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Modeling A Reverse Osmosis Desalination Plant: A Practical Framework Using Wave Software

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Abstract

Seawater desalination is a highly successful and effective method of obtaining fresh water from saline water sources. Reverse osmosis (RO) is a key and pivotal technology in seawater desalination as it produces high-quality freshwater from seawater with low energy consumption, in comparison to alternative technologies. However, the practical modelling of a comprehensive full-scale RO system is challenging due to fluctuating operating conditions stemming from seasonal variations and progressive fouling of the membrane during prolonged filtration operation. This study presents a comprehensive modeling framework for a seawater reverse osmosis (SWRO) desalination plant using DuPont's Water Application Value Engine (WAVE) software. The modeled system integrates ultrafiltration (UF) for pretreatment and ion exchange (IX) polishing for post-treatment, which reflects the actual operational structure of the Victoria & Alfred Waterfront desalination plant in Cape Town, South Africa. The model simulates the hydraulic and separation performance under steady-state conditions, using plant-specific data for feed salinity, pressure, flow rates, and membrane configuration. Results demonstrate the WAVE model's capability to accurately predict key performance parameters, including permeate flow, energy consumption, recovery rate, and total dissolved solids (TDS) removal. Simulated results indicate improved recovery (45.7% vs. 31%) and reduced specific energy consumption (5.91 kWh/m³ vs. 6.58 kWh/m³) compared to actual plant data. The study validates the model's predictive accuracy and highlights its application in optimizing system design, minimizing operational costs, and guiding future desalination infrastructure development under varying operational conditions.

Keywords: WAVE, Ultrafiltration, Pretreatment, Reverse Osmosis, Desalination, Seawater, RO membrane, RO Model.

1. Introduction

Seawater desalination is considered a viable solution for producing drinkable water from seawater, especially as global freshwater resources are rapidly depleting. In recent years, reverse osmosis (RO) has emerged as a leading desalination technology [1], [2]. This technology adopts a semi-permeable membrane for water purification, effectively removing organic compounds, metals, and toxic substances that are typically difficult to eliminate with conventional water treatment processes [3]. RO has been increasingly employed in water

treatment, particularly for seawater and brackish water desalination in water-scarce regions. However, the technology has its limitation which includes membrane fouling, high energy demand, and high brine waste generation. The membrane fouling, which results from an accumulation of foulants in the feed solution on the membranes' surface, is another significant problem for RO systems [4]. Membrane fouling is a complex process where various foulants accumulate on the membrane surface, decreasing its permeability and increasing energy demands. A suitable pretreatment process is typically implemented to reduce fouling, which also requires

energy for operation [5]. RO desalination technology requires significant energy to pressurize the feed flow and overcome the osmotic pressure of the solution. While technological advancements over the years have greatly reduced the energy requirements, these still remain high [6]. Additionally, the disposal of RO rejected brine from the system is a great environmental concern for marine ecosystems [7]. The advancements in membrane performance have expanded the versatility applicability of RO technology for water desalination across a wider range of pH, pressure, and temperature, and the technology is characterized by low energy consumption, operation at relatively low temperatures, an abridged system footprint, and lower overall water production costs However, RO technology performance is principally dependent on the quality of the feed water and the operating conditions. Therefore, a reliable RO model is crucial for an efficient desalination process [8], [9].

Given that the performance of an RO system is heavily influenced by its design and operating conditions, access to reliable RO models is crucial to ensure efficient system planning and operation [10]. While numerous computer models are available to assist engineers in designing RO plants, the majority primarily emphasize performance evaluation of individual RO modules rather than comprehensive optimization of the process for energy efficiency and water quality. Only a limited number of studies have concentrated on developing advanced RO models aimed at optimizing membrane modules and overall desalination plant performance [11], [12], 13]. However, the influence of different design and operational parameters on the performance of RO desalination systems has not been thoroughly explored using these existing models. This paper aims to develop a WAVE-based model capable of simulating the efficiency of a full-scale seawater reverse osmosis desalination plant while accounting for the influence of operating conditions.

Operating parameters such as recovery ratio, salinity, and temperature were quantitatively evaluated, and the RO desalination system was optimized with respect to energy consumption and brine discharge [14].

This study presents a novel application of DuPont's Water Application Value Engine (WAVE) software for the full-scale simulation and optimization of a seawater reverse osmosis (SWRO) desalination plant, uniquely

integrating ultrafiltration pretreatment, two-stage reverse osmosis processing, and ion exchange polishing into a unified modeling framework. Contrary to existing models that focus on isolated RO components, this work is distinguished by its direct validation against real-world operational data from the V&A Waterfront desalination facility in Cape Town, achieving high predictive accuracy across key performance metrics. The model not only quantifies improvements in system recovery and specific energy consumption but also identifies critical operational bottlenecks and proposes optimization strategies for enhanced plant efficiency. This research extends the conventional use of WAVE software beyond membrane sizing to comprehensive system simulation, providing a scalable and practical tool for design, performance forecasting, and adaptive infrastructure planning in waterstressed regions.

The next section of the paper presents the Victoria and Alfred (V & A) desalination plant in Cape Town, South Africa and the studied system. Section 3 discusses model development using WAVE software, while Section 4 details the system configuration and operational regimes of the desalination process. Section 5 outlines the equations governing WAVE and the general water desalination process. Section 6 describes the methodology used in this study, and Section 7 focuses on modelling and simulation for efficient separation. Section 8 explores key design considerations, and Section 9 discusses the simulation results. Section 10 concludes the review paper.

2. Studied System

The V&A desalination plant in Cape Town's waterfront is a containerised facility that produces 2 million litres per day (MLD) of potable water from saline water sourced from the Atlantic Ocean. It comprises three treatment trains: the first and second each produce 500,000 litres per day, while the third generates 1 MLD, totalling a daily capacity of 2 MLD. The trains are designated as 500-3, 500-4, and 1000-10. The plant's key systems include the intake, raw water pretreatment unit with cartridge filters, high-pressure pump, reverse osmosis (RO) membrane unit, energy recovery device, and post-treatment system.

3. Model Development

This study details modelling a seawater reverse osmosis (SWRO) desalination plant using modelling software and validated with operational data from an already existing facility in Cape Town. Various operational stages of the desalination process will be efficiently simulated during the study to reflect a complete water treatment system from source works to clear water. The process will encompass the entire plant control system and replicate full-scale plant operations, and its versatility will make it suitable for diverse research applications, such as performance analysis, and health monitoring. Dupont's Water Application Value Engine (WAVE), a leading software for reverse osmosis (RO) membrane design, will be employed in this RO modelling study.

The key inputs for this software are:

- 1. Project details
- Water Source/analysis
- 3. Temperature / pH
- 4. Product water volume requirement

In response to the given inputs, the software calculates the feed water's Total Dissolved Solids (TDS) and its scaling tendency. Based on these results, the software makes decisions regarding the use of acid/anti-scalant dosage and helps in selecting the type and size of the membrane. It also sets the initial membrane configuration and estimates the number of membrane pieces. Typically, for a flow rate of 5 m3/hr, 8-inch membranes are recommended. After receiving this data, the software produces output related to the following parameters:

- 1. Detailed analysis of the permeate and rejected water.
- 2. Scaling tendency of the water.
- 3. Net head pressure requirement.
- 4. Concentration polarisation (beta factor).

The membrane system computer models listed have demonstrated effectiveness when used according to the manufacturer's guidelines, but they have certain limitations. Designers must understand these limitations to ensure the correct application of data outputs during the design phase of the reverse osmosis membrane system. There are countless configurations of membranes, pumps, energy recovery mechanisms, and more that can be considered for a SWRO desalination system [15].

4. Configuration of Water Desalination System

This study applied DuPont's WAVE water solution software to simulate a reverse osmosis (RO) desalination system. Figure 1 illustrates the four distinct steps involved in the reverse osmosis desalination process. Before entering the ultrafiltration (UF) pretreatment system, the water from the system feed source passes through a strainer equipped with fine and coarse screens to eliminate any floating particles in the feed stream.

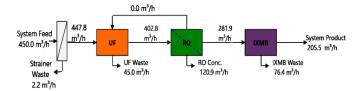


Figure 1. UF, RO, IX system configuration.

The ultrafiltration unit comprised six online trains, each containing 34 1.86-meter-long Integralflux SFP-2860 XP modules that are internally branched and interlocked in tandem. The module occupies a total area of 51 m with a diameter of 0.225 m as shown in Table 1. The module provided a total volume of 35 litres. A CIP water source is provided from the RO permeate flux for the UF system.

The UF permeate is pumped at an elevated pressure with a high-pressure pump (HPP) as feed water to the RO desalination system, and the feed water flows across a semi-permeable membrane barrier as shown in Figure 2. The solvent flows through the membrane faster than the dissolved solids. The difference in this flow rate results in the separation of the solids from the solvent. The solvent which in this case is pure water passes through the membrane with a very low salt concentration. The concentrated water or brine is left behind as waste to be disposed of.

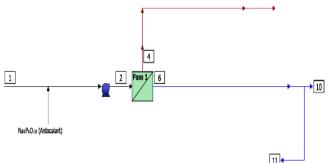


Figure 2. RO system configuration.

| Trains | | Module Details | Module Details | | | | | |
|-------------------|-------------------------|------------------------------------|------------------------------|---------------------|--|--|--|--|
| Trains | | Name: IntegraFlux SFP- | Name: IntegraFlux SFP-2860XP | | | | | |
| Online Trains | 6 |) f 1 | 51 m ² | 540.62 | | | | |
| Standby Trains | adant Trains 0 Length | | | 549 ft ² | | | | |
| Redundant Trains | | | | 73.2 in | | | | |
| Total Trains | Diameter Weight (empty) | | 0.225 m | 8.9 in | | | | |
| Max Office Trains | | | 48 kg | 106 lb | | | | |
| Modules/Train | 34 | Weight (water filled) Water Volume | 83 kg 35.0 L | 183 lb | | | | |
| Total Modules | 204 | water volume | 33.0 L | 9.2 gal | | | | |

Table 1. UF System size and module details.

The reverse osmosis system is configured as a twostage pressure vessel (PV) setup. It has a seawater RO (SWRO) production capacity of 9,000 m³ per day, operating at a recovery rate of 70%, while the ultrafiltration (UF) process is designed to achieve a 90% recovery rate, and the IX polish (post-treatment) system is designed with a 72.9% recovery rate. The ultrafiltration (UF) permeate produced during the pretreatment stage met the required water quality standards for RO feed, with total suspended solids (TSS) not exceeding 10 mg/L, turbidity below 1.7 NTU, and a silt density index (SDI) of 2.5 or less. This feed water is then pressurized using a high-pressure pump (HPP) before entering the reverse osmosis (RO) system, which is configured into two pressure vessel (PV) stages consisting of 36 PVs in the first stage and 18 in the second., with each PV having six seamaxxTM - 440i elements installed. Specifically, it is essential to highlight that the retentate from the first-stage pressure vessels, which serves as the feed water for the second-stage PVs in the RO process, was not further pressurized by an interstage booster pump (IBP), and the difference in intake feed pressures between the first-stage and second-stage PV systems confirms this. This inlet pressure difference was calculated as an average of 0.3 bar (i.e., pressure drops within the first stage PV) during the studied period of the RO operation. Sodium hypochlorite, hydrochloric and citric acids are used as chemical agents for the CIP to remove organic and inorganic foulants from the membranes separately.

5. Governing Equation

According to Anqi, et al. [16], who studied twodimensional steady and transient flows in the feed channel of a reverse osmosis (RO) membrane system, assuming incompressible flow and constant fluid physical properties, including a constant diffusion coefficient. The equations for fluid motion and concentration fields are provided below.

The continuity:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

The conservation of momentum:

$$\frac{\partial u_i}{\partial t} + U_j \frac{\partial u_i}{\partial x_i} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + v \frac{\partial^2 U_i}{\partial x_i \partial x_i}$$
(2)

and the mass transport equation:

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = D \frac{\partial^2 c}{\partial x_j \partial x_j}$$
 (3)

Where D represents the diffusion coefficient, ρ is the density, and μ is the viscosity. The velocity components are u1 = u and u2 = v, with summation indices i and j. The spatial coordinates are x1 = x and x2 = y, time is t, pressure is p, and the kinematic viscosity ($v = \mu/\rho$) is v.

According to Filmtec [17], the performance of a reverse osmosis (RO) system is primarily determined by its feed pressure (or permeate flow when feed pressure is unspecified) and salt passage. The permeate flow (Q) through an RO membrane is mathematically expressed as proportional to the product of the wetted surface area (S) and net driving pressure (ΔP - $\Delta\pi$), with the constant membrane proportionality being the permeability coefficient commonly known as A - value, as shown in the water permeation equation.

$$Q = (A)(S)(\Delta P - \Delta \pi \tag{4}$$

Salt passage in reverse osmosis occurs through diffusion, with the salt flux (NA) directly proportional to the salt concentration difference across the membrane.

This relationship is characterized by the proportionality constant, which is the salt diffusion coefficient also known as B-value, where C_{fc} represents the average feed-concentrate concentration and C_p is the permeate concentration.

$$N_A = B(C_{fc} - C_p) \tag{5}$$

Where.

 $C_{fc} = feed - concentrate$ average concentration

 $C_p = Permeate Concentration$

Element-to-Element method is used to calculate the performance of a specified design as shown below.

5.1. Element-to-element approach

The equations below show the design equations for projecting RO system performance and individual element performance. The water permeation equation is expanded to Eq. 6 to determine the values of A, ΔP , and $\Delta \pi$ from Eq. 4.

Permeate flow of Element i(gpd):

$$Q_{i} = A_{i}\pi_{f}S_{E}(TCF)(FF)\left(P_{ff} - \frac{\Delta P_{fci}}{2} - P_{pi} - \pi + \pi_{pi}\right)$$
 (6)

Average Concentrate-side osmotic pressure

$$\pi = \pi_i \left(\frac{C_{fc}}{C_f} \right) P^f \tag{7}$$

Average Permeate-side osmotic pressure

$$\pi_{pi-\pi_{fi}}(1-R_1) \tag{8}$$

Ratio: arithmetic Average Concentrate-side to feed concentration for Element i

$$\frac{C_{fci}}{C_{fi}} = \frac{1}{2} \left(1 + \frac{C_{ci}}{C_{fi}} \right) \tag{9}$$

Ratio: Concentrate to feed concentration for Element i

$$\frac{c_{fi}}{c_{fi}} = \frac{1 - Y_i (1 - R_i)}{(1 - Y_i)} \tag{10}$$

Fredwater osmotic pressure:

$$\pi_i = 1.12(273 + \tau) \sum m_i \tag{11}$$

Temperature correction factor for RO and NF membrane

$$TCF = EXP \left[2640 \left(\frac{1}{298} - \frac{1}{273 + \tau} \right) \right] T \ge 25^{\circ} C$$
 (12)

$$TCF = EXP \left[3020 \left(\frac{1}{298} - \frac{1}{273 + \tau} \right) \right] T \le 25^{\circ} C$$
 (13)

Concentration Polarization factor for 8-inch Elements

$$Pf_i = EXP(0.7Y_i) \tag{14}$$

System recovery:

$$Y = 1 - [(1 - Y_i)(1 - Y_2)..(1 - Y_n)]$$

$$= 1 - \prod_{i=1}^{n} (1 - Y_i)$$
(15)

Permeate Concentration:

$$C_{pj} = B(C_{fc})(Pf_i)(TCF)\frac{S_E}{O_i}$$
(16)

Where Q_i is the Permeate flow of Element i(gpd), $A_i\pi_f$ is the Membrane permeability at 25°C for element i. a function of the average concentrate side osmotic pressure (gfd/psi, S_E is the membrane surface area per element (ft²), TCF is the Temperature correction factor for membrane permeability, FF is Membrane fouling factor, P_{ff} is Feed pressure of Element I (psi), ΔP_{fci} is Concentrate-side pressure drop for Element I (psi), P_{pi} is Permeate pressure of Element I (psi), π_{i} is Average concentrate-side (psi), π_{fi} is Feed osmotic pressure of Element I, P_{fi} is Feed osmotic pressure of Element I, P_{fi} is Feed osmotic pressure of Element I, P_{fi} is Feed concentration for system (ppm), P_{fi} is Feed pressure of Element I (psi), P_{fi} is Permeate-side (psi)

After being transformed into Eq. 16, the permeate concentration can be derived from Eq. 5. These equations are applicable to the ith element in a sequence of n elements in a series flow configuration, as indicated by the subscript i. Starting with a given set of conditions, Eq. 6 is solved iteratively for each of the n elements to accurately assess system performance. For salt (Eq. 10) and water (Eq. 16), solutions are based on mass balances for each element and correlations for specific parameters, including concentrate-side flow resistance (Δ Pfc), temperature correction factor for water permeability (TCF) (Eqs. 12 and 13), polarization factor (pfi) (Eq. 14), and membrane permeability coefficient for water (Ai (π i)).

For RO membranes, permeability is influenced by the average concentrate concentration or osmotic pressure. Solutions often employ averages of hydraulic and osmotic pressures on the feed and permeate sides. In cases of low recovery rates, accurate results can be achieved using arithmetic averages of inlet and outlet conditions. However, as outlet parameters are initially unknown, iterative calculations remain necessary.

Based on the analysis in [18], the theoretical expressions for specific energy consumption (SEC) and permeate flux (J_v) are given by:

$$SEC = \frac{E_{bp} + E_{hp} + E_{sp}}{Q_p} \tag{17}$$

$$J_{v} = \frac{Q_{p}}{A} \tag{18}$$

Where: E_{bp} , E_{hp} and E_{sp} represent the energies consumed by the booster pump, high-pressure pump and supply pump respectively, Q_p represents the permeate water flow rate and A is the membrane area.

The specific energy consumption (SEC) of the plant is further determined by:

$$SEC = \frac{W_{pump}}{Q_p} \tag{19}$$

$$W_{pump} = \frac{\Delta P * Q_f}{\eta_{pump}} \tag{20}$$

Where W_{pump} is the work done by the pump, ΔP is the pressure differential Q_f is the feed flow rate, and η_{pump} is the pump efficiency [19].

According to [20], [21], [22], salt rejection, R_s , and the total mass balance, Q_fC_f is calculated using:

$$R_s = 1 - \frac{TDS_p}{TDS_f} \tag{21}$$

$$Q_f C_f = Q_p C_p - Q_r C_r (22)$$

The permeate water flow rate is determined by the equation below:

$$Q_p = Q_f - Q_r \tag{23}$$

$$Q_p = n_i W \int_0^L J_v dz \tag{24}$$

Where C_f , C_p and C_r represent the feed, permeate and rejected salts mass concentrations, respectively, Q_r is the rejected water flow rate, and n_i , L and W represent the number of leaves, length and width of the RO module.

Concentration polarization ϕ , resulting from impermeable salt accumulation on the membrane surface, is expressed by:

$$\emptyset = \frac{C_m - C_p}{C_b - C_p} = e^{\frac{J_v}{k}} \tag{25}$$

Where k is the mass transfer coefficient and C_b is the bulk solution solute concentration [23].

The temperature (TMP*) is defined by:

$$TMP^* = TCF * TMP (26)$$

Temperature correction factor (TCF) is a factor that takes into cognisance the effect of the temperature [24].

6. Methodology

This study adopted a structured modeling approach to evaluate the performance of a seawater reverse osmosis desalination system which incorporate ultrafiltration (UF), reverse osmosis (RO), and ion exchange (IX) stages. The general procedure comprised the following steps:

- 1. **System Configuration:** A process flow including UF pretreatment, two-stage RO, and IX polishing was established based on the actual layout of the V&A desalination plant.
- Data Collection: Plant operating data such as feedwater total dissolved solids (TDS), temperature, pressure, flow rate, and specific energy consumption (SEC) were gathered over a 12-month period to support model setup and validation.
- 3. **Software Tool:** The DuPont WAVE (Water Application Value Engine) software version 1.83 was used to simulate the full process. This tool integrates membrane performance models with hydraulic and thermodynamic calculations across UF, RO, and IX units.
- 4. **Input Specification:** Technical inputs, which includes membrane element characteristics,

design recovery, system pressure, cleaning cycles, and fouling assumptions, were defined based on manufacturer specifications and plant documentation.

- Model Execution: A model case was established under nominal operating conditions. The system was simulated under steady-state assumptions to determine key outputs such as permeate quality, recovery, and energy consumption.
- 6. **Performance Comparison:** Simulated results were compared with measured operational data to evaluate the accuracy of the model. Any observed discrepancies were addressed through parameter tuning within the modeling constraints.

The model excluded seasonal changes for simplicity; however, design guidelines note that surface feedwater quality can vary with seasons and recommend modeling average case conditions. Membrane ageing was also idealized: by setting the fouling factor to 1.00, we assumed membranes remain like-new throughout. This neglects any gradual flux decline or salt passage increase. In reality, fouling factors less than 1.00 (for example, 0.75 after 3 years) account for performance loss. By combining ultrafiltration for pretreatment and ion exchange for posttreatment within the RO framework, the study provides a robust model framework. This approach ensures efficient hydraulic performance and cost-effective desalination, offering valuable insights for design engineers in the development of high-performance seawater desalination systems.

This section outlines the overall design and modeling process. Detailed simulation lucidity, calibration results, and performance evaluation are discussed in the next section.

7. Modeling and Simulation

This section presents the modeling and simulation approach used to evaluate the performance of the seawater reverse osmosis (SWRO) desalination plant. Employing DuPont's WAVE software, the study simulates the integrated process, which includes ultrafiltration

pretreatment, reverse osmosis, and post-treatment, under realistic operating conditions to predict system behavior, assess energy efficiency, and optimize key performance parameters.

7.1. System modeling

Post-treatment is defined as the process of stabilizing the permeate flow from the desalination system to prepare it for distribution. Most alkaline mineral components are larger than the pores of a typical RO membrane, preventing their passage while allowing permeate flux to flow through easily. Consequently, the permeate becomes very acidic, which is harmful to human consumption and can damage equipment.

7.2. Model input

The WAVE model tool can be used to model or size new desalination systems or evaluate the performance of an existing system. When developing a new ultrafiltration system, it's crucial to understand the essential inputs required for an accurate and efficient design. Some examples of these inputs include information about the feed supply, quality, temperature range, and the necessary feed flow or system net production. For a given type and quality of a feed water source, applying appropriate design principles is very essential. These design principles stem from extensive experience and research in relevant fields. Design guidelines include effective operational flow, length of filtration cycles, or frequency of chemical cleaning. Once this information has been entered into the system design software, a detailed UF, RO, and IX system design report is created, showing an overall process flow diagram, module selection, size, and number of inhalations, the size of the water and chemical tanks, the process parameters and sequence tables, estimates, chemicals consumption among other things. The feed water quality shown in Table 2 was entered into the computer model, while the permeate water quality is the information output of the computer model. The actual total dissolved solids content of the raw water was obtained from the seawater database.

Table 2. Input data table.

| Parameter | Unit | Value |
|---------------------------------|----------------------|---------------|
| Feed water classification | Not applicable | Surface water |
| Pretreatment | Silt density index | < 1 |
| Permeate flow per train | Cubic meter per hour | 289.1 |
| Recovery rate | Percent | 70 |
| Membrane fouling/flow factor | Not applicable | 1.00 |
| Stages | Number | 2 |
| Pressure vessels – first stage | Number | 36 |
| Pressure vessels – second stage | Number | 18 |
| Elements per vessel | Number | 6 |
| Membrane element selection | Not applicable | |
| Area per element | Square meter | 40.9 |
| Feed Stream pH adjustment acid | Not applicable | Hydrochloric |

7.2.1. Input justification

The model design is based on the simulation and development of a movable solar-powered reverse osmosis membrane 2 million gallons per day (MGD) packaged facility that treats seawater and/or brackish water of high salinity. The feed source for this model is seawater from an inexhaustible source of the ocean, with its properties derived from the physicochemical analysis of the source work. A silt density index (SDI) of less than 1 was adopted because the seawater has been tested to have the less fouling potential of suspended solids, and this is further established with the selection of a 70 % recovery rate due to the low TDS of the system. A fouling factor that accounts for flow loss due to fouling of 1.00 was adopted for this model because the system vis-à-vis the membranes is still new with an expected less fouling/scaling tendency. One online RO train with two stages of treatment comprising 36 PVs and 18 PVs respectively for stage 1 and stage 2 was selected to ensure a highly efficient desalination process by removing a considerable percentage of brine concentration and delivering improved permeate flow of World Health Organization (WHO) standard potable water.

The water type is selected from the Feed Water tab. The solid content properties (NTU, TSS, SDI) and the organic content (TOC) are inputted with the temperature and pH values. Please note that the pH value in WAVE is defined as $-\log 10$ of the H + concentration (mol / L). In the case of a solution of fixed composition, the concentration of H + cum the pH value is a function of temperature due to the temperature dependence on the

equilibrium constants. Table 2 shows the input data overview.

It is important to note that in reverse osmosis (RO), TDS refers to "total dissolved solids" and excludes dissolved CO₂, whereas in the ion exchange (IX) modules, TDS refers to "total dissolved solutes" which includes dissolved CO₂. When designing ion exchange systems, important factors to consider include the water quality, the quantity and cost of chemicals, and the size and shape of the containers. Designing these systems is not a one-size-fits-all approach, as there are various trade-offs to be considered. This is similar to the designs of ultrafiltration (UF) systems.

7.3. Model – UF, RO, IX polishing

feedwater Total Dissolved Solids (TDS) concentration was determined by the model, using input values for Total Suspended Solids (TSS), turbidity, organic Total Organic Carbon (TOC), and feedwater temperature. The designed TDS represented a design value of 44,352 mg/L of ions of SiO₂ and B(OH)₃ but does not include NH₃ and CO₂. This designed TDS accounts for the feedwater quality and the minimum requirements for the total designed head of the reverse osmosis feed pump, and it is specific to the project location. The chosen temperature of the feed flow aligns with the maximum documented temperature of 25°C for the feed source. Considering the influence of TDS and temperature on the membrane supply pressure, it might not be necessary to include a design margin for both parameters. This evaluation is based on the site-specific water quality. This model specifies a designed feed flow of 450 m³/h and a permeated flow of 205.5 m³/h, with a maximum system recovery of 70%. This model adopts clean reverse osmosis membranes and includes a fouling factor of 1.00 in the membrane system computer model.

Two similar reverse osmosis membranes were modelled for this system. Table 3 provides detailed flow and performance data for a two-stage reverse osmosis (RO) system using SeamaxxTM-440i membrane elements. In Stage 1, 36 pressure vessels PVs) each containing 6 elements process 401.5 m³/h of feedwater at 70.9 bar, producing 273.3 m³/h of permeate with an average flux of 30.9 L/m²·h and a permeate TDS of 284.1 mg/L. Stage 2 receives 129.1 m³/h of feed at 69.8 bar across 18 PVs and yields 8.67 m³/h of permeate at a lower average flux of 2.0 L/m²·h and TDS of 5,134 mg/L. The table also shows the pressure drop and flow rates for concentrate streams, providing insight into the hydraulic and separation performance across each stage. The table also shows that both model membrane elements provided a surface area of 3,679 m². Each membrane manufacturer offers comparable high-productivity, low-pressure options, as illustrated by the modelled membrane elements.

7.4. Model output – Ultrafiltration (UF)

The summary of the output data calculated by each design model run is presented below. We refer to Figure

1, which shows the system flow of the desalination process model from the feed source to the system product. A designed system flow of 450 m³/h is admitted into the system through a coarse and fine strainer. The strainer offers a little resistance to the flow by the filtration process, which reduces the system flow to 447.8 m³/h before entering the UF pretreatment process. Following the UF treatment, the RO feed water has a flow rate of 402.8 m³/h, which is further diminished to 281.9 m³/h after the RO membrane treatment before entering the post-treatment process. The potable water output after the IX polishing process has a final flow rate of 205.5 m³/h.

Table 4 summarizes key operational parameters for the system configuration and output across four stages of the seawater desalination process: strainer, ultrafiltration (UF), reverse osmosis (RO), and ion exchange mixed bed (IX MB) polishing treatment processes. It shows the input feed water and product water parameters developed by the model tool for each treatment process and the overall system recovery for the design. The system starts with a feed flow rate of 450.0 m³/h and maintains a consistent temperature of 25°C throughout all stages. The total dissolved solids (TDS) reduce significantly from 45,696 mg/L at the strainer to 117.1 mg/L after IX polishing. The system operates at a maximum pressure of 71.2 bar in the RO stage, with pH adjusted from 7.0 to 5.9 in the final polishing stage. Overall, the system consumes 5.91 kWh/m³ of energy, delivers a final product flow of 205.5 m³/h, and achieves a recovery rate of 45.7%.

| RO flow Table (stage Level) – Pass1 | | | | | | | | | | | | | | |
|-------------------------------------|--------------------------------|-----------------------|------|------------------------|--------------------------|------------------------|-------------------------|------------------------|------------------------|------------------------|------------------------|----------------------|------------------------|-----------------------|
| | Elements | ts #PV #Els Per PV | #E1a | Feed | | Concentrate | | | | Permeate | | | | |
| Stage | | | | Feed Flow (m³/h) | Recirc Flow (m³/h) | Feed press (bar) | Boost Press (bar) | Conc Flow (m³/h) | Conc Press (bar) | Press Drop (Bar) | Perm Flow (m³/h) | Avg Flux (LMH) | Perm Press (bar) | Perm TDS (mg/L) |
| 1. | Seamaxx TM -440i | 36 | 6 | 401.5 | 0 | 70.9 | 0 | 129.1 | 70 | 0.9 | 273.3 | 30.9 | 0 | 284.1 |
| 2. | Seamaxx TM -440 | 186 | 6 | 129.1 | 0 | 69.8 | 0 | 120.5 | 68.6 | 1.2 | 867 | 2 | 0 | 5,134 |

Table 3. RO membrane modelled.

| - | | Strainer | Ultrafiltration | Reverse osmosis | IX MB Polish | | |
|--------|---------------------------------------|-----------------------|-----------------------|-----------------|--------------------|--|--|
| | Flow Rate (m ³ /h) | 450.0 | 447.8 | 402.8 | 281.9 | | |
| | TDS (mg/L) | 45,696.0 ^b | 44,352.0 ^b | 44,352.0a | 117.1 ^b | | |
| Feed | рН | 7.0 | 7.0 | 7.0 | 5.9 | | |
| | Pressure (bar) | 1.2 | 1.2 | 71.2 | 2.1 | | |
| | Temperature (⁰ C) | 25.0 | 25.0 | 25.0 | 25.0 | | |
| | Specific Energy (kWh/m³) | 5.91 | | | | | |
| System | Feed Flow Rate (m ³ /h) | 450.0 | | | | | |
| | Product Flow Rate (m ³ /h) | 205.5 | | | | | |
| | Recovery (%) | 45.7 | | | | | |

Table 4. UF, RO, IX model overview.

Based on the information provided, the WAVE modelling tool generated the UF process flow diagram as shown in Figure 3.

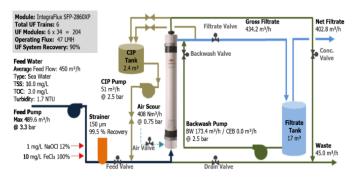


Figure 3. UF system flow diagram.

The flow diagram shows the process flow and operating conditions of the ultrafiltration pretreatment system using IntegraFlux SFP-2860XP membrane modules. The system includes six UF trains, each with 34 modules, providing a total recovery of 90% at an operating flux of 47 LMH. Seawater feed enters at 450 m³/h and passes through a 150 µm strainer with 99.5% recovery. Sodium hypochlorite and ferric chloride are dosed for fouling control. The gross filtrate produced is 434.2 m³/h, while the net filtrate is 402.8 m³/h after eliminating 45.0 m³/h of waste. The system includes a CIP tank (2.4 m³), CIP pump (5.1 m³/h), air scour system (408 Nm³/h), and backwash pump (173.4 m³/h), operating at 2.5 bar. Filtrate is stored in a 17 m³ tank before transfer to the RO stage. The flow diagram also illustrates various pressure regimes for the UF treatment process, starting from the feed pump with a pressure of 3.3 bar. Sodium hypochlorite and ferric chloride are added in percentages of 12% and 100% respectively immediately after the feed

pump to prevent fouling of the UF membrane. The UF feed water is further passed through a fine strainer to trap any floating impurities in the flow before reaching the membrane. The backwash of the membrane is carried out with the filtrate from the UF process using a backwash pump at 2.5 bar. The UF recovery is 90 %.

Six online trains were modelled for the system, with WAVE determining the module count per train based on the flux and duration recommendations, with each train consisting of 34 modules. The module type adopted for this design is InegraFlux SFP - 2860XP. a total number of 204 modules are used in the 6 trains with individual train flow rates of 67.1 bar. The model calculates UF system recovery to optimise hydraulics and maintain intake pressure for the RO system, with RO permeate water designated for the CIP water source. WAVE employs three durations in developing the CIP process, which are:

- Chemical soaking duration: This is the time within which the UF module is soaked in each chemical during CIP.
- Duration of heating step: This is the time required daily to heat the CIP chemicals from the design temperature of the UF system to the CIP temperature to determine the system energy consumption.
- Duration of CIP recycling: This is the time during which the CIP solution is expected to move around through which the UF Module circulates.

WAVE establishes specifications for the increase in pressure drop across the UF membrane known as transmembrane pressure (TMP) between successive backwash steps, acid/alkaline CEB, and CIP per hour.

These specifications aid in estimating the energy requirements for ultrafiltration, taking into account the accumulation of solids or fouling of the UF membrane during operation.

7.5. Model output – Reverse Osmosis (RO)

WAVE generated the RO process flow diagram based on the information provided in the modeling tool. The flow diagram indicates the system components and how they are arranged for an effective RO desalination system. Details of the RO system flow diagram and configuration have been given in the Desalination System Configuration. The RO system flow diagram shows the different systemic flow rates from the RO feed source (UF product flux) through the high-pressure pump (HPP) to the concentration and product feed. It also indicates different pressure regimes for the RO treatment process, starting from the high-pressure pump to the RO concentrate.

The RO system was modelled to include only one pass with one online train, and WAVE was used to calculate the number of elements per train. The flow factor used in this model which accounts for flow loss due to fouling, is 1.00, as this model was for a new system.

The risk of scaling resulting from chemical adjustments in the RO process can be best assessed by using the Langelier saturation index (LSI), the Stiff & Davis index (S&DI), and the saturation percentage for certain salts such as CaSO4, BaSO4, SrSO4, CaF2, Mg(OH)2, and SiO2. WAVE also simulated the scaling risk for the RO membrane process being. It uses colour coding to flag any percentage saturation of salts with values greater than 100, as well as LSI and S&DI values greater than 0, to alert the designer.

7.6. Model output – Ion Exchange (IX) polishing

Figure 4 illustrates the process flow and water balance of the ion exchange mixed bed (IXMB) polishing system in a seawater desalination plant. The system receives 281.9 m³/h of feed water per online train and delivers a net product flow of 205.5 m³/h after IX treatment. One train operates while another is in standby or regeneration. The system consumes 275.8 m³/h of design flow, with part of the water diverted for regeneration—6.08 m³/h from

the feed side and 70.33 m³/h from the product side. Regeneration and waste processes generate 80.54 m³/h of total waste, including chemicals, with a TDS of 9666.42 mg/L. The diagram also indicates use of cation (SAC) and anion (SBA) resins and includes degassing to remove dissolved CO₂ before polishing.

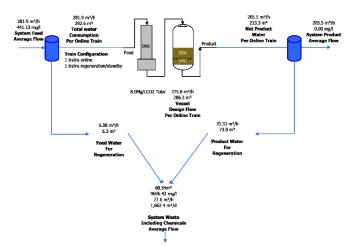


Figure 4. IX system flow diagram.

The resin volume and operating cycle for this model were calculated based on the input specifications. The IX system configuration as shown in Figure 4, depicts WAVE software calculating the feed and product flow rates for the designed system, set at 281.9 m³/h and 205.5 m³/h, respectively. The system input flow is expected to be the same as the operating flow due to the inclusion of a standby train in the model. The IX overall system recovery, as shown in Figure 4, is 72.9%. Specific velocity (BV/h) was selected and used for the regeneration frequency, and as a result, the operating flow, the specific velocity value and the resin volume became fixed. The operating cycle length is calculated using the vessel size recommended by WAVE. WAVE also configured and developed the model parameters based on the resin's arrangement/choice (SAC, SBA) and the selected regeneration system (MB: internal regeneration) from the IX initialization window. The estimated run time for the IX process is 1.04 hours, while the expected regeneration time based on the design model and calculations is 4.27 hours. Hydrochloric acid and sodium hydroxide are used as regenerants for the cation and anion resins, respectively. The selected resin for this model is Amberlite (SAC, SBA), loaded one on top of the other in the MB internal regeneration vessel.

8. Design Consideration

The data in the UF, RO, and IX model output provides the expected operating conditions of the system. This information is used to size and select the system feed pumps, the interstage booster pumps (if any), and energy recovery equipment to meet the system's operating requirements. The UF backwash is scheduled to be repeated several times, depending on the fouling tendencies of the UF membrane modules. The frequency of the UF CIP is 1-3 months, adjusted based on the operating conditions. The CIP operation begins with a backwash sequence and ends with a backwash sequence. Given the comparatively high frequency of mini-CIP (usually once or twice a week), automating the procedure is recommended to save labour costs. The current auxiliary system for standard CIP is exploited for more frequent and shorter chemical cleanings in mini-CIP, eliminating the need for extra installation or hardware. The mini-CIP takes approximately 30 minutes and involves three steps: a standard backwash pre-cleaning, a heated chemical solution recirculation with a soaking period and in between intermittent air scour, and a final backwash post-cleaning. If the fouling is extensive, this phase may take longer, possibly reaching or exceeding 12 hours. It is worth noting that the mini-CIP replaces the CEB rather than the typical intensive CIP program, which may still be required regularly. The water quality analysis of the RO model revealed that monovalent ions such as Na+ and Cl- were predominant. Among the divalent ions, K2+ showed the highest concentration at 7.33 mg/L, while Mg2+ and SO42- had relatively lower concentrations at 3.45 mg/L and 4.66 mg/L, respectively.

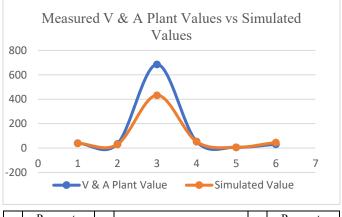
9. Result and Discussion

This section presents the result of the model study in comparison to the measured data from the V & A desalination plant. Table 5 presents the result of the model study in comparison to the measured data from the V & A desalination plant. The table indicates that the measured feed pressure and permeate flow values are 39.8 m³/h and 53.4 bar, respectively, while the simulated values are 39.73 m³/h and 52.67 bar. The simulated results demonstrate a reduction in specific energy consumption (SEC) from 6.58 kW/h to 5.91 kW/h and an increase in system recovery from 31% to 45.7%.

Table 5. Plant measured data in comparison to WAVE simulated data.

| Parameter | V & A Plant Value | Simulate d Value | Varian ce (%) | |
|---------------------------------------|-------------------------|---------------------|------------------|--|
| Permeate Flow [m3/h] | 39.8 | 39.73 | 0.2 | |
| Permeate TDS [mg/l] | 685.5 | 433.2 | 36.8 | |
| Feed Pressure [Bars] | 53.4 | 52.67 | 1.4 | |
| Specific Energy Consumption [kW/h] | 6.58 | 5.91 | 10.2 | |
| Recovery | 31 | 45.7 | 32.2 | |

The comparison of measured and simulated data offers insights into the performance of the reverse osmosis (RO) desalination system and the reliability of the simulation model. The simulated results of the RO were compared with operating data from the V&A desalination plant (Figure 5). The permeate flow rate showed minimal variance between plant and simulated data, confirming the robustness of the predictive model and its accuracy in forecasting permeate flow, replicating the system's hydraulic performance. This accuracy is critical for optimizing operations and ensuring consistent freshwater output.



| 1 | Permeate flow | 2 | Feed TDS | | Permeate TDS |
|---|------------------|---|--------------------------------|---|-----------------|
| 4 | Feed Pressure | 5 | Specific Energy Consumption | 6 | Recovery |

Figure 5. Measured V & A desalination plant data Vs simulated data.

Furthermore, the simulated feed pressure data aligned closely with the measured values, indicating that the model effectively estimates the system's hydraulic pressure requirements. Feed pressure is crucial as it directly affects energy consumption and system

reliability, further reflecting the simulation's reliability in predicting the RO system's mechanical operation.

However, the simulated feed total dissolved solids (TDS) were significantly lower than the actual plant value. This discrepancy may stem from model assumptions, such as a higher efficiency of the pretreatment system (e.g., ultrafiltration). In reality, variations in raw seawater quality or inadequate pretreatment could lead to higher feed TDS. This highlights the need to validate the model under diverse feed water conditions to enhance its robustness.

A reduction in permeate TDS generally improves water quality, as noted by [25] and [26], who found that increased feed pressure decreases permeate TDS, thereby enhancing permeate flux and salt rejection while reducing specific energy consumption (SEC). The significant difference between measured and simulated permeate TDS suggests that the model predicts lower salinity than actual plant performance, likely due to assumptions of ideal operating conditions with minimal fouling or scaling. Real-world factors such as fouling, scaling, or partial bypass flow could elevate permeate TDS, and adjusting the model to account for these conditions could enhance its predictive accuracy.

The simulated SEC result indicates lower energy consumption than the plant operational data. However, achieving theoretical SEC can be challenging due to concentration polarization, hydraulic resistance, and membrane fouling [27]. The 10.2 percent variance from the measured data suggests significant positive impacts on energy consumption, potentially reducing operational costs. This variance may also arise from idealized simulation assumptions, such as less fouling, lower feed TDS, and higher recovery rates, which all lower energy demands. In practice, factors like membrane ageing, fouling, and pump inefficiencies could increase energy consumption. Iterative tuning (and/or WAVE's default sizing routine) was used for this model rather than any metaheuristic. Although Genetic Algorithm or simulated annealing was not used for this work, future work could explore this to further improve efficiency of the system.

The notable variance in recovery rate indicates that the simulation predicts a higher water recovery capacity than what the plant currently achieves. In real-world

operations, recovery is often constrained by scaling, fouling, and operational safety margins to prevent membrane damage. The high simulated recovery rate represents optimal conditions, which would necessitate improved pretreatment and regular maintenance to achieve in practice.

The resulting permeate concentration is 156.5 mg/L (Na+), while the other ions are not detected by the model due to their absence or low concentration. The brine concentration, at 433.2 mg/L TDS, is within the acceptable range for the system recovery rate of 45.7%, and this can also be further confirmed with the equation (R / (1 - R) = cb / cf) with a rejection of 99.9 % [28]. The output from the computer models of the RO membrane system raised warnings regarding the concentrations of calcium sulfate, barium sulfate, strontium sulfate, and calcium fluoride, which have surpassed their individual solubility limits in the reverse osmosis concentrate flow stream. An antiscalant is required for this model to prevent chemical compounds in the feed/concentrate stream from precipitating and causing membrane scaling. The pH of the post-treatment water was measured at 7.18, indicating that the water is safe for consumption.

10. Conclusion and Recommendation

This study aims to develop a reliable predictive model for seawater reverse osmosis (SWRO) membrane desalination systems. The Water Application Value Engine (WAVE) simulation model shows a theoretical improvement in system performance, especially in predicting hydraulic parameters such as permeate flow and feed pressure. Furthermore, it indicates significant improvements in operational parameters, such as specific energy consumption (SEC) and system recovery. Notably, the reduction in SEC was achieved without requiring membrane replacement, leading to a reduction in the plant's overall operational costs.

To strengthen future modelling efforts, it is recommended that the model should be validated across various operational scenarios, including seasonal changes and membrane cleaning cycles, to ensure reliability under diverse conditions. Overall, the simulations provided insights into operational variables and system performance, including feed pressure, concentration, and velocity across membranes and resins, along with their

interactions. The model also provides a robust framework for understanding RO system performance.

With further refinements, the model can effectively facilitate the design of efficient seawater desalination systems, boost RO plant productivity, reduce operational costs, and enhance system efficiency.

Conflicts Interest Statement

The authors declare that they have no known conflicts financial interests or personal relationships that could have influenced the work reported in this article' or authors should disclose any potential conflicts of interest that could be perceived as influencing the research or its outcomes.

Data Availability Statement

Supplementary materials and data used in this research are accessible upon request. For access, please contact the corresponding author via email:

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