | 500 kPa | 4000 kPa | Capital: UPC coefficient \( b \) |
| Variable A: \( \delta \)             | 25% | 75% | Capital: UPC coefficient \( m \) |

Table 2

| General performance | Min | Max | Impact factors |
|---------------------|-----|-----|----------------|
| Availability        | 90% |     | O&M: Share general 50% |
| Technology lifetime | 10 years |     | O&M: UPC coefficient \( b \) |

| Feed limits         | Min | Max | Impact factors |
|---------------------|-----|-----|----------------|
| Bicarbonate         | - mg L\(^{-1}\) | - mg L\(^{-1}\) | CO\(_2\) conversion factor 0.62 kg m\(^{-3}\) |
| Calcium             | - mg L\(^{-1}\) | - mg L\(^{-1}\) | O&M: UPC coefficient \( b \) 2.31 |
| Chloride            | - mg L\(^{-1}\) | - mg L\(^{-1}\) | O&M: UPC coefficient \( m \) 0.26 |
| Flow rate           | - m\(^3\) h\(^{-1}\) | - m\(^3\) h\(^{-1}\) | O&M: Share general 50% |
| Iron                | 0 mg L\(^{-1}\) | 35,000 mg L\(^{-1}\) | O&M: UPC coefficient \( b \) |
| Pressure            | 100 kPa | 4000 kPa | O&M: Share general 50% |
| Salinity            | 0 mg L\(^{-1}\) | 16,025.64 mg L\(^{-1}\) | O&M: Share general 50% |
| Temperature         | 0 °C | 45 °C | O&M: Share general 50% |
| TOC                 | 0 mg L\(^{-1}\) | 35,000 mg L\(^{-1}\) | O&M: Share general 50% |

| Test conditions     | Min | Max | Impact factors |
|---------------------|-----|-----|----------------|
| Feed salinity       | 2000 mg L\(^{-1}\) |     | O&M: Share general 50% |
| Flow rate           | 1.79 m\(^3\) h\(^{-1}\) |     | O&M: Share general 50% |
| Pressure            | 15.50 Pa |     | O&M: Share general 50% |
| Product salinity    | 7 mg L\(^{-1}\) |     | O&M: Share general 50% |
| Recovery ratio      | 15% |     | O&M: Share general 50% |
| TDS removal rate    | 99.7% |     | O&M: Share general 50% |
| Temperature         | 25 °C |     | O&M: Share general 50% |
| TOC removal rate    | 66% |     | O&M: Share general 50% |

A.2. Technology evaluation method

(BW)RO is one of the most common and fastest growing desalination technologies in the world [9,38]. Its benefits are a small physical footprint, modular design, automated control, and relatively low cost [9,24,35]. Since this technology is well researched, there are abundant amounts of literature on the topic of (BW)RO modelling. However, many of these evaluations are either too detailed for the scope of the DESALT model [14,36,39] or were not in a format that could be easily included in the DESALT model [37,40–45]. As a result, it was necessary to develop a custom evaluation method.

The (BW)RO evaluation method was adapted from existing models where the given parameters determine the required membrane area [24,46,47]. In this approach, the primary driving force is the hydraulic pressure while the recovery ratio operates as a secondary variable.

To begin, the permeate water flow rate \( Q_{\text{perm}} \) is determined through its direct relation to both the recovery ratio \( \delta \) and the feed water flow rate \( Q_{\text{feed}} \) [46–48].

\[
Q_{\text{perm}} = \frac{Q_{\text{feed}}}{1 - \delta} \tag{A1}
\]

The removal rate of the system \( R_{\text{sys}} \) is also directly related to \( \delta \) [47]. \( R_{\text{sys}} \) is typically found in (BW)RO data sheets, however, this value is only valid under the specified test conditions [47]. It is therefore necessary to use the test conditions in combination with Eq. (A2) to determine the removal rate of the membrane \( R_{\text{mem}} \). Eq. (A2) is then reapplied using the given operating conditions to determine the actual \( R_{\text{sys}} \).

\[
R_{\text{sys}} = 1 - (1 - \delta)^{1/R_{\text{mem}}} \tag{A2}
\]

The \( R_{\text{sys}} \) under the given operating conditions is then used to determine the concentration in the permeate water \( C_{\text{perm}} \) based on the feed water concentration \( C_{\text{feed}} \) [5,47]. Note that this method is used for all TDS components listed in Table 2. Additionally, the same methodology is used for TOC, however, the corresponding \( R_{\text{sys}} \) and \( R_{\text{mem}} \) need to be used.

\[
C_{\text{perm}} = (1 - R_{\text{sys}}) \cdot C_{\text{feed}} \tag{A3}
\]

As stated previously, \( \delta \) is treated as a secondary variable thus it is a given value per evaluation. With this approach, \( Q_{\text{perm}} \) remains constant in the evaluation. However, the transport of water across the membrane per area of membrane (i.e. the average permeate flux) is not fixed since it is directly related to the applied pressure and feed water temperature [5,36,49]. These are reflected in the calculation of the average permeate flux \( J \) through the water permeability coefficient \( a_{\text{w}} \), the net driving pressure \( \text{NDP} \) as explained in Appendix A.3, and the temperature correction factor \( \text{TCF} \) as explained in Appendix A.4.

\[
J = a_{\text{w}} \times \text{NDP} \times \text{TCF} \tag{A4}
\]

Next, a mass balance approach is applied which is based on dividing the parallel flow of water along the membrane into subsections. These
subsections are then used for mass balances of both the flow rate and salt flux. The flow rate mass balance states that the amount of water crossing the membrane for a given subsection is based on both J and the surface area of the membrane subsection (S).

\[
\frac{dQ}{dx} = -J \cdot S
\]  

(A5)

The salt flux mass balance follows a similar relation in which the concentration of salt entering the subsection \( (C_{\text{conc}, x}) \) in combination with the flow rate relation (Eq. (A5)) is directly related to the concentration of the permeate stream at given point x \( (C_{\text{perm}, x}) \). It should be noted that for the purposes of the mass balance, the concentration of salt entering the first subsection \( (C_{\text{conc}, 1}) \) is equal to the feed concentration entering the (BW)RO system, while the output from the first subsection would be the input to the next subsection.

\[
\frac{d(Q \cdot C_{\text{conc}, x})}{dx} = -J \cdot S \cdot C_{\text{perm}, x}
\]  

(A6)

The equation for the required membrane area \( (A_{\text{req}}) \) is then developed through the derivation of both Eqs. (A5) and (A6). This equation is then expanded to show the correlation between \( A_{\text{req}} \) and TCF, applied pressure \( (\Delta P) \), osmotic pressure \( (\pi_{\text{feed}}) \), feed water conditions, and the technology parameters. The equation is evaluated over the length of channel from the input (feed) to the output (con)

\[
A_{\text{req}} = \frac{1}{\Delta P - \pi_{\text{feed}} \cdot \eta_{\text{feed}} \cdot \frac{Q_{\text{feed}, x}}{Q_{\text{perm}, x}}} \int_{Q_{\text{feed}, x}}^{Q_{\text{conc}, x}} \frac{1}{\eta_{\text{perm}}} \frac{dQ}{dx}
\]  

(A7)

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

\[
Q_{\text{installed}} = Q_{\text{test}} \cdot \left[ \frac{A_{\text{req}}}{A_{\text{test}}} \right]
\]  

(A8)

(BW)RO energy use is assumed to be only the electrical energy required for the hydraulic pump. Therefore, the total energy use per hour \( (E_{\text{total, hour}}) \) is simplified to the pumping power which is based on \( P_{\text{feed, sec}} \), feed flowrate per second \( (Q_{\text{feed, sec}}) \), and pump efficiency \( (\eta_{\text{pump}} 80\%) \) [26,50,51].

\[
E_{\text{total, hour}} = \Delta P \cdot Q_{\text{feed, sec}} \cdot \eta_{\text{pump}}
\]  

(A9)

Abdulbaki et al. developed a cost function based on technology type and plant capacity. This method breaks down the unit production costs \( (\text{UPC}) \) into capital and yearly operations and maintenance \( (\text{O&M}) \) [28]. The capital UPC correlation determined by Abdulbaki et al. (first term in Eq. (A10)) matches with other publications such as Wittholz et al. (2008) who found that the larger the installation capacity, the smaller the UPC [52].

The total capital costs \( (C_{\text{Cap}}) \) are then calculated using this correlation with the installed capacity \( (Q_{\text{installed, day}}) \) and the expected daily production of water \( (Q_{\text{perm, day}}) \). Note that the given constants \( (b_{\text{cap}} \text{ and } m_{\text{cap}}) \) are presented in Abdulbaki et al. and are also given in Appendix A.2.

\[
C_{\text{Cap}} = (b_{\text{cap}} \cdot Q_{\text{installed, day}}) \cdot Q_{\text{perm, day}}
\]  

(A10)

The annual O&M costs \( (C_{\text{OM, year}}) \) must be broken out to account for changes in operating conditions (i.e. energy use) and site-specific information (i.e. cost of energy). Three aspects of O&M costs were identified. Specifically, membrane replacement costs \( (C_{\text{OM, mem}}) \), pumping costs \( (C_{\text{OM, pump}}) \), and general costs \( (C_{\text{OM, gen}}) \). The method for calculating each is presented in Appendix A.5.

\[
C_{\text{OM, year}} = C_{\text{OM, mem}} + C_{\text{OM, pump}} + C_{\text{OM, gen}}
\]  

(A11)

The total UPC adjusted \( (\text{UPC}_{\text{adj}}) \) is then determined using the aforementioned \( C_{\text{Cap}} \) and \( C_{\text{OM, year}} \) as well as the annual permeate water flow rate \( (Q_{\text{perm, year}}) \), plant availability \( (\alpha 90\%) \), and expected lifetime \( (l) \) [28,52]. In this case the UPC is defined as the total cost per cubic meter produced.

\[
\text{UPC}_{\text{adj}} = \frac{C_{\text{Cap}} + C_{\text{OM, year}}}{Q_{\text{perm, year}} \cdot \alpha \cdot l}
\]  

(A12)

The final step of the (BW)RO evaluation method is calculating the CO₂-equivalent (CO₂-eq). This is achieved using Tarnacki et al.’s conversion rate method where it was found that 0.624 kg of CO₂-eq is created for every cubic meter of permeate water produced by (BW)RO [53]. The total CO₂-eq of the system over its lifetime is then based on the given conversion factor \( (\epsilon_{\text{CO}_2} 0.624 \text{ kg m}^{-3}) \) and \( Q_{\text{perm, year}} \).

\[
\text{CO}_2\text{eq} = \epsilon_{\text{CO}_2} \cdot Q_{\text{perm, year}} \cdot l
\]  

(A13)

### 3. Net driving pressure

The net driving pressure \( (\text{NDP}) \) is the driving force behind the transport of water and salt through the membrane [5,36]. The \( \text{NDP} \) is the difference of the applied pressure difference \( (\Delta P) \) and the osmotic pressure difference \( (\Delta \pi) \) [5,36,47]. Though the \( \text{NDP} \) varies across the length of the membrane, the aim of the evaluation method is the overall result. Therefore Eq. (A14) is based on the averages over the length of the channel.

\[
\text{NDP} = \Delta P - \Delta \pi = P_{\text{feed}} - P_{\text{perm}} - \pi_{\text{feed}} + \pi_{\text{perm}}
\]  

(A14)

There are three methods for calculating \( \pi \): physics based, general relation, and hybrid. The physics based equation is derived from the van’t Hoff equation based on the gas constant \( (R_{\text{gas}}) \), temperature \( (T) \), and the sum of the molarities of ions and non-ionic compounds \( (m_i) \) [5,36].

\[
\pi = R_{\text{gas}} \times T \times \sum m_i
\]  

(A15)

The general relation is that \( \pi \) will increase by 77 kPa for every 1000 mg L\(^{-1}\) increase in salt concentration \( (\beta : 0.077\text{ kPa (mg L}^{-1}\text{)}^{-1}) \) [5,36]. The
hybrid approach uses a similar relation, however, the conversion factor ($\beta$) is non-fixed and instead defined by the feed water composition $[5,36]$.

\[ \pi \approx \beta \cdot C \]  
(A16)

In keeping with the reasonable complexity guideline from Table 3, the hybrid approach is used. In this research, $\beta$ is determined using the DuPont Manual for the Calculation of Osmotic Pressure which includes several inputs including (but not limited to) pH, salinity, and temperature.

A.4. Temperature correction factor

The effect of the feed water temperature ($T$) is represented as a temperature correction factor (TCF) $[36,47,70]$. The general relation accepted in literature is that for every degree above the standard temperature ($T_{std}: 20 ^\circ C$) the TCF will increase by 3% $[5,49,71]$. This is represented in Eq. (A17), where $\alpha$ is between 2500 and 3000 $[5,49,71]$. Through empirical based testing, Dow Chemical Company (2013) determined more specific values for $\alpha$ based on $T$ being above $T_{std}$ ($\alpha: 2640$) or below ($\alpha: 3020$).

\[ TCF = \exp \left[ \alpha \times \left( \frac{1}{T_{std}} - \frac{1}{T} \right) \right] \]  
(A17)

A.5. O&M costs

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

\[ \mathcal{C}_{OM, mem} = n \cdot \frac{l_{mem}}{l} \cdot c_{mem} \]  
(A18)

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

\[ \mathcal{C}_{OM, pump} = c_{energy} \cdot E \]  
(A19)

$\mathcal{C}_{OM, gen}$ are based on the relations presented in Abubaki et al. (first term in Eq. (A20)), the product flow rate per day ($Q_{prod, day}$), and a general O&M conversion factor ($\eta_{OM, gen}$) $[28,52,73]$. This conversion factor is the percentage of O&M costs that do not include membrane replacement or energy consumption. Per existing literature this value is estimated to be 50% $[5,52,73,74]$.

\[ \mathcal{C}_{OM, gen} = b_{OM, gen} \cdot Q_{installed, day} \cdot n_{m} \cdot Q_{perm, day} \cdot \eta_{OM, gen} \]  
(A20)

A.6. Validation

The technical performance of the (BW)RO evaluation method was compared to the expected general relations found in the support documentation for the Reverse Osmosis System Analysis software (ROSA) $[51]$. Per ROSA documentation, it is expected that the removal rate will decrease rapidly as the recovery ratio approaches 100%, and the average permeate flux has a linear relation with the feed pressure. As can be seen in Fig. A1a, both general relations occur through the (BW)RO evaluation method.

The accuracy of the (BW)RO evaluation method was first tested by comparing the specific energy performance to Sarai Atab et al. $[35]$. This was done by first applying the same inputs found in Sarai Atab et al. and then comparing. As shown in Fig. A1b, the results of the evaluation method are similar with that in Sarai Atab et al. The same method was used for evaluating the accuracy of the unit production costs (UPC) as compared to Wittholz et al. $[52]$. In this case, Wittholz et al. only provided an average non-pressure dependent cost curve. As can be seen from Fig. A1c, this evaluation method is more accurate at higher product flow rates, thus this methodology should not be relied upon at lower product flow rates with higher applied pressures.

**Fig. A1.** Verification of the (BW)RO evaluation method: (a) general performance for the removal rate and average permeate flux as compared to ROSA’s expected general relations $[51]$; (b) specific energy performance of the (BW)RO evaluation method based on the recovery ratio and applied pressure and compared to Sarai Atab et al. results which operated at 30E5 Pa $[35]$; and (c) cost performance of the (BW)RO evaluation method based on the product flow rate and applied pressure as compared to the average cost curve presented by Wittholz et al. $[52]$. 
### Appendix B. Electrodialysis evaluation method

#### B.1. ED technology parameters

| ED technology parameters | Min      | Max      | Impact factors          |
|--------------------------|----------|----------|-------------------------|
| General                  |          |          |                         |
| Driving force: $V_{cp}$  | 0.05 V   | 0.20 V   | Capital: UPC coefficient b 6772.04 |
| Variable A: $\delta$     | 50%      | 80%      | Capital: UPC coefficient m −0.22 |
| Variable B: $N_{cp}$     | 500      | 250,000  | $CO_2$ conversion factor 0.41 kg m$^{-3}$ |
|                          |          |          | O&M: UPC coefficient b 2.41 |
|                          |          |          | O&M: UPC coefficient m −0.26 |
|                          |          |          | O&M: Share general 50% |
| General performance      |          |          |                         |
| Availability             | 90%      |          |                         |
| Technology lifetime      | 20 years |          |                         |
|                          |          |          |                         |
| Feed limits              |          |          |                         |
| Bicarbonate              | - mg L$^{-1}$ | - mg L$^{-1}$ | Membrane diffusivity 2.00E-12 m$^{2}$ s$^{-1}$ |
| Calcium                  | - mg L$^{-1}$ | - mg L$^{-1}$ | Membrane height 1.30E-4 m |
| Chloride                 | - mg L$^{-1}$ | - mg L$^{-1}$ | No. cell-pairs 500 |
| Flow rate                | - m$^{3}$ h$^{-1}$ | - m$^{3}$ h$^{-1}$ | Membrane (CEM) 0.969 |
| Iron                     | 0 mg L$^{-1}$ | 35,000 mg L$^{-1}$ | Permeability (AEM) 0.975 |
| Magnesium                | mg L$^{-1}$ | mg L$^{-1}$ | Resistance (AEM) 1.77E-4 Ω m$^{2}$ |
| Pressure                 | 100 kPa  | 200 kPa  | Resistance (CEM) 1.89E-4 Ω m$^{2}$ |
| Salinity                 | 0 mg L$^{-1}$ | 16,000 mg L$^{-1}$ | Shadow effect (x) 1.471 |
| Temperature              | 0 °C     | 45 °C    | Shadow effect (y) 1.212 |
| TSS                      | 0 mg L$^{-1}$ | 35,000 mg L$^{-1}$ | Spacer height 1.55E-4 m |
| Test conditions          |          |          |                         |
| Feed salinity            | - mg L$^{-1}$ |          | Water permeability (AEM) 1.75E-14 m$^{3}$ Pa$^{-1}$ s$^{-1}$ m$^{-2}$ |
| Flow rate                | - m$^{3}$ h$^{-1}$ |          | Water permeability (CEM) 2.16E-14 m$^{3}$ Pa$^{-1}$ s$^{-1}$ m$^{-2}$ |
| Pressure                 | Pa       |          |                         |
| Product salinity         | - mg L$^{-1}$ |          |                         |
| Recovery ratio           | - %      |          |                         |
| TDS removal rate         | - %      |          |                         |
| Temperature              | - °C     |          |                         |
| TOC removal rate         | - %      |          |                         |

#### B.2. Technology evaluation method: electrodialysis

Electrodialysis (ED) is the most common application of ion exchange membranes and has increased in popularity due to its efficiency and ability to operate without pretreatment [54–56]. ED evaluation methods are broken down into either simplified or advanced models [19,57–62]. Simplified models are often case specific since they rely on numerous assumptions. Advanced models focus on the detailed processes and are typically either theoretically or semi-empirically based [19,58–62]. Theoretical approaches are very specific to the internal processes, thus they can often neglect systems level application effects. Thus, a semi-empirical approach was found to best fit a systems level application. Two semi-empirical models were selected and merged based on their individual scopes: Campione et al. and Wright et al. [61,62]. The Campione evaluation method is a one-dimensional approach which assumes operations remain below the limiting current [61]. This approach is based on a mass balance along the length of the ED channel that is divided into sub-cells. Wright uses a similar mass balance approach, however, expands to include systems level impacts such as the energy use due to pumping.

The ED evaluation method developed uses the applied cell pair voltage ($V_{cp}$) as the primary driving force. This is because $V_{cp}$ is what forces ions in the diluate channels to move through the alternately charged membranes into concentrate channels [54]. Additionally, two secondary variables were included: $\delta$ and number of membrane cell pairs ($N_{cp}$).

$\delta$ directly relates to the flow rate in the diluate ($Q_{dil}$) and concentrate ($Q_{conc}$) channels (Eqs. (B1) and (B2), respectively). It should be noted that $Q_{dil}$ directly relates to the channel velocity and thus is inversely related to the salt removal rate.

$$Q_{dil} = \delta \cdot Q_{tot}$$  \hspace{1cm} (B1)

$$Q_{conc} = (1 - \delta) \cdot Q_{tot}$$  \hspace{1cm} (B2)

This evaluation method is based on two transfer processes: salt transport and water transport. Salt transport (i.e. the total salt flux, $J_{total,x}$) is the sum of the transport methods for each sub-cell located at point $x$. The transport methods include the conductive flux ($J_{cond,x}$) and the (back) diffusion occurring at each membrane ($J_{diff,x}^{AEM}$ and $J_{diff,x}^{CEM}$). More information on these transport methods can be found in Appendix B.3.

$$J_{total,x} = J_{cond,x} + J_{diff,x}^{AEM} + J_{diff,x}^{CEM}$$  \hspace{1cm} (B3)

Water transport (i.e. the total water flux, $q_{total,x}$) is also calculated as the sum of the transport methods for each sub-cell. These transport methods include both electroosmotic ($q_{qeous,x}$) and osmotic ($q_{osm}^{AEM}$ and $q_{osm}^{CEM}$) transport mechanisms, further detailed in Appendix B.4.

$$q_{total,x} = q_{qeous,x} + q_{osm}^{AEM} + q_{osm}^{CEM}$$  \hspace{1cm} (B4)

The mass balance for the bulk salt concentration is developed for both the diluate channel (Eq. (B5)) and concentrate channel (Eq. (B6)). This mass balance states that the change in the total amount of salt present in a given sub-cell is directly related to both the channel width ($b_{chan}$) and $J_{total,x}$.
Note that the total amount of salt is defined as the product of the flow rate \((Q_x)\) and the concentration \((C_x)\) at given point \(x\).

\[
\frac{dQ_{\text{dil, }x} \cdot C_{\text{dil, }x}}{dx} = -b_{\text{ chan}} \cdot j_{\text{total, }x}
\]  

(B5)

\[
\frac{dQ_{\text{conc, }x} \cdot C_{\text{conc, }x}}{dx} = b_{\text{ chan}} \cdot j_{\text{total, }x}
\]  

(B6)

The mass balance for the flow rate distributions is also developed for both the dilute and concentrate channels, Eqs. (B7) and (B8), respectively. This mass balance is similarly reliant on \(b_{\text{ chan}}\) as well as \(q_{\text{total, }x}\). The change in the dilute flow rate is seen as equal and opposite to the change in the concentrate flow rate.

\[
\frac{dQ_{\text{dil, }x}}{dx} = -b_{\text{ chan}} \cdot q_{\text{total, }x}
\]  

(B7)

\[
\frac{dQ_{\text{conc, }x}}{dx} = b_{\text{ chan}} \cdot q_{\text{total, }x}
\]  

(B8)

Using the feed water conditions as the initial system, the conditions of ordinary differential equations are solved using a Python solver (ODIENT). The output of the derivation is the concentration and flow rate for both channels at the outlet. Eqs. (B1) and (B9) are then used to determine \(\delta \) and \(R_{\text{sys}}\), respectively.

\[
R_{\text{sys}} = \frac{C_{\text{conc}}}{C_{\text{dil}}}
\]  

(B9)

The ED stack is viewed as an analogous DC circuit where the total cell voltage \((V_{\text{total}})\) is directly related to the potential across each membrane in the cell-pair \((V_{\text{mem, }y}\) see Appendix B.7) as well as the channel. The potential across the channel is seen as the product of the current density \((i_{x, y}\) see Appendix B.8) and the total resistance \((R_{\text{total, }x}\) see Appendix B.9). The total voltage per cell-pair is then multiplied by \(N_{\text{cp}}\).

\[
V_{\text{total}} = N_{\text{cp}} \cdot (V_{\text{mem, }y} + i_{x, y} \cdot R_{\text{total, }x})
\]  

(B10)

The total current \(i_{\text{total}}\) is then calculated as the sum of \(i_{x, y}\) for all sub-cells multiplied by the cell-pair membrane area \(A_{\text{cp}}\) divided by the number of sub-cells used \(n_{\text{subcell}}\).

\[
i_{\text{total}} = \frac{A_{\text{cp}} \cdot \sum i_{x, y}}{n_{\text{subcell}}}
\]  

(B11)

In this evaluation, the total energy \((E_{\text{total}})\) is used comprised of two components: the energy used in the ED process and the energy used to pump the water through the channels. Note that the energy for the electrode reactions is neglected. While the energy used in the ED process is the product of Eqs. (B10) and (B11), the energy used from pumping is based on Eq. (A9) and assuming the pressure difference is 1 bar.

\[
E_{\text{total}} = V_{\text{total}} \cdot i_{\text{total}} + \frac{\Delta P \cdot Q_{\text{feed, sec}}}{\eta_{\text{pump}}}
\]  

(B12)

To keep the cost calculation for ED consistent with (BW)RO, Eq. (A10) is again applied. However, though Abdulbaki et al. provides relations and constants \((b_{\text{ up}}, m_{\text{ up}})\) for multiple technologies, ED was not included in their results [28]. Therefore, constant values for ED were derived from the data presented in Wittholz et al. so that they could be applied in the same format as Abdulbaki et al. (see Appendix B.2).

O&M costs for ED are broken up in a similar method as (BW)RO, with the three aspects being membrane replacement \((C_{\text{OM, mem}})\), energy \((C_{\text{OM, elec}})\), and general costs \((C_{\text{OM, gen}})\). These terms are further explained in Appendix B.10. Once the annual O&M costs are found, the UPC is determined through Eq. (A12).

\[
C_{\text{OM, year}} = C_{\text{OM, mem}} + C_{\text{OM, elec}} + C_{\text{OM, gen}}
\]  

(B13)

The CO₂eq for ED is calculated using Eq. (A13) with a conversion factor of 0.41 kg of CO₂ per cubic meter of product water. This was determined through the values presented in Raluy et al. and extrapolated from the findings in Youssef et al. [63,64].

### B.3. Salt flux across membrane

Conductive flux \((J_{\text{cond, }x})\) is the main salt transport mechanism in ED [61]. It is calculated along the length of the cell pair and is directly related to the ionic current \((i_{x, y})\) which is related to the applied cell voltage \((V_{\text{cp}})\). In addition to \(i_{x, y}\), \(J_{\text{cond, }x}\) is also dependent on the transport number for the counter ion per membrane \((t_{\text{CEM, counter}} & t_{\text{AEM, counter}})\) and the Faraday constant \((F: 96,485 \text{ s A mol}^{-1})\).

\[
J_{\text{cond, }x} = \frac{(t_{\text{CEM, counter}} - (1 - \gamma_{\text{AEM}}) \cdot t_{\text{AEM}}) \cdot i_{x, y}}{F}
\]  

(B14)

The second process is back-diffusion salt transport \((J_{\text{diff}}^{\text{EM}}(x))\) caused by the difference in the concentrations of the diluate and concentrate channels \((C_{\text{EM, dil}} \& C_{\text{EM, conc}})\) respectively. This is represented by Fick’s law and is calculated for both AEM and CEM membranes using the appropriate diffusion coefficient \((D_{\text{EM}})\) and membrane height \((h_{\text{EM}})\).

\[
J_{\text{diff}}^{\text{EM}}(x) = -\frac{D_{\text{EM}} \cdot (C_{\text{EM, conc}} - C_{\text{EM, dil}})}{h_{\text{EM}}}
\]  

(B15)

The salt concentrations at the interfaces \((C_{\text{channel, }y})\) are calculated through Eq. (B16), where \(k_m\) is the mass transfer coefficient related to the Sherwood number presented in Appendix B.4 [62].
\[ C_{channel,y}^{\text{IEM}} = C_{channel,y}^0 \frac{(I_{\text{channel}} - I_{\text{ion}}) \cdot i_{channel,y}}{F \cdot k_m} \]  

(B16)

**B.4. Dimensionless numbers**

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

\[ \Re = \frac{2 \cdot \rho \cdot v \cdot h}{\mu} \]  

(B17)

\( v \) is determined using the flow rate \( Q \) and the cell-pair dimensions \( W \& h \) and number \( N_{cp} \) [19].

\[ v = \frac{N_{cp} \cdot h \cdot W}{Q} \]  

(B18)

The Schmidt number \( \Sc \) is the ratio of \( \mu \) to \( \rho \) and diffusivity \( D \). The general relation is the relative thickness of the hydrodynamic layer and mass-transfer boundary layer.

\[ \Sc = \frac{\mu}{\rho \cdot D} \]  

(B19)

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

\[ Sh = \frac{k_m \cdot d_e}{D} = \frac{1}{4} \cdot \Re \cdot \Sc \]  

(B20)

These dimensionless numbers are then used to determine \( k_m \).

\[ k_m = \frac{Sh \cdot D}{2 \cdot h} \]  

(B21)

**B.5. Water flux across membrane**

Water transport over the membrane is primarily caused by the difference in osmotic pressure \( \Delta \pi_{\text{IEM}} \), see Appendix B.6) and the water permeability of the membrane \( L_w^{\text{IEM}} \).

\[ q_{\text{ion}}^{\text{IEM}} = \Delta \pi_{\text{IEM}} \cdot L_w^{\text{IEM}} \]  

(B22)

Additionally, water transport also occurs as a result of water being dragged by ions across the membrane (electroosmosis). This is calculated based on the water transport number \( t_{\text{H}_2\text{O}} : 7 \), the total flux of salt across the membrane \( J_{\text{total}, \text{x}} \), the molar mass of water \( M_{\text{H}_2\text{O}} : 18.02 \, \text{g mol}^{-1} \), and density of the water \( \rho_{\text{NaCl}} : 1029 \, \text{kg m}^{-3} \).

\[ q_{\text{osm}, \text{x}} = \frac{t_{\text{H}_2\text{O}} \cdot J_{\text{total}, \text{x}} \cdot M_{\text{H}_2\text{O}}}{\rho_{\text{NaCl}}} \]  

(B23)

**B.6. Osmotic pressure using Pitzer’s correlation**

The osmotic pressure \( \pi_{\text{channel}}^{\text{IEM}} \) is calculated based on the concentration in the channel \( C_{\text{channel}, \text{y}}^{\text{IEM}} \), the gas constant \( R_g : 8.31 \, \text{J mol}^{-1} \text{K}^{-1} \), temperature \( T \), van hoff constant \( \nu : 1.87 \), and Pitzer’s correlation \( \psi_{\text{channel}}^{\text{IEM}} \).

\[ \pi_{\text{channel}}^{\text{IEM}} = C_{\text{channel}, \text{y}}^{\text{IEM}} \cdot R_g \cdot T \cdot \psi_{\text{channel}}^{\text{IEM}} \]  

(B24)

The osmotic coefficients \( \psi \) can be estimated by using Pitzer’s correlation presented below.

\[ \psi - 1 = -A_1 \cdot \sqrt{\varphi} \left[ 1 + b \cdot \varphi + m \cdot B \right] + m^2 \cdot C \]  

(B25)

\[ B = B^{(0)} + B^{(1)} \varphi e^{-\sqrt{\varphi}} \]  

(B26)

\( A_1 \) is the Debye-Huckel constant (0.3915 at 25 °C), \( b' \) is 1.2, \( m \) is the molarity of the electrolyte, and \( \alpha \) is the fixed constant (2 kg0.5 mol-0.5). Meanwhile, the nature of the electrolyte is represented in \( B^{(0)}, B^{(1)}, \) and \( C \) which are 0.06743, 0.3301 and 0.00263, respectively [73].

**B.7. Electrical potential across the membrane pair**

The electrical potential across each membrane pair \( (V_{\text{mem}, \text{y}}) \) is seen as the sum of potential across each membrane \( (V_{\text{y}}^{\text{IEM}}) \) [62].

\[ V_{\text{mem}, \text{y}} = V_{\text{y}}^{\text{IEM}} + V_{\text{y}}^{\text{CEM}} \]  

(B27)

The potentials are determined based on the activity coefficient of the solution, transport numbers of the counterions, and the concentrations [62].
\[ V_{\text{IEM}}^i = \frac{(2 \cdot \text{IEM} - 1) \cdot R_x \cdot T}{F} \log \left( \frac{Y \cdot C_{\text{IEM}}^{\text{IEM}}}{X \cdot C_{\text{IEM}}^{\text{IEM}}} \right) \]  

(B28)

**B.8. Current density**

As stated in Campione et al., the relation between the current density \((i_{x,y})\) and the cell pair voltage \((V_{cp})\) is crucial to the evaluation process [61]. The relation is stated to be that \(i_{x,y}\) is equal to \(V_{cp}\) minus the non-ohmic voltage drop \((V_{\text{drop},x})\) see Campione et al., Page 83 divided by the total resistance \((R_{\text{total}})\).  

\[ i_{x,y} = \frac{V_{cp} - V_{\text{drop},x}}{R_{\text{total}}} \]  

(B29)

**B.9. Total area resistance**

The total area resistance is defined as the sum of the resistances across each channel and across each membrane [61]. Note that while Wright et al. includes the resistance of the boundary layer, Campione et al. have chosen to neglect this aspect.

\[ R_{\text{total},x} = R_{b,x,y}^b + R_{x,y}^b + R_{\text{IEM}}^b + R_{x,y}^\text{CEM} \]  

(B30)

The resistance across each channel is based on the channel thickness \((h_{\text{channel}})\), shadow factor \((f_{s,\text{channel}})\), equivalent conductivity \((\Lambda_{x,\text{channel}})\), and the concentration in the channel \((C_{x,\text{channel}})\) [61].  

\[ R_{\text{channel},x,y} = f_{s,\text{channel}} \cdot \frac{R_{\text{channel}}}{\Lambda_{x,\text{channel}} \cdot C_{x,\text{channel}}} \]  

(B31)

The resistance of the membrane \((R_{\text{IEM}}^b)\) as presented by Campione et al. is based on the experimental data provided by Galama et al. [61,76]. Here it is stated that the resistance of the membrane is inversely related to the concentration (see Campione et al., Page 90)

**B.10. Islam’s correlation**

Islam’s correlation (Eq. (B32)) estimates the equivalent conductivity based on the molar concentration, electrolyte temperature and a series of constants as presented in Eqs. (B33) through (B36) [77].

\[ \Lambda_x = \left( \frac{B_1'(C) \cdot \sqrt{C}}{1 + B_1'(C) \cdot a \cdot \sqrt{C}} \right) \left( 1 - \frac{B_1'(C) \cdot \sqrt{C}}{1 + B_1'(C) \cdot a \cdot \sqrt{C}} \right)^F(C) \]  

(B32)

\[ B_1'(C) = \frac{50.29 \cdot 10^8}{\sqrt{\xi_1 T}} \]  

(B33)

\[ B_1(C) = \frac{82.50}{\eta_1 \sqrt{T} \sqrt{C}} \]  

(B34)

\[ B_2'(C) = \frac{8.204 \cdot 10^5}{(\varepsilon \cdot T)^{1/2}} \]  

(B35)

\[ F(C) = \frac{0.2929 \cdot B_1(C) - 1}{0.2929 \cdot B_1(C) \cdot a \cdot \sqrt{C}} \]  

(B36)

In Islam’s correlation the viscosity (Eq. (B37)) and dielectric constant (Eq. (B38)) depend on the salt concentration [78].

\[ \eta = \eta_0 (1 + 0.0061 \sqrt{C} + 0.078 C + 0.013 C^2) \]  

(B37)

\[ \varepsilon = \varepsilon_0 - 15.2 C + 3.64 C^2 \]  

(B38)

**B.11. O&M costs**

Since ED is a newer technology, there is less data available to accurately model its costs. As such, several approximations were applied to conform the available data to the evaluation process. Extreme caution should be taken when considering the ED cost results.

The membrane replacement cost \((C_{\text{OM, mem}})\) is determined by the number of cell pairs \((N_{cp})\), cell pair membrane area \((A_{cp})\), their expected lifetime \((l_{\text{mem}})\) vs. the plant life time \((l)\), and the cost per membrane area \((c_{\text{mem}})\).

\[ C_{\text{OM, mem}} = N_{cp} \cdot A_{cp} \cdot \frac{l_{\text{mem}}}{l} \cdot c_{\text{mem}} \]  

(B39)

The energy costs \((C_{\text{OM, elec}})\) are calculated based on the local cost of electricity \((c_{\text{energy}})\) and the amount of energy consumed \((E_{\text{total}})\).

\[ C_{\text{OM, elec}} = c_{\text{energy}} \cdot E_{\text{total}} \]  

(B40)

Due to the limited amount of information regarding how ED O&M costs are divided at various scales, the general relation found in Strathmann (2004) was used as a starting point [68]. A general relation for the O&M costs was determined based on the linear relation between the applied voltage and the O&M UPC. This relation was then applied to the estimated O&M costs calculated in Eq. (A10) where the general O&M conversion
factor is viewed as the ratio between the cell voltage and the maximum applied cell voltage.

\[ \eta_{OM, \text{gen}} = \frac{h_{\text{OM}} \cdot Q_{\text{installed, day}}}{h_{\text{OM}} \cdot Q_{\text{dil, day}} \cdot \eta_{\text{OM, gen}}} \]

(B41)

B.12. Validation

Less information was available regarding the performance of ED. In terms of technical performance, the general relation for UPC and applied voltage presented in Strathmann were used [68]. It can be seen in Fig. B1a that the evaluation method behaves similarly to what was expected, however, there are some notable differences in the capital UPC. Strathmann found that the capital UPC increases at lower applied voltages. This is because the active area would need to increase to account for the lower performance at lower voltages. The ED evaluation method, however, does not show an increase at the lower applied voltage. This is because the capital cost is based on the capacity, which is related to the number of cell-pairs, not the applied voltage. Though effective at giving a general capital cost it is a reminder that with newer technologies, an accurate cost calculation is more difficult to achieve. Therefore, the results should be seen as indicators and not final values.

Fig. B1. Verification of the ED evaluation method: (a) general cost performance relations resulting from the ED evaluation method and compared to the general relations found in Strathmann [68]; and (b) salt concentrations of the diluate and concentrate channels for both the ED evaluation method and the results from Tedesco [58].

The accuracy of the ED evaluation method was tested using an electrodialysis model developed by Tedesco et al. [58–60]. As can be seen from Fig. B1b, the concentration of salt in both the concentrate and diluate channels grow and decrease at different rates. However, the output from the channel is similar in both models. Since the DESALT model is primarily concerned with the inputs and outputs of the channel, the variation within the channel can be neglected.

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