

SHAPE-OPTIMIZATION OF MEMBRANE CHANNELS
TOWARDS IMPROVED SEAWATER DESALINATION

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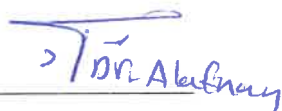
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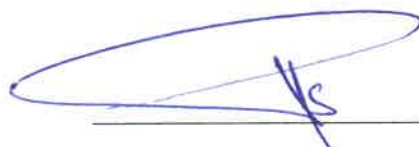
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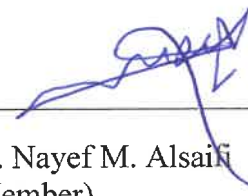


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|To my inspiring father & my caring mother |

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LIST OF ABBREVIATIONS

CDFP	:	Concentration Dependent Fluid Property
CFD	:	Computational Fluid Dynamics
CNT	:	Carbon Nanotube
MD	:	Membrane Distillation
MOF	:	Metal Organic Framework
MSF	:	Multi-Stage Flashing
PER	:	Performance Enhancement Ratio
PPM	:	Parts Per Million
RO	:	Reverse Osmosis
SDG	:	Sustainable Development Goal
SEC	:	Specific Energy Consumption
SR	:	Salt Rejection
TDS	:	Total Dissolved Solids

|

ABSTRACT

Full Name : Hasan Mansour Ahmad AlShafei
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This study explores a method to optimize the reverse osmosis process through shape reconfiguration of feed channels. Computational Fluid Dynamic (CFD) simulations were conducted to calculate water flux and viscous dissipation losses. An economic performance metric combining both variables to evaluate the new models was developed and defined as the profitability rate. The profitability rate represents the difference between the value of product water and the operational cost attributed to energy consumption. The bottom boundary curve in the simulation model represents the interface between feed channel and the permeate collection channel. This boundary was constructed using a variety of three mathematical profiles – comprising the Logistics, Gompertz, and third-order Polynomial functions for the purpose of investigating their effect on the optimization trials. The most promising outcomes were achieved using the Logistics function, with a profitability increasing by 12.2% relative to the baseline design. Sensitivity analyses were conducted to examine how the values of permeate water and the feed Reynolds number affect the optimal shape, represented through the channel-integral-depth parameter. The channel integral depth reflects the curvature of the membrane wall boundary relative to the conventional flat membrane wall used in the baseline design. It was revealed that the optimum channel integral depth saturates to a maximum when the water permeate value exceeds a transition point – where the product water value dominates over the energy cost. Water feed flow and the rate of viscous dissipation losses are proportional to feed Reynolds number, translating to both larger product revenue and operational cost at higher feed flow rates. Accordingly, a critical Reynolds number was observed that produces the maximum optimal channel integral depth. Using our shape optimization procedure, it was demonstrated that geometrical reconfiguration of the feed channel generates a positive rate of return.

ملخص الرسالة

الاسم الكامل: حسن بن منصور بن أحمد الشافعي

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تقوم هذه الدراسة باستكشاف طريقة لتحقيق الدرجة المثلى في عملية التناضح العكسي من خلال إعادة تشكيل قنوات التغذية. عمليات محاكاة ديناميكية السوائل الحسابية استخدمت من أجل حساب التدفق المائي وخسائر تبديد المائع. لقد تم تطوير مقياس أداء اقتصادي شامل لكل من المتغيرين لتقييم النماذج الجديدة وعرف بالمعدل الربحي. المعدل الربحي يمثل الفرق بين قيمة الناتج المائي والتكاليف التشغيلية المرتبطة باستهلاك الطاقة. يمثل المنحنى السفلي في نموذج المحاكاة الواجهة بين قناة التغذية وحاجز الغشاء. هذا المنحنى قد شكّل باستعمال ثلاث دوال رياضية، وهي الدالة اللوجستية ودالة جومبيرتز والدالة المتعددة الحدود من الدرجة الثالثة. الدالة اللوجستية حققت أفضل النتائج حيث أن المعدل الربحي زاد بنسبة 12.2% بالنسبة إلى التصميم الأساسي. لقد أجريت تحاليل الاستجابة من أجل دراسة تأثير قيم الناتج المائي ورقم رينولدز للدخيل على شكل القناة الأمثل، والذي تم تمثيله من خلال العمق التكاملي للقناة. العمق التكاملي للقناة يمثل درجة الانحناء لحاجز الغشاء بالنسبة إلى الحاجز المستوي المتواجد في التصميم الأساسي. اكتشف البحث أن العمق التكاملي للقناة في شكل القناة الأمثل قد وصل إلى الحد الأقصى عندما تجاوزت قيمة الناتج المائي نقطة انتقالية لأن ثمن الماء تعدى على تكلفة الطاقة. بما أن كلاً من الناتج المائي الإجمالي ومعدل خسائر تبديد المائع يتناسبان طردياً مع رقم رينولدز لتدفق الماء الدخيل، فإن إيرادات الإنتاج وتكاليف التشغيل يزدان مع زيادة تدفق الماء الدخيل. لهذا السبب فإن هنالك قيمة محددة لرقم رينولدز من حيث وصول العمق التكاملي للقناة إلى النسبة العليا. من خلال استعمال أسلوب الامتياز الأمثل فقد تم استنتاج أن إعادة التشكيل لقناة الدخيل قد أدت إلى عائد ربحي.

CHAPTER 1

INTRODUCTION

1.1 History of Reverse Osmosis Spiral Wound Module Development

The earliest recorded documentation of the membrane separation principle based on osmotic pressure dates to 1748, following observations by Abbe Nollet. A significant milestone in the development of modern Reverse Osmosis (RO) technology occurred in 1948, when Dr. Gerald Hassler at the University of California, Los Angeles (UCLA), began investigating the osmotic properties of cellophane. Initially, Dr. Hassler hypothesized that osmosis involved surface evaporation, vapor permeation, and subsequent surface condensation on the opposite side of the membrane. However, it is now understood that osmosis primarily involves the diffusion of different solutes across the membrane at contrasting rates [1].

The first patented design of a reverse osmosis (RO) spiral-wound membrane module was introduced in 1963 by Gulf General Atomics. A deconstructed representation of the spiral-wound membrane configuration is presented in Figure 1. A cross-sectional area of spiral wound consists of two membrane sheets placed back-to-back with a permeate collector channel sandwiched between them, forming a single membrane “leaf”.

Modern RO spiral-wound membranes are typically composed of three layers: polyester support web, polysulfone interlayer, and polyamide barrier. The last layer is positioned adjacent to the feed channel. The objective of the first two layers is to provide support and structure for the last layer. They are highly porous to facilitate water permeability. The polyamide barrier, on the other hand, enables high salt rejection. This membrane family was developed to achieve lower salt rejection with relatively higher operating pressure compared to the other membrane family, cellulose acetate membranes.

Each membrane layer is adjoined by a feed spacer layer on one side, and a permeate spacer layer on the other. These spacers are critical in shaping the hydrodynamic behavior within the RO module. They disrupt the flow and enhance mixing near the membrane surface, thereby mitigating concentration polarization [2, 3]. Feed spacers are commonly created from polypropylene material, where the typical channel height is about 0.8 mm [4]. In contrast, the permeate spacer channel height ranges between 0.2 and 0.3 mm [5]. All membrane leaves are helically wound around a central perforated permeate collection tube. The tube collects permeate water from each membrane leaf, while the remaining brine continues to flow through the feed channels. A fraction of feedwater permeates through the membrane, passing through the permeate spacer and into the central tube for collection.

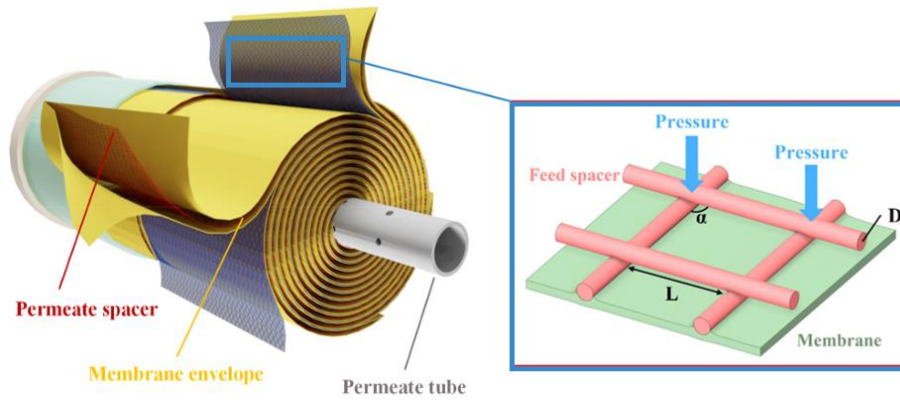


Figure 1 Deconstructed presentation of a spiral-wound RO module

These elements feature high packing density with small footprints, offering a simpler framework for maintenance, plumbing, and system design compared to other RO configurations. These advantages significantly accelerated the adoption of RO desalination processes [6].

1.2 Reverse Osmosis Terminology

The RO process can be described using key terms that provide a comprehensive understanding of its operational principles. These terms include water salinity, chemical potential, semipermeable membrane, permeate recovery rate, net driving pressure, salt passage and rejection, average permeate flux, specific permeability, and the concentration polarization factor.

Water salinity refers to the concentration of dissolved ions in water, typically expressed in parts per million (ppm). It is a critical parameter influencing the osmotic pressure and, consequently, the performance of RO systems. Chemical potential, a thermodynamic

quantity, represents the free energy per unit of a substance available for release or absorption during chemical reactions or phase transitions. In the context of RO, differences in chemical potential drive molecular transport across the membrane. These differences arise from gradients in salinity, temperature, and ionic composition, dictating both the direction and the magnitude of water and solute movement.

The semipermeable membrane serves as a selective barrier, allowing water molecules to pass through while rejecting dissolved salts and other solutes. This selectivity depends on the membrane's physical pore size and chemical properties. The permeate recovery rate is defined as the ratio of the volumetric flow rate of the product water (permeate) to that of the feed water, reflecting the efficiency of water extraction.

The net driving pressure (NDP) is the effective pressure driving water transport across the membrane. It is calculated as the difference between the applied feed pressure and the sum of osmotic pressure and system pressure losses, such as those due to flow resistance in the feed and brine channels. Salt passage quantifies the fraction of salts passing through the membrane and is defined as the ratio of salt concentration in the permeate to the average feed salt concentration. Salt rejection, conversely, represents the percentage of salts retained by the membrane, calculated as:

$$\text{Salt Rejection (\%)} = \left(1 - \frac{C_p}{C_0}\right) \times 100\%$$

Where C_p is the salt concentration in permeate water, and C_0 is the salt concentration in the feed.

Average permeate flux represents the volumetric flow rate of permeate normalized by the total membrane area, providing a measure of water production efficiency. Specific permeability, also known as specific flux, is a key performance parameter defined as the average permeate flux divided by the net driving pressure. It reflects the membrane's ability to produce water under given operating conditions.

The concentration polarization factor describes the ratio of salt concentration at the membrane surface to that in the bulk solution. This factor reflects the propensity for salts to accumulate at the membrane interface, which can exacerbate fouling and scaling. Proper management of concentration polarization is critical to maintaining system performance and longevity.

These terms collectively form the foundation for understanding and optimizing the performance of reverse osmosis systems.

1.3 Mechanism Theories of Reverse Osmosis

Osmosis is a natural process where water flows through a semipermeable membrane from an area of low solute concentration to an area of higher solute concentration. The driving force for this movement is the difference in chemical potential, which is a function of the solute concentration. For simplicity, this work focuses on the salt concentration difference as a proxy for chemical potential, given that it is easier to measure and has a direct influence on osmotic pressure in reverse osmosis processes. This is because salt concentration difference is easily measured and calculated, and since salt concentration is the predominant factor affecting chemical potential in reverse osmosis process. Osmosis

occurs until water flow reaches equilibrium when the concentration difference becomes zero between the two compartments in a batch process. In a steady-state process, water flow is governed by convection in addition to diffusion; the flow is continuous due to constant fluid motion. Reverse osmosis involves applying external pressure that exceeds the osmotic pressure due to the concentration difference. This overcomes the natural osmotic tendency and forces water to flow from the compartment with higher solute concentration to the compartment with lower solute concentration.

Reverse osmosis membranes are selectively permeable, allowing only water molecules to pass through while rejecting salts and other solutes. As water moves from the feed to the permeate channel, salt ions accumulate on the feed side of the membrane, creating a counteracting force that opposes the direction of permeate flux. To mathematically describe this behavior, several theories have been formulated to relate performance with operational conditions. Theories of reverse osmosis transport propose different mechanisms based on concepts from irreversible thermodynamics, diffusion, and capillary flow. These theories offer distinct pathways for molecular transport and are used to explain the performance of reverse osmosis under varying operational conditions [7]. This section covers examples corresponding to each theory. The examples for transport model theories are the Spiegler-Kedem-Katchalsky model, solution-diffusion (nonporous) model, and pore flow (porous) model.

1.3.1 Spiegler-Kedem-Katchalsky Model

Kedem, O., and Katchalsky, A., 1958 [8] developed a theoretical model for the reverse osmosis process through non-equilibrium thermodynamics equations. A central assumption is that non-equilibrium state can be divided into isothermal local equilibrium

subsystems as illustrated in Figure 2. This approach allows for the detailed for the detailed analysis of the osmotic and hydraulic pressures involved in the reverse osmosis process. While both water chemical potential and pressure are lower at the permeate channel side, water concentration remains fixed across the feed and permeate channels. The mathematical formulae treat concentration and pressure gradients in a series of infinitesimal parts. These equations are expressed below.

$$J_W = -P_W \left(\frac{dp}{dy} - \sigma \frac{d\pi}{dy} \right) \quad (1.1)$$

$$J_S = -P_S \frac{dc_S}{dy} + (1 - \sigma) J_W c_S \quad (1.2)$$

$$\sigma = -\frac{L_{pD}}{L_p} \quad (1.3)$$

Where J_W is water flux, J_S is salt flux, π is osmotic pressure, c_S is surface salt concentration, P_W is local hydraulic permeability, σ is reflection coefficient, L_{pD} is kinetic cross-effect coefficient between driving forces of pressure and concentration, L_p is kinetic filtration coefficient, and y is position along transport direction in the feed channel.

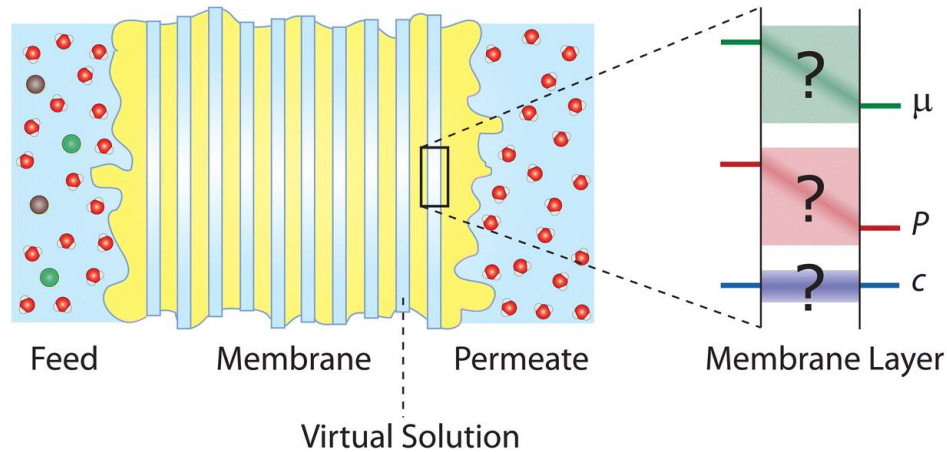


Figure 2 Microscopic representation of the Spiegler-Kedem-Katchalsky model. The diagram illustrates the chemical potential of water (green) and the pressure drop across the membrane layer, while the water concentration (blue) is depicted as being equivalent on both sides of the membrane.

Although the Spiegler-Kedem-Katchalsky model is less frequently discussed in modern membrane research, it remains a fundamental framework for understanding reverse osmosis. Their thermodynamic principles continue to serve as a foundation for subsequent theoretical developments in osmosis transport theory. Building on these thermodynamic principles, later research introduced alternative models for osmosis, including the Solution-Diffusion Model, which assumes a different mechanism for solute and solvent transport.

1.3.2 Solution-Diffusion Model (non-porous)

The Solution-Diffusion model, first proposed by Lonsdale et al. in 1965 [9], assumes of a perfectly non-porous membrane, where transport occurs via dissolution and diffusion rather than through pores. It is believed that salt transportation in membranes is through a concentration gradient, which adheres to Fick's first law of diffusion. As shown in Figure 3, the model assumes that water and salt molecules partially dissolve into the membrane,

diffuse across it, and then partition out of the membrane on the other side. The pressure within the membrane is assumed to be equivalent to feed pressure, whereas water concentration decreases as molecules diffuse through the barrier. The transport of water and salt ions are assumed to be independent of each other. This assumption simplifies the model by treating each component separately, despite the potential interactions between water and solute. Later works by Paul and Ebra-Lima improved the theory by incorporating the effect of the pressure gradient by assuming constant pressure profile across the membrane layer. Mathematical formulae (1.4) – (1.7) describe water and salt fluxes as per the Solution-Diffusion (non-porous) model.

$$J_W = A (\Delta P - \Delta \pi) \quad (1.4)$$

$$A = \frac{D_W K_W \bar{V}_W c_W(y=0)}{lRT} \quad (1.5)$$

$$J_S = B (C_S[y = 0] - C_S[y = l]) \quad (1.6)$$

$$B = \frac{D_S K_S}{l} \quad (1.7)$$

Where J_W is water flux, J_S is salt flux, π is osmotic pressure, c_S is salt concentration, l is membrane layer thickness, T is temperature, R is ideal gas constant, D_i and K_i are diffusion and partition coefficients for component “i”, $\bar{V}$ is partial molar volume, A is water permeability constant, B is salt permeability constant, and y is position along transport direction in the feed channel.

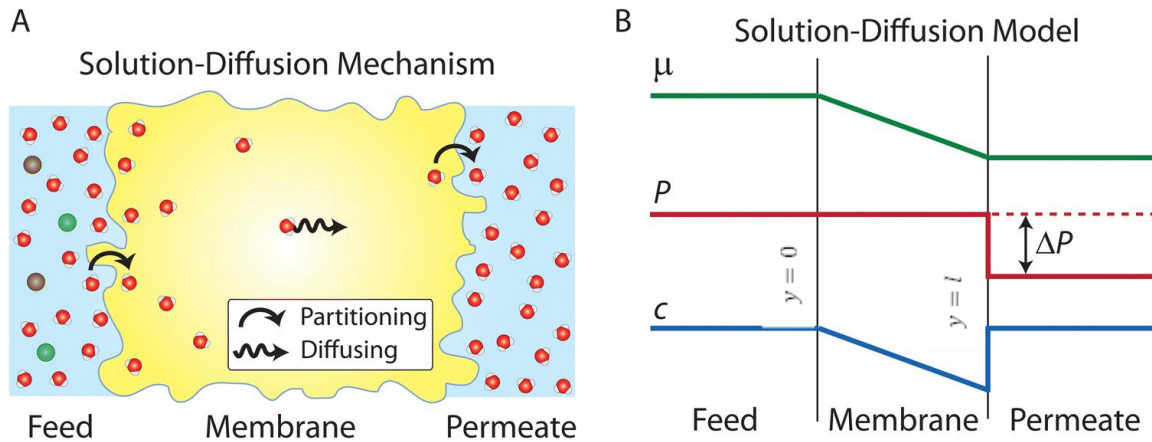


Figure 3 Microscopic representation of the Solution-Diffusion model. The diagram illustrates the water chemical potential (green) and water concentration (blue) decreasing across the membrane layer, while the pressure (red) remains constant within the membrane and equivalent to the feed channel pressure.

Having explored the non-porous approaches in reverse osmosis models, an alternative approach is through the porous mechanism of water transport. Pore-Flow Model, which operates on the assumption of flow through micropores within the membrane, introduces a different perspective on how water and solutes move in reverse osmosis processes. This model, based on Darcy's law, emphasizes the role of pressure gradients in driving water transport, offering insights into the behavior of membranes with porous structures.

1.3.3 Pore-Flow Model (porous)

Sourirajan, S., 1963 [10] had proposed water transport in cellulose acetate membranes to follow a viscous type of flow mechanism. His model was called preferential sorption – capillary flow, which is derived from generalized capillary flow. The model states that through external pressure, solute and solvent molecules permeate through micropores of the membrane, which is illustrated in Figure 4. In this process, the solvent is preferentially adsorbed by the pore walls, while the solute is rejected due to the membrane's physiochemical characteristics. The Pore-Flow Model assumes that water transport is

driven by a pressure gradient within the membrane, with a constant concentration of solute. The mechanism is based on the movement of water through micropores, which is influenced by the pressure difference across the membrane. Pore-Flow Model is derived from Darcy's law as described in equation (1.8).

$$J_W = k \frac{dP}{dy} \quad (1.8)$$

Where J_W is water flux, k is Darcy law coefficient, P is pressure profile within membrane, and y is position along transport direction. Darcy law coefficient is dependent upon water viscosity and membrane structure and porosity.

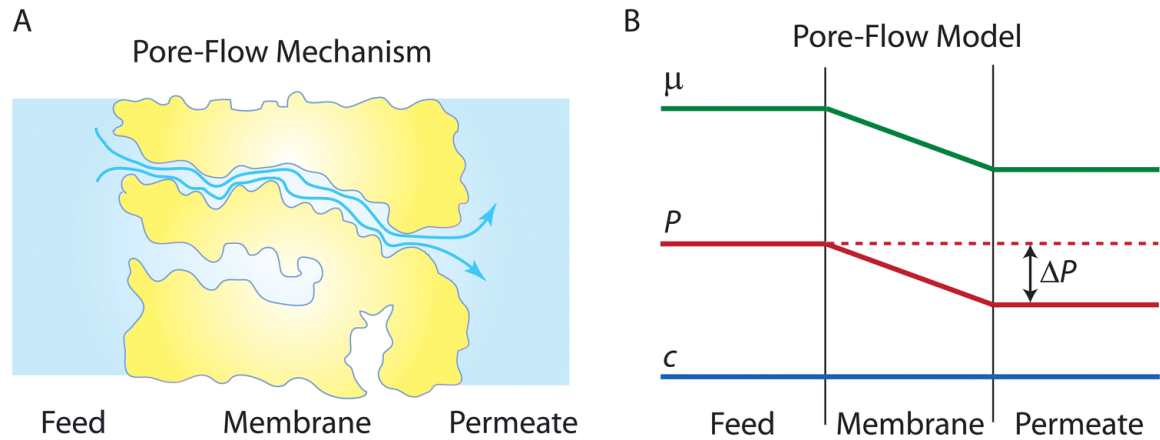


Figure 4 Microscopic representation of the Pore-Flow model. The diagram illustrates the water chemical potential (green) and pressure (red) decreasing across the membrane layer, while the water concentration (blue) remains constant throughout the membrane.

1.4 Study Objective

Spiral-wound membranes are the most widely adopted configuration in Reverse Osmosis (RO) systems due to their compact design and operational efficiency. A fundamental

parameter in evaluating membrane performance is water salinity, typically expressed as total dissolved solids (TDS). The acceptable TDS levels vary depending on the intended application. For example, potable water is recommended to have a salt concentration of about ~500 ppmw [11], whereas water for industrial applications, such as feedwater for boilers, requires TDS levels below 10 ppmw [12]. In contrast, seawater typically has a salinity of 35,000 ppmw [13].

This significant disparity between the salinity of feed water and the desired purity of product water necessitates the use of highly selective membranes capable of effectively rejecting salt ions. However, as salts are excluded from permeating through the membrane, they tend to accumulate at the membrane-feedwater interface. This accumulation increases local osmotic pressure and inhibits water transport, thus requiring higher applied feed pressures to maintain desired flux rates; ultimately resulting in elevating energy consumption.

This study addresses the economic trade-offs inherent in RO operation by proposing a novel approach: optimizing the feed channel geometry to simultaneously enhance water production and reduce energy demand. To this end, a key performance indicator referred to as the Profitability rate, is introduced as the primary objective in the shape optimization framework. This metric integrates the economic value of the produced water with the cost of mechanical work input, offering a holistic evaluation of system performance.

The novelty of this research lies in presenting an optimum feed shape design that enhances operational cost-effectiveness of water purification processes. This approach modifies the conventional feed channel design by introducing curvature along the membrane layer to

maximize the profitability rate. Shape optimization represents an advanced strategy that offers a more economically viable solution for desalination applications. This work aspires to revolutionize the manufacturing industry of spiral wound membranes since it elevates economical profitability of RO processes.

Technological advancement offers ways to purify water resources with high salinity to be consumed for residential and commercial purposes. Two technologies currently dominate the market for water purification. The first is multi-stage flashing (MSF). It evaporates saline water, which is condensed as high-purity water. The second is Reverse Osmosis (RO). RO is a purification process that utilizes membranes selectively permeable to water ions in the feed stream. Other recent emerging technologies involve carbon nanotube (CNT) membranes [14], metal organic frameworks (MOFs) [15], and membrane distillation (MD) [16]. In comparison with thermal desalination, RO offers more energy efficiency. Typically, seawater RO has a Specific Energy Consumption (SEC) between 3-6 kWh/m³, whereas MSF has an SEC of 21-59 kWh/m³, as reported by Stillwell and Webber [15]. The SEC of other commercialized water purification processes are listed and summarized by Stillwell and Webber [17] in Table (1).

Table 1 Typical SEC for commercialized water purification technologies

Technology	Specific Energy Consumption (SEC) in Electric Energy Equivalent (kWh/m³)
Seawater Reverse Osmosis	3 – 6
Multi-vapor Compression	7 – 15
Forward Osmosis	10 – 68
Membrane Distillation	3 – 22
Multi-stage Flashing	21 – 59
Multiple Effect Distillation	15 – 57
Multiple Effect Boiling	30

The SEC is one approach to measure economic viability of water treatment technology. An alternative approach is profitability rate, which was adopted in this work to assess economic feasibility by combining water product value and power consumption cost. The computed profitability rates vary between regions due to changes in water prices and energy tariffs. For example, the water value in Denmark is 3.3 \$/m³ [18], while in Italy it drops to 0.88 \$/m³ [19]. These prices are influenced by many factors, such as governmental subsidies and taxes, available water resources, and wastewater treatment recycling policies. Similarly, energy tariff costs fluctuate by region. In 2023, average electricity prices for household consumers in Europe had reached 0.31 \$/kWh [20], while in the GCC countries, such as Qatar, the energy tariff can be as low as 0.032 \$/kWh [21]. In comparison, Saudi Arabia has a potable water cost of 1.96 \$/m³ [22] and an energy tariff of 0.05 \$/kWh [23]. Optimization trials were carried out using the permeate water price and energy unit cost for Saudi Arabia to compute the profitability rate by way of example. Additional trials were conducted by varying the water product price to expand the model for a comprehensive outcome.]

CHAPTER 2

LITERATURE REVIEW

2.1. RO Feed Channel Shape Manipulation

The performance of RO can be manipulated by varying the feed channel shape profile. Zemour et al., 2021 [24] numerically simulated the performance of reverse osmosis using two channel configurations. The first configuration featured a channel bounded by a membrane on one side and a wall on the other, while the second configuration had membranes on both sides. The results indicated that water recovery and concentration polarization varied between the two configurations. Additionally, their numerical simulation was validated with experimental work at two-gauge pressures, 8.99 barg and 14.0 barg. The impact of mean flow velocity on permeate flow was studied, with the mean absolute error being below 4.5% for the high-pressure dataset. The novelty of this study lies in presenting an optimal membrane shape that enhances operational cost-effectiveness of water purification processes. This approach modifies the conventional feed channel design by introducing curvature along the membrane layer to maximize the profitability rate.

A potential counterargument to the abovementioned proposal is that the benefits from modulating feed channel shape can instead be achieved using feed spacers, which has been extensively studied in RO systems. Feed spacers have two primary roles in feed channels. While the first is to separate membrane leaves apart to allow for feed flow, the second is

to promote turbulence. Consequently, this enhances fluid mixing along with mass transfer [25]. There are numerous feed spacer arrangements and filament types as shown in figure 5. For example, the spacers can be arranged through a ladder, submerged, or wavy structure [26]. Similarly, geometrical filaments can be modified to be circular, elliptically deformed, octagonal, or rectangular [27].

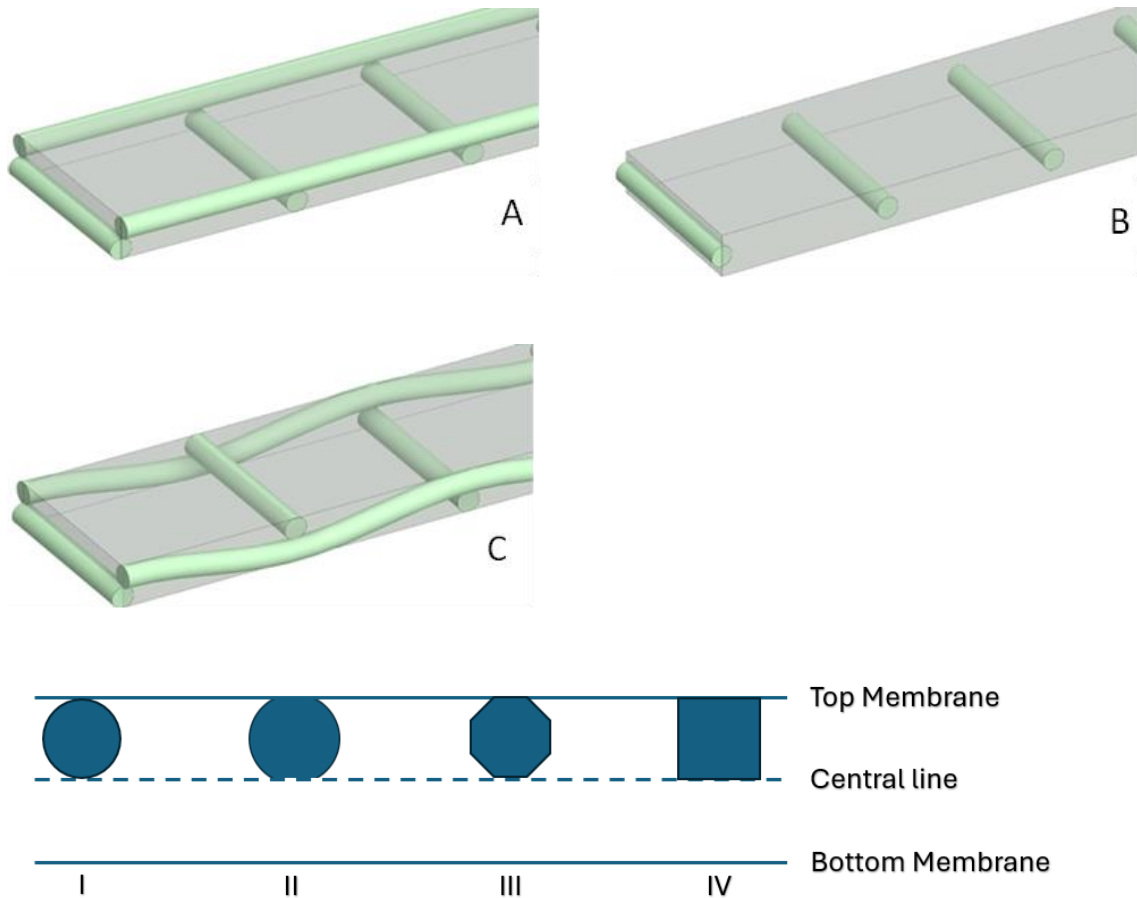


Figure 5 The potential arrangements for spacers in the feed channel are presented by the above three types: (A) ladder, (B) submerged, and (C) wavy. The cross-sectional areas for spacer filaments are demonstrated, where they can be (I) circular, (II) elliptically deformed, (III) octagonal, or (IV) rectangular.

Haidari et al., 2018 [28] presented a comprehensive study on the optimal design of feed spacers for RO systems. Spacers introduce turbulence to the water flow inside the feed channel, reducing the retarding effect of concentration polarization. Feed spacers generate significant increase in channel pressure losses ranging between 2.5 and 160 times that of a spacer-free channel [28]. There are additional setbacks with feed spacers application. Their surfaces offer a susceptibility to biofouling. Vrouwenvelder et al., 2011 [29] investigated the consequences induced by spacer biofouling, which were found to introduce a more severe outcome to energy consumption than membrane biofouling. Nevertheless, the conclusion has sparked debate in the literature, with some scholars objecting to the relative severity of spacer fouling [30], while others support the findings [31].

Configuration of feed spacers can be modulated to fit the optimum feed channel shape design. Haaksman et al., 2017 [32] proposed an arrangement for feed spacers where filament thickness is alternating longitudinally along the feed direction. The collected results demonstrated that the alternating strand thickness approach was highly efficient in converting mechanical energy into shear stress. Accordingly, longitudinal reduction of filament strand thickness will be incorporated with the optimum shape design, thereby offering a synergistic strategy for maximizing water production efficiency and minimizing energy consumption.

Hitherto, no previous work was published proposing the shape optimization of reverse osmosis membrane layers. The existing literature on geometrical optimization has primarily focused on feed spacer design. Bucs et al, 2014 [33], Gu et al., 2017 [34], and Toh et al., 2020 [35] are few examples of scholars who had studied the optimization of feed spacer geometry to improve reverse osmosis performance and minimize concentration

polarization effects. They examined multiple geometric variations for feed spacers using Computational Fluid Dynamics (CFD) numerical simulations.

2.2. Shape Optimization in Fuel Cells

Although shape optimization in RO systems has not been extensively studied, similar methodologies have been successfully employed in fuel cell research, where channel geometry plays a crucial role in system performance. In typical fuel cells, hydrogen and oxygen gases are introduced from opposite ends to generate water and electrical power. The system architecture includes two gas diffusion layers and two catalyst layers, symmetrically arranged around a central membrane layer.

Analogously, RO membrane sheet incorporates a feed spacer channel, which can conceptually be compared to the gas diffusion layer in fuel cells. Both configurations are adjoined by membrane layers that serve as selective transport barriers. The hydrodynamics within the gas diffusion layer of a fuel cell and the feed spacer channel of an RO membrane are governed by the Navier-Stokes equations, highlighting the shared fluid dynamics framework between the two systems. Furthermore, molecular transport through the membrane layers in both technologies follows Fick's second law of diffusion.

Due to these fundamental similarities in fluid flow and mass transport behavior, fuel cell research offers valuable insights that can inform the optimization of RO systems. Several notable studies have demonstrated the effectiveness of shape optimization in enhancing performance metrics in fuel cells. Notable examples include studies by Chen et al., 2006 [36], Al-Smail & Novruzzi, 2011 [37], and Korkischko et al., 2017 [38]. These studies examined different channel geometries and evaluated numerical simulation outcomes

based on multiple key performance indicators, such as hydrogen flux, showcasing the potential of shape optimization techniques in improving transport efficiency.

Chen et al., 2006 [36] varied the internal structures and external shapes of polymer electrolyte membrane (PEM), assessing results based on steady state net power output and fuel cell start-up time. They followed a multi-objective optima approach to solve for the optimum geometric design responding to quick step loads and large power densities. The multi-objective problem was constituted of two levels. The first level is the internal structure, which focused over the dimensional allocation of fuel cells compartments, including anode, cathode, and electrolyte. The second level is the external aspect ratios between fuel cell width and height over its length. It was concluded that there exists a trade-off between steady state net power output and start-up time. It was also revealed that the geometric variables vary depending on cell total volume. Nonetheless, research scope should be further expanded by performing sensitivity analysis while varying the channel membrane length.

Al-Smail & Novruzi, 2011 [37] investigated oxygen concentration on a catalyst layer, outlet vapor fraction, and pressure drop in a hydrogen fuel cell cathode air channel. They reduced the hydrogen fuel cell cathode air channel into a two-dimensional isothermal model. The model was comprised of two gas channels delivering hydrogen and air, two gas diffusive layers composed of porous carbon material, two catalyst layers, and a central specially treated porous membrane layer. The gas channel, diffusive layer, and catalyst layer form the anode at the hydrogen side, while they form the cathode at the air side. The anode catalyst layer split hydrogen molecules into protons and electrons, where the membrane layer conducts only positively charged protons, whereas the blocked electrons

travel through an external circuit. The migrated protons, transferred electrons, and oxygen in air react at the cathode catalyst layer with presence of platinum to produce water and an electric current. The cathode channel longitudinal shape was therefore optimized to enhance performance of hydrogen fuel cells. By solving a series of partial differential equations (PDEs), it was found that there exists a unique solution coupled with an optimum channel shape design.

Korkischko et al., 2017 [38] modified the shape of proton exchange membrane fuel cells to maximize current density generation. In comparison with Al-Smail & Novruzi, 2011 [37], Korkischko et al., 2017 [38] sought to vary cross-sectional shapes of gas flow channels while keeping the areas constant. The objectives were to maximize electrical power output and improve the fuel cell durability. Numerical modeling and simulation techniques through CFD software, COMSOL Multiphysics version 5.3, were employed along with experimental applications to find the optimum cross-sectional area shapes. The outcome for optimum shape was revealed to be an inverted trapezoidal for both the anode and cathode flow channels. Furthermore, the agreement between empirical data and simulation outputs proves the accuracy and precision of numerical simulation to geometrically optimize flow channel shape.

These studies demonstrate that the application of shape optimization has yielded promising results for fuel cells. This research seeks to expand shape optimization to reverse osmosis membranes, as they share similar attributes with fuel cells concerning molecular transport mechanism. The novelty of this study lies in presenting an optimal membrane shape that enhances operational cost-effectiveness for water purification. This approach reconfigures the membrane shape profile from a conventional feed channel with uniform height by

applying curvature along the membrane layer to maximize the profitability rate. Optimizing the membrane shape represents an advanced strategy that offers a more economically advantageous solution for desalination applications.

CHAPTER 3

METHODOLOGY

3.1 Process Background & Overview

The membrane system, which includes the membrane elements housed in pressure vessels and a high-pressure pump constitutes the heart of the RO plant. Figure 6 illustrates a macroscopic overview of the reverse osmosis process. Seawater is pumped from atmospheric pressure to a feed pressure adequate to overcome the osmotic pressure. Desalinated water flows from feed channel to a central tube passing through semipermeable membranes. In this study, permeate water and reject water pressures were set at atmospheric pressure and 60 barg, respectively. The feed volumetric flow rate was preserved by adjusting the feed velocity, $\hat{U}_f$, as the inlet boundary was modified during optimization. Specifically, as the inlet boundary expanded downward, the velocity is proportionally reduced to maintain a constant volumetric flow of 1.09 m³/hr. Such a flow rate corresponds to an inlet velocity of 300 mm/s as in the baseline case. Additionally, feed salt concentration was set at 35,000 ppmw to be modeled as seawater. The length of the reverse osmosis membrane is set to be one meter long, corresponding to the standard used in industrial applications [39].

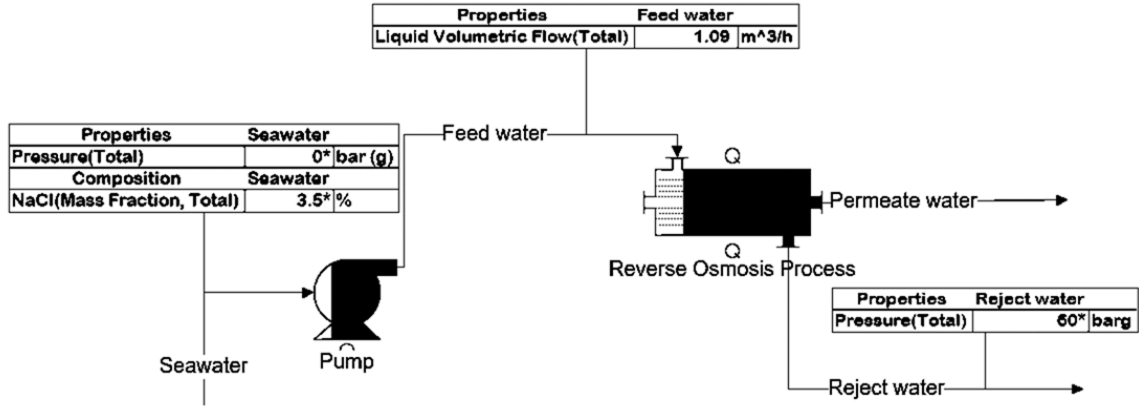


Figure 6 Overview of a reverse osmosis process arrangement depicting a seawater feed with a concentration of 3.5 wt%, and a pump discharge pressure of 60 barg applied upstream of the RO process.

3.2 Model Simulation Setup

The study focuses on the microscopic scale of the reverse osmosis membrane process. Water behavior inside the feed channel was simulated using COMSOL Multiphysics version 6.1. This software contains several numerical simulation packages to perform Computational Fluid Dynamical (CFD) analysis. CFD is the process of predicting fluid behavior following the conservation of laws of momentum, energy, and mass. CFD works by linearizing conservation laws and conducting extensive computations across multiple cells. The collection of such cells is referred to as the mesh.

The RO membrane sheets were modeled as a two-dimensional frame, neglecting the third dimension (sheet width) due to the high aspect ratio and negligible variations associated with laminar flow. The model framework consists of a single layer representing the feed channel, with a symmetry line employed as the top boundary. The base thickness of the feed channel was set at 1.0 mm. The cross-section channel area in the xy-plane was

maintained constant to impose a constraint during the optimization trials. This constraint ensured that the quantity of the membrane module's material sheet remained consistent with the conventional baseline model. Furthermore, the feed volumetric flow rate was kept fixed by adjusting the feed velocity. As the inlet barrier expanded downward during the optimization trials, the velocity was reduced to maintain consistent volumetric flow. To capture the steep transport gradients near the sublayer region, the mesh at the membrane wall boundary was refined to a high resolution. Figure 7 illustrates the base geometry of a half-domain feed channel, with each boundary side numbered: the inlet (1), the top symmetry line (2), the outlet (3), and the bottom barrier (4). The permeate channel modelling is excluded since it has negligible contribution over the simulation outcome. The half-height, H , and axial length, L , of the feed channel are set at 1 mm and 1 m, respectively, for the baseline case. Saline feed water enters boundary 1, where the feed flow is modeled as fully developed flow profile. The membrane is modelled as fully salt-rejecting, allowing only water to pass through, with both the intrinsic rejection, $R_i (\equiv 1 - c_p/c_w)$, and water permeability, A , considered uniform along its length.

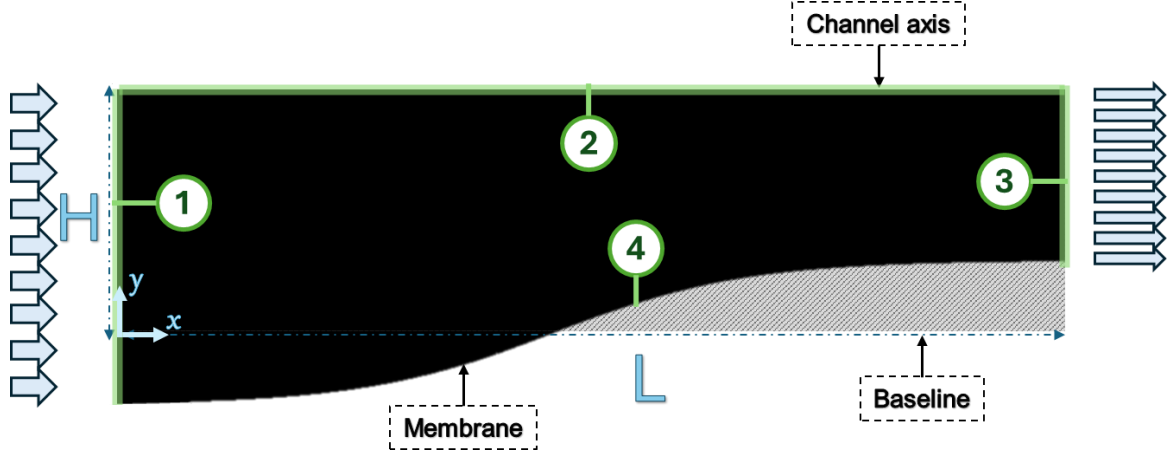


Figure 7 Two-dimensional side elevation of the feed channel with four boundaries. Boundary (1) represents the inlet, (2) is the axial line of symmetry, (3) is the outlet, and (4) is the membrane barrier, the shape of which is to be optimized.

3.3 Numerical Optimization Modelling

The single-objective optimization problem in this work is the maximization of profitability rate, which is expressed in Eq. 3.1. The profitability rate is calculated from the difference of permeate water revenue and operational costs attributed to power consumption.

$$E = Q_m w - \Delta P_f * Q_f * e \quad (3.1)$$

Where E is profitability rate (\$/hr), Q is volumetric flow (m^3/hr), ΔP is pressure difference from atmospheric pressure (Pa), w is the product value (\$/ m^3), e is specific energy cost (\$/kWh), while subscripts f and m represent feed and permeate streams, respectively.

The behavior for salt accumulation at the membrane barrier is governed by diffusive and convective components. Diffusive flux is the transport of mass governed by salt concentration gradient, whereas convective flux is the transport of mass due to bulk fluid motion, which is proportional to fluid y -component velocity. Figure 8 shows salt flux

components plotted along the y-axis at two x-coordinate locations, which are 50-mm and 950-mm from the origin point along a one-meter length.

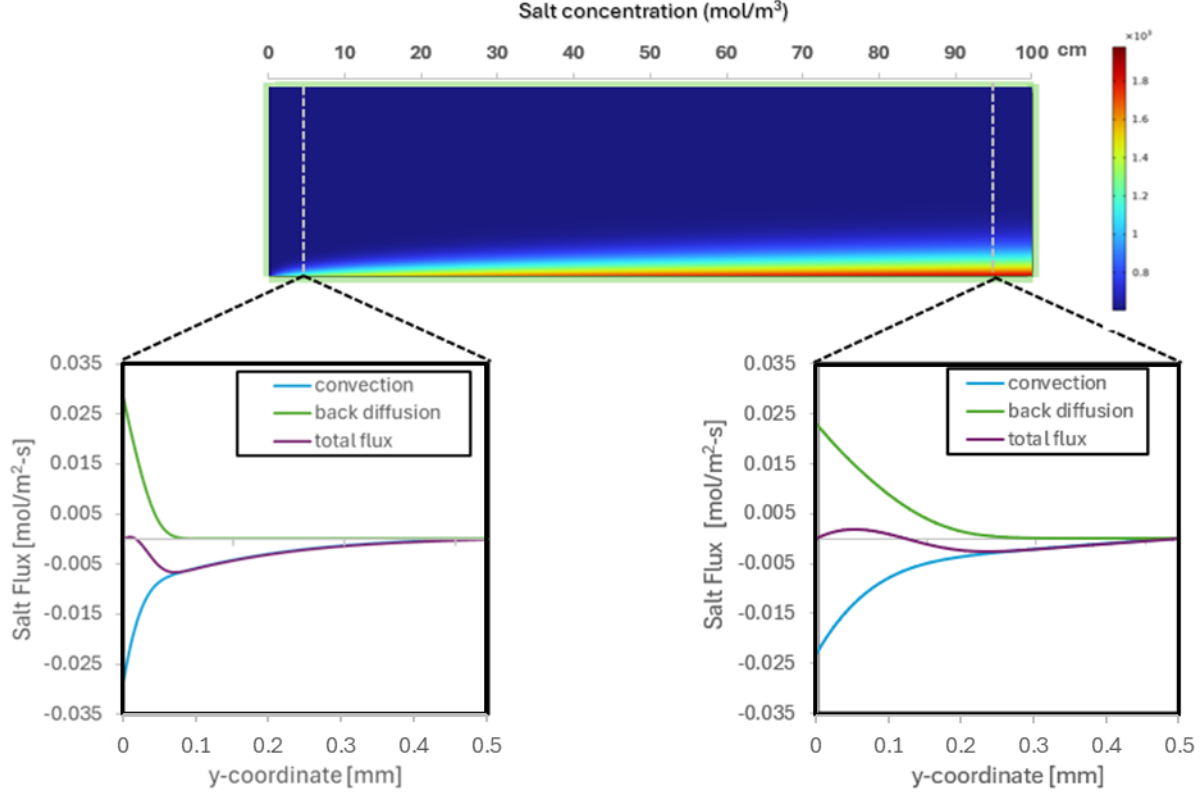


Figure 8 Convective and diffusive components of salt flux and their total at lengths (a) 50 mm and (b) 950 mm of a one-meter channel. These plots explain the accumulation of salt over the membrane layer.

The general direction for diffusive flux is upward (positive), whereas for convective flux is downward (negative). The total flux at both ends of y-axis must be zero given the boundary conditions imposed over boundary (2) for symmetry, and boundary (4) for zero salt flux. This relationship can be described by the spatial integration of the convection-diffusion equation.

$$\nabla \cdot (-\mathcal{D}_s \nabla c + v * c) = R \quad (3.2)$$

$$\rightarrow \int_{\Gamma_x} R(y') dy' = c * v - \mathfrak{D}_s \frac{\partial c}{\partial y} \quad (3.3)$$

Where ∇ is spatial differentiation, $\mathfrak{D}_s$ is salt diffusivity coefficient, c is salt concentration, v is the orthogonal velocity component above the membrane boundary, while R is the creation/destruction rate of salt.

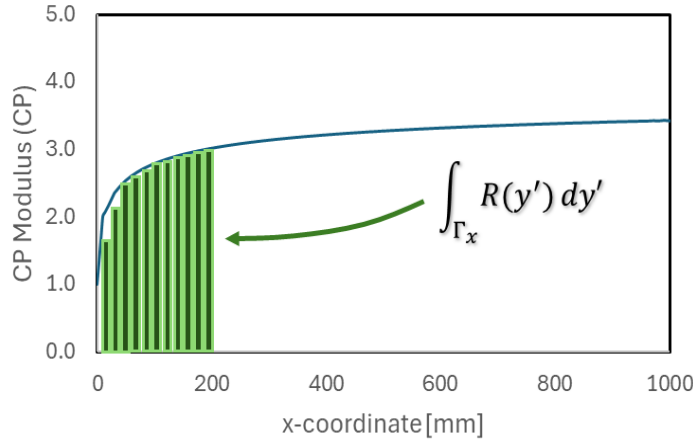


Figure 9 Salt accumulation within a narrow unit area describes membrane salt differential along the x-axis.

The LHS in Eq. 3.3 describes the differential unit volume indicated in figure 9 along the x-coordinate. Concentration gradient in Eq. 3.3 can be assumed as linear given that the salt height is within the hydrodynamic sublayer [40]. Moreover, normal velocity can be substituted with the water flux formula, which incorporates fluid hydrodynamic pressure and osmotic pressure. Recombination of these parts produces Eq. 3.6 which is like Eq. 3.7.

$$\frac{\partial c}{\partial y} \approx \frac{\Delta c}{\delta_h} \text{ if } y \leq \delta_h \quad (3.4)$$

$$v = A * (\Delta P - RT\Delta c) \quad (3.5)$$

$$\rightarrow \int_{\Gamma_x} R(y') dy' = \left(A * P(x) + RT * c_p - \frac{\mathcal{D}_s}{\delta_h} \right) \mathbf{c} - (A * RT) \mathbf{c}^2 + \frac{\mathcal{D}_s}{\delta_h} c_f \quad (3.6)$$

$$f(x; A, B, c) = Ac - Bc^n \quad (3.7)$$

Eq. 3.7 is the differential formula for a group of solutions known as growth functions. Examples of growth functions include Logistics function and Gompertz function [41, 42]. These two functions were selected to model the boundary membrane layer since it was hypothesized that by adapting to salt accumulation, its adverse effect will be negated resulting in a maximized net flux. As channel height reduces as per the growth functions, convective flux will dominate diffusive flux and water flux will be maximized. Polynomial function was also selected to simulate a free shape. Third-order polynomial function was chosen specifically since it has the same number for degrees of freedom as the other previous functions. The numerical basis equations are written as follows:

I. Logistics wall equation

$$s(x) = \beta_0 + \beta_1 / [1 + \beta_2 \exp(-\beta_3 x)] \quad (3.8)$$

II. Gompertz wall equation

$$s(x) = \beta_0 + \beta_1 \exp[-\beta_2 \exp(-\beta_3 x)] \quad (3.9)$$

III. Polynomial wall equation

$$s(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 \quad (3.10)$$

Since a fixed channel cross sectional area is imposed as a constraint, the intercept coefficient, β_0 , can be computed through a relationship with the other coefficients. For example, Eq. 3.11 details the relationship between the intercept coefficient and the other coefficients in the polynomial wall function.

$$A_{base} = A_{opt}, \text{ where } \left(A = \int_0^L y_{Top} - y_{Bottom} dx \right) \quad (3.11a)$$

$$\int_0^L H - 0 dx = \int_0^L H - s(x) dx \quad (3.11b)$$

$$H * L = H * L - \int_0^L s(x) dx \quad (3.11c)$$

$$\int_0^L s(x) dx = 0 \quad (3.11d)$$

$$\int_0^L \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 dx = 0 \quad (3.11e)$$

$$\rightarrow \beta_0 = -\left(\frac{1}{2}\beta_1 L + \frac{1}{3}\beta_2 L^2 + \frac{1}{4}\beta_3 L^3\right) \quad (3.11f)$$

Accordingly, each shape function has three geometrical degrees of freedom expressed through the coefficients: $\beta_1, \beta_2, \text{ and } \beta_3$. This number of degrees of freedom offers sufficient flexibility for optimization while ensuring reproducibility, as the control parameters remain consistent across all optimization trials.

The COMSOL Multiphysics package includes multiple optimization numerical techniques, which can be categorized as gradient-based or gradient-free. The Gradient-based technique computes the exact analytical derivative of an objective function. The optimal point is reached by stepping from the initial guess point either to find a local maximum point or a local minimum point. To find a maximum, the algorithm dictates the program to step in the same direction as the gradient since this is aligned with the steepest ascent. In contrast, to find a minimum, the algorithm dictates the program step in the opposite direction from the gradient since this is aligned with steepest descent. The Gradient-free technique, on the other hand, samples the objective function at different positions within the control variable range. Modulating variables affecting geometry can only be performed through Gradient-free techniques. This is because geometrical variations lead to changes in finite element

meshes. As a result, these changes generate noise induced from superimposing varying discretization errors over the pointwise movement of Gradient-based methods [43].

3.4 Momentum & Mass Transport

3.4.1 Fluid Physical Characteristics

The physical properties, such as density, viscosity, and diffusivity, were simulated using empirical correlations established in the Concentration Dependent Fluid Property (CDFP) models [44]. These CDFP models were essential in predicting accurate osmotic pressure and mass transportation phenomena by reflecting water behavior at any given sodium chloride salt concentration. The models for density, viscosity and diffusivity are represented by equations (3.12), (3.13), and (3.14), respectively. Table 2 lists the empirical parameters for CDFP equations.

$$\rho = A_{\rho} + B_{\rho} * c \quad (3.12)$$

$$\mu = A_{\mu} + B_{\mu} * c \quad (3.13)$$

$$\mathfrak{D} = A_D + B_D * c + C_D * c^2 + D_D * c^3 \quad (3.14)$$

Table 2 Empirical parameters constituting physical models of saline water [44]

<i>Characteristics</i>	<i>Symbol</i>	<i>Value</i>	<i>Unit</i>
<i>Density</i>			
	A_{ρ}	999	kg/m^3
	B_{ρ}	0.04099	kg/mol
<i>Viscosity</i>			
	A_{μ}	0.001004	$Pa * s$
	B_{μ}	$8.377 * 10^{-8}$	$m^2 * kg/(mol * s)$

<i>Diffusivity</i>	A_D	$1.370 * 10^{-9}$	m^2/s
	B_D	$-0.2780 * 10^{-12}$	$m^5/(mol * s)$
	C_D	$0.3199 * 10^{-15}$	$m^8/(mol^2 * s)$
	D_D	$-0.2015 * 10^{-18}$	$m^{11}/(mol^3 * s)$

The equations are embedded as packages in the numerical simulation software. On the other hand, Table (3) lists the range of parameters considered in the channel dimensions and fluid dynamics, demonstrating the extent and scope of the study. The channel length (L), membrane characteristic permeability (A), and energy unit cost (e) are fixed throughout the study. Similarly, feed channel area (xy-plane) is fixed and imposed as a constraint, such that the product of length (L) and base height (H) is maintained. Feed Reynolds number (Re), which is defined as the ratio of inertial to viscous forces within a fluid, is calculated by multiplying feed mass flux with channel thickness and divided by dynamic viscosity. Both feed Reynolds number (Re) and water permeate value (w) were selected to be varied during the sensitivity analyses. Feed concentration (c_0) and back pressure (P_0) are kept as constant and used as boundary conditions.

Table 3 List of parameters along with their range of values

Parameter	Symbol	Value	Unit
Channel length	L	1000	mm
Nominal Channel half-height	H	0.5	mm
Membrane permeability	A	9.8×10^{-12}	m/s/Pa
Reynolds number	Re	20 – 900	
Feed concentration	c_0	604	mol/m ³
Back pressure	P_0	60	barg
Density	ρ	see Eq.3.5	kg/m ³
Viscosity	μ	see Eq.3.6	Pa.s
Diffusivity	$\mathcal{D}$	see Eq.3.7	m ² /s
Permeate value	w	$10^{-7} - 10^3$	\$/m ³

Energy unit cost	e	3.68×10^{-8}	\$/J
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3.4.2 Governing Equations & Boundary Conditions

The fluid viscous behavior in the feed layer is categorized as laminar flow. Physical simulation of laminar flow is numerically expressed through Navier-Stokes equations, which have the general form expressed in equations (3.15 – 3.17).

$$\rho (u \cdot \nabla) \mathbf{u} = \nabla \cdot [-p \mathbf{I} + \mathbf{K}] + \mathbf{F} \quad (3.15)$$

$$\mathbf{K} = \mu(\nabla \cdot \mathbf{u} + (\nabla \cdot \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \quad (3.16)$$

$$\rho \nabla \cdot \mathbf{u} = 0 \quad (3.17)$$

Where ρ is solution density, $\mathbf{u}$ is velocity vector, u is tangential velocity to bulk motion (x-component), v is normal velocity to bulk motion (y-component), p is external pressure, $\mathbf{F}$ is body forces vector, and μ is solution dynamic viscosity.

The boundary conditions are feed velocity, reject pressure, and velocity components at top and bottom boundaries. Feed velocity normal to boundary (1) and effluent pressure normal to boundary (3) are determined by user based upon process conditions. Throughout the simulations, feed volumetric rate and effluent pressure were kept constant at 1.09 m³/hr and 60 barg, respectively. Feed volumetric rate of 1.09 m³/hr is equivalent to a Reynolds number of 336. Tangential velocity (x-component) first-order derivative with respect to y-axis $\left(\frac{\partial u}{\partial y}\right)$ at top boundary is zero due to symmetry. Tangential velocity (u) to bottom layer

(4) is zero, whereas normal component (v) is computed following water flux equation of Solution-diffusion model.

$$J_w = A (\Delta P - \Delta \pi) \quad (3.18)$$

The mathematical formulae modelling transport of dilute species in the feed channel have the general form below.

$$\nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i \quad (3.19)$$

$$\mathbf{J}_i = -D_i \nabla c_i \quad (3.20)$$

Where $\mathbf{J}_i$ is the mass flux, c is concentration, R is rate of generation/consumption, and D is diffusivity coefficient. Each of these parameters represent component “i”, which can either be water (w) or salt (s).

This form indicates that two concentration boundary conditions are required. The first boundary condition is the inlet salt concentration at boundary (1). The second condition is zero salt diffusive flux at boundary (4). This second condition is added assuming a perfect impermeable barrier with negligible salt permeability constant (B). The boundary conditions are summarized in Table (4).

Table 4 Boundary conditions for Navier-Stokes and mass transport packages

Boundary ID	Navier-Stokes		Mass transport	
1	$u_1 = \dot{Q}_0 / \Delta y_1$	normal flow	$c_1 = c_o$	inlet mass fraction
2	$\partial u / \partial y _2 = 0$	Symmetry	$\mathbf{n} \cdot (-\mathfrak{D} \nabla c + c \mathbf{u}) = 0$	Symmetry
3	$P_3 = P_0$	Backpressure	$\mathbf{n} \cdot \nabla c = 0$	Open boundary
4	$u = 0, v = J_w(x)$	Membrane wall	$\mathbf{n} \cdot (-\mathfrak{D} \nabla c + c \mathbf{u}) = 0$	zero salt transport

CFD uses finite volume method to linearly discretize the partial differential equations over a domain of subdivided cells, known as mesh. Convergence of these equations across the finite mesh with respect to the boundary conditions creates a numerical unique solution. Accordingly, the accuracy of generated solutions is significantly impacted by the size and shape of mesh.

3.5 Mesh Verification & Validation

3.5.1 Mesh Structure

To ensure the numerical model's accuracy and reliability, it is crucial to verify the laminar flow and dilute species mass transfer equations to yield results consistent with experimental data reported in the literature for similar setups. The simulation is modelled using FEM, which requires a well-defined mesh to solve the governing equations accurately. Figure 10 illustrates an example of a structured mesh used in our simulations.

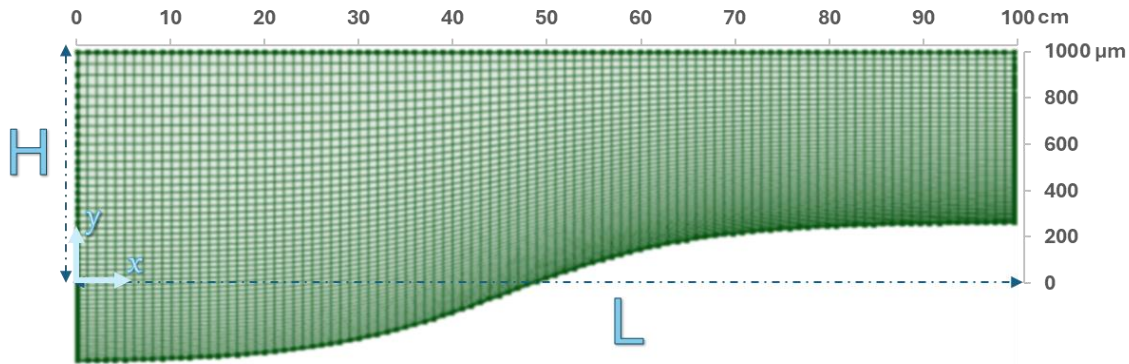


Figure 10 Example rectangular mesh with 5000 elements, denser near membrane (bottom layer).

The total number of cells is 5,000 with 100 elements in the x-direction and 50 elements in y-direction. The horizontal width of cells was distributed uniformly across the x-

dimension. On the other hand, the heights of cells were adjusted to decrease exponentially as they move down along the y-dimension, where the ratio of top cells is four times that of the bottom cells. The refinement of cells near membrane wall was conducted since it is essential to accurately reflect concentration polarization and ultimately water flux. As a result of steep transport gradients near sublayer area, the size of cells at that region has a significant impact over the simulation outcome. In contrast to a nonuniformed distribution of cells, a mapped configuration produces organized results with minimal processing time.

3.5.2 Mesh Verification

One of the fundamental checks for simulation reliability is ensuring mesh resolution independence. This step confirms that the simulation results are not affected by the chosen mesh size. Given that profitability rate, E , depends on both the overall permeate production, $\dot{Q}_P$, and hydraulic loss term, $\Delta P \dot{Q}_f (= TVD)$, as described in Equation (3.1), it is instructive to verify mesh independence for both components. Figure 11a illustrates the dependence of these two parameters on the average element size. Both parameters become independent of mesh size below approximately $1000 \times 10^{-4} \text{ mm}^2$, indicating that E is also independent of mesh size under these conditions within a tolerance of 0.1%. Similarly, the tolerance for water flux and pressure drop are below 0.05%. This finding suggests the chosen mesh resolution is adequate for accurate simulations.

Mesh independence can also be evaluated by adjusting the element size and analyzing its impact on spatial profiles. A key spatial profile selected for model verification is permeate flux $J_w(x)$. Figure 11b shows water flux along the membrane wall boundary while varying the mesh size. The output results become invariant when the average mesh size is below

$1000 \times 10^{-4} \text{ mm}^2$. The observed output consistency for both figures confirms that adapted mesh resolution is adequate to generate reproducible results.

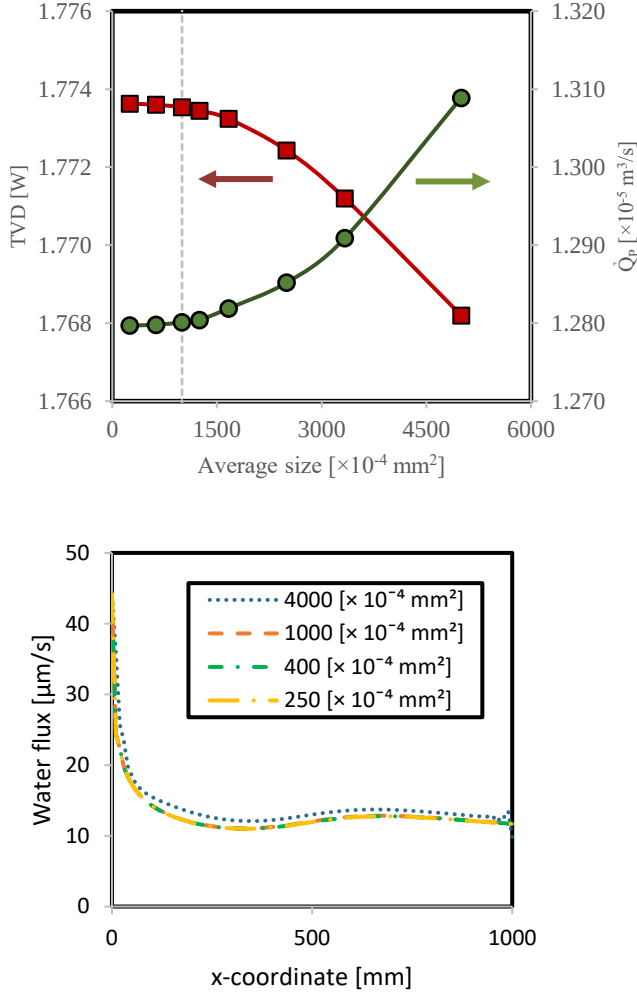


Figure 11 (a) Influence of mesh element size on Total Viscous Dissipation, TVD, and overall permeate flow rate, Q_p ; (b) permeate flux profile at the membrane surface at different mesh element sizes. Computation error with mesh size of 0.1 mm^2 is below 0.1%

3.5.3 Model Validation

The developed model was validated by testing it in comparison with experimental work performed by Alexiadis et al., 2007 [45]. The experiments varied transmembrane pressure

and feed velocity for each group, while the channel dimensions and feed concentration were kept unchanged. Table (5) summarizes the simulation parameters and experimental operating conditions for validation paper. Table (6) compares the results between our simulation and Alexiadis et al., 2017 [45] work.

Table 5 Simulation structure and mesh parameters and experimental operating conditions adapted by Alexiadis et al., 2017 paper [45]

Parameters	
Cells across the x-coordinate [#]	100
Cells across the y-coordinate [#]	50
Channel Length [mm]	260
Channel Height [mm]	2.5
Operating Conditions	
Water Permeability Coefficient [m/s/Pa]	8.756E-12
Inlet Velocity [m/s]	128.450
Feed Concentration [mol/m ³]	34.223
Transmembrane Pressure drop [kPa]	1398.7

Table 6 A summary for the results obtained by this work in comparison with the validation paper [45]

Results	Reference Experiment	This Work
Permeate Flux [L/m ² /hr]	36.98	36.34
Wall Concentration at x = 200 mm	72.55	95.81

One of the defining measurement parameters was the water flux, which was used for this model verification. Figure 12 shows model outcomes simulating experimental operating conditions in comparison with experimental results. The average model water flux errors were 6.6%, 6.5%, and 4.6% for transmembrane pressures of 9.9 barg, 11.9 barg, and 13.9 barg, respectively. These computed errors agree with the outcomes reported by Alexiadis et al., 2017 [45] where they compared their CFD simulation with run experiments. This

indicates that this study CFD simulation and reliable and consistent with other experimental research works.

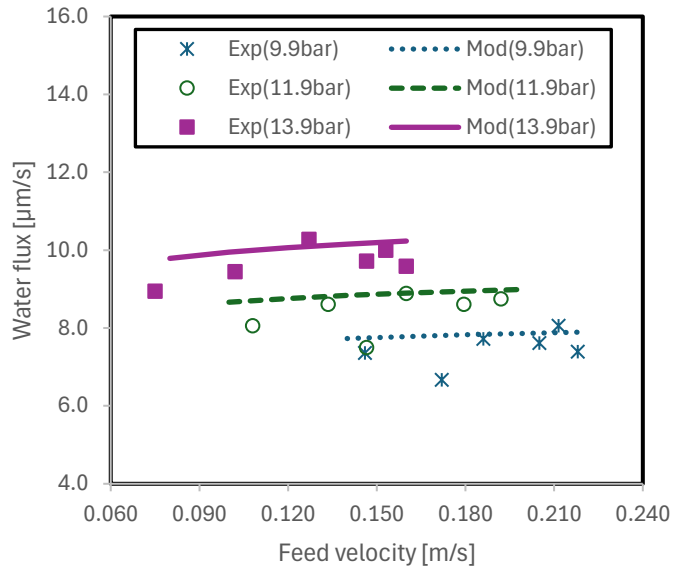


Figure 12 Model validation with experiments [45] using water fluxes

CHAPTER 4

RESULTS & DISCUSSION

4.1 Manual Optimization via Numerical Models

Consecutive trials to optimize profitability rate were performed while varying the numerical models describing membrane wall boundary. Feed channel geometrical shape impacts convective and diffusive water fluxes along the y-dimension since it plays a role in controlling fluid hydraulic pressure. These selected numerical models are Logistics function, Gompertz function, and Polynomial third-order function. The optimum shapes corresponding to each numerical function were analyzed based on velocity and salt concentration contour profiles, permeate water fluxes, and membrane wall concentrations. Additionally, Performance Enhancement Ratio (PER) is introduced to evaluate both permeate water flux and membrane wall concentration in the modified shapes relative to the conventional baseline design. PER is calculated by dividing each variable of the optimum shapes over the baseline.

4.1.1 Logistics Wall Function

The optimum shape adopting the Logistics function is illustrated in Figures 13 (a-b) demonstrating velocity and concentration profiles across feed channel. The optimum shape features a smooth reduction in the channel cross-sectional area until the end area becomes 50% that of the inlet area. The optimization study showed that maximum profitability corresponds to a contracting area. The profitability rate for this shape is reported to be \$746

per year, which is 12.2% higher than the base model. The total integrated permeate flow had increased by 5.4%, while total dissipation losses also increased by 84%. The rise in dissipation losses is because the influence of operational costs is minimal since the power unit cost is relatively low compared with the product unit price. Figure 14 shows water flux along the permeate channel, where the flux was initially lower than the base water flux. The permeate water flux PER increases gradually and exceeds 100% at an x-coordinate above 400 mm. As the channel cross-sectional area is reduced, water axial velocity increases. Figure 15 shows the optimum shape concentration polarization (CP), where it sharply increases until it saturates at 3.3 above 300 mm. The sharp increase in salt concentration is attributed to low feed axial velocity permitting salt accumulation over the membrane layer. As the channel cross sectional area is reduced, shear rate increases resulting in lower concentration polarization in the optimum shape relative to the baseline design.

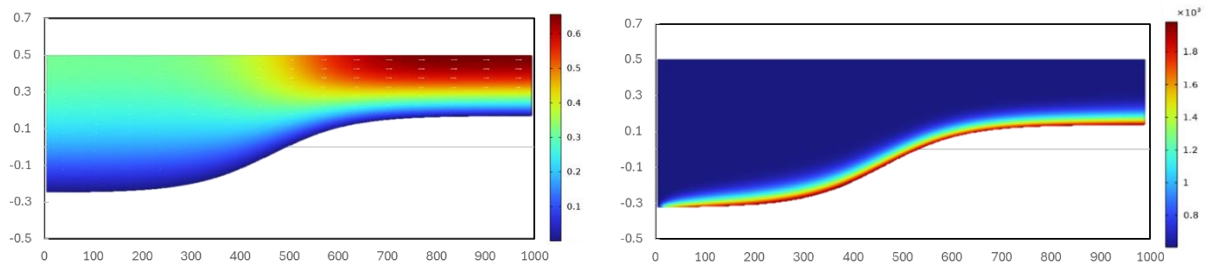


Figure 13 Optimal channel configuration following Logistic wall function. Velocity profile shade plot is presented in (a) and concentration shade plot is presented in (b)

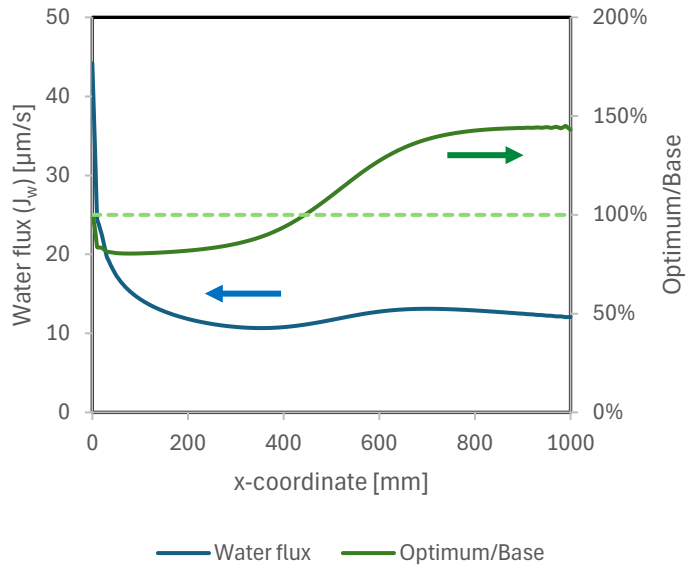


Figure 14 Water flux profile (blue) at optimum shape configured following Logistic wall function. The ratio between water fluxes at this optimum shape relative to the original base shape (green)

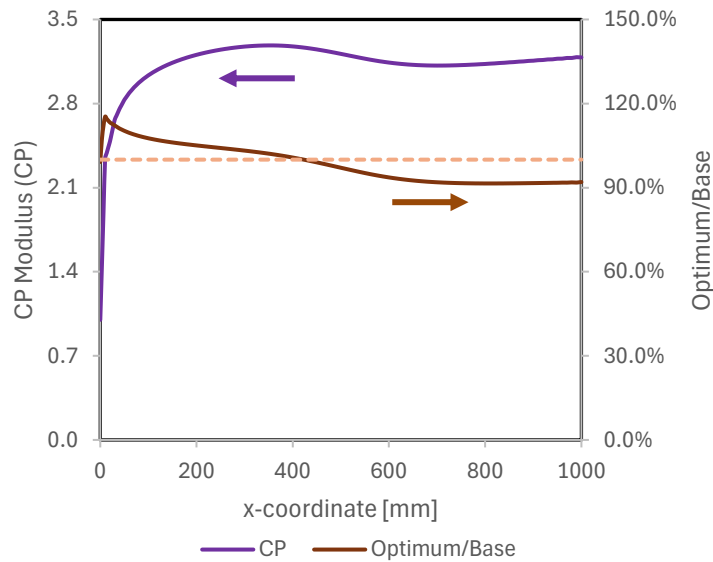


Figure 15 Concentration polarization profile (purple) along the membrane layer at optimum shape configured following Logistic wall function. The ratio between salt concentrations at this optimum shape relative to the original base shape (red)

4.1.2 Gompertz Wall Function

The optimum shape adopting the Gompertz function is illustrated in Figures 16 (a-b) demonstrating velocity and concentration profiles across feed channel. The optimization study showed that maximum profitability corresponds to a contracting area. The profitability rate for this shape is \$716 per year, which is 8% higher than the baseline model. The total integrated permeate flow had slightly increased by 3%, whereas total dissipation losses are higher by only 22%. Figure 17 shows water flux over the permeate channel. The optimum shape water flux initially falls below base model water flux prior to recovering and exceeding it at an x-coordinate of 250 mm. This behavior is ascribed to a low water pressure near the feed channel inlet relative to the base shape, yet it is overturned due to steep curvature promoting water axial velocity. Figure 18 illustrates the concentration polarization profile as it increases sharply, followed by a gradual rise toward a saturation limit of 3.2. The membrane salt concentration at the optimum shape is slightly below the base model since the high shear rate slows off the incremental rate of salt accumulation.

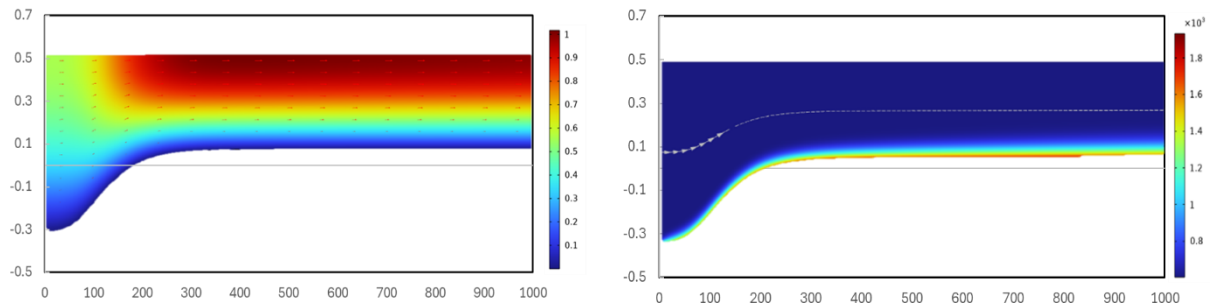


Figure 16 Optimal channel configuration following Gompertz wall function. Velocity profile contour is presented in (a) and concentration profile is presented in (b)

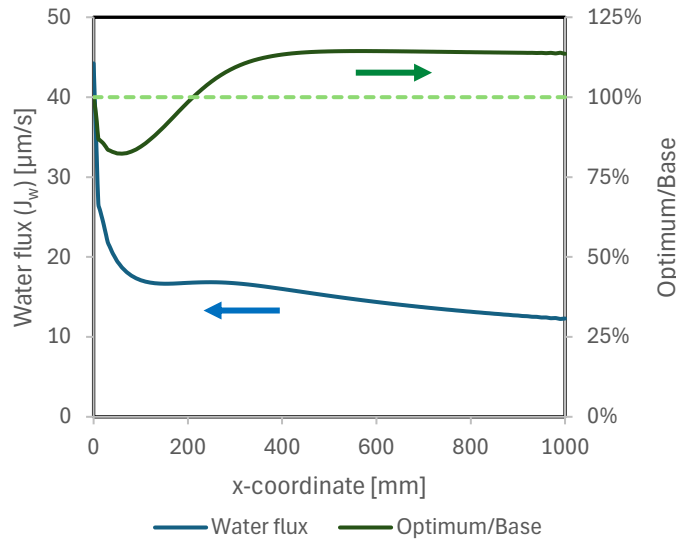


Figure 17 Water flux profile (blue) at optimum shape configured following Gompertz wall function. The ratio between water fluxes at this optimum shape relative to the original base shape (green)

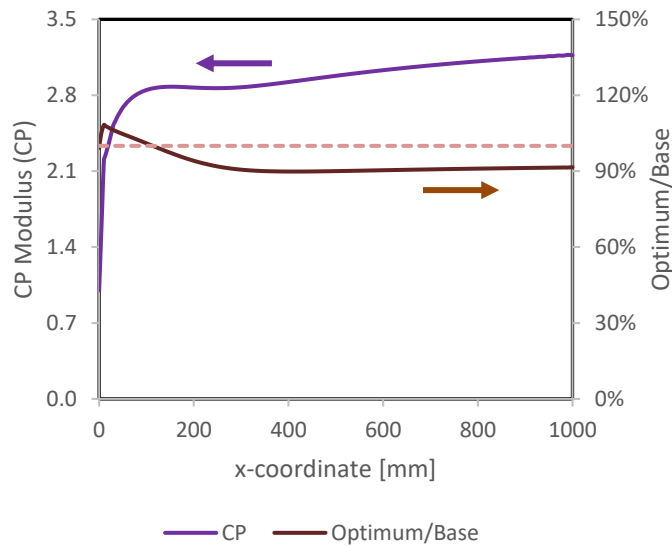


Figure 18 Concentration polarization profile (purple) along the membrane layer at optimum shape configured following Gompertz wall function. The ratio between salt concentrations at this optimum shape relative to the original base shape (red)

4.1.3 Polynomial (3rd-order) Wall Function

The optimum shape adopting third-order polynomial function is illustrated in Figures 19 (a-b) demonstrating velocity and concentration profiles across feed channel. The optimization study showed that maximum profitability corresponds to a contracting area. The profitability rate for this shape is \$ 773 per year, which is 16.2% higher than the base model. The total integrated permeate flow had increased by 7.3%, while the total dissipation losses had surged such that it had become 5.6 times the losses found in the conventional design. As per Figure 20, water flux PER initially drops to below 75%, then it increased exponentially until it exceeds 100% at an x-coordinate above 700 mm and reached 256% towards the channel outlet. The exponential increase is attributed to the steep curvature resulting in a sharp reduction of channel cross-sectional area. Figure 21 illustrates salt concentration along the membrane boundary layer. In contrast to the other models, this channel's concentration polarization decreases after peaking at a limit of 3.3. This observation is due to the continuously steep positive slope of the boundary wall leading towards an exponential increase in shear rate, effectively dissipating wall concentration near the end of feed channel and allowing water flux to rise again.

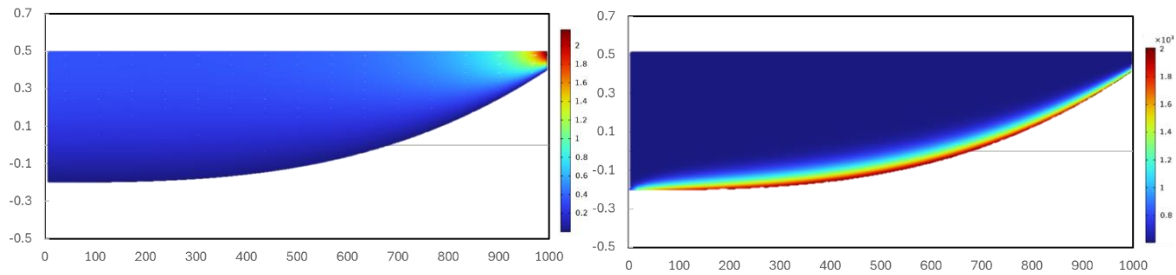


Figure 19 Optimum channel configuration following Polynomial third order wall function. Velocity profile contour is presented in (a) and concentration profile is presented in (b)

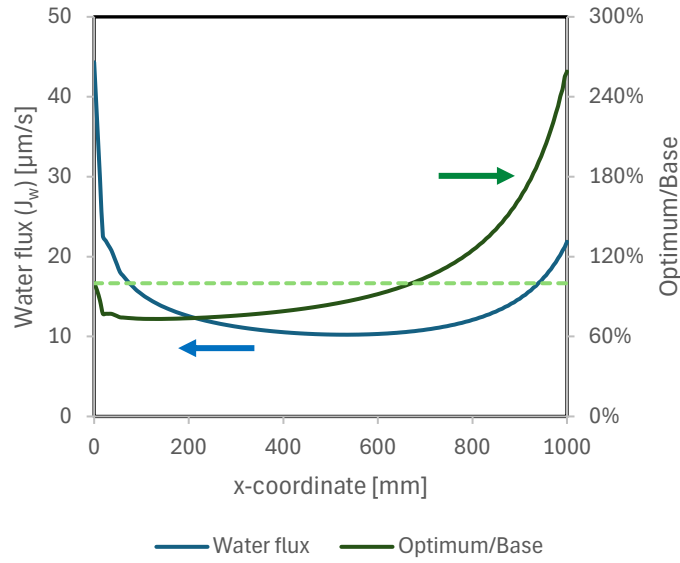


Figure 20 Water flux profile (blue) at optimum shape configured following Polynomial third-order wall function. The ratio between water fluxes at this optimum shape relative to the original base shape (green)

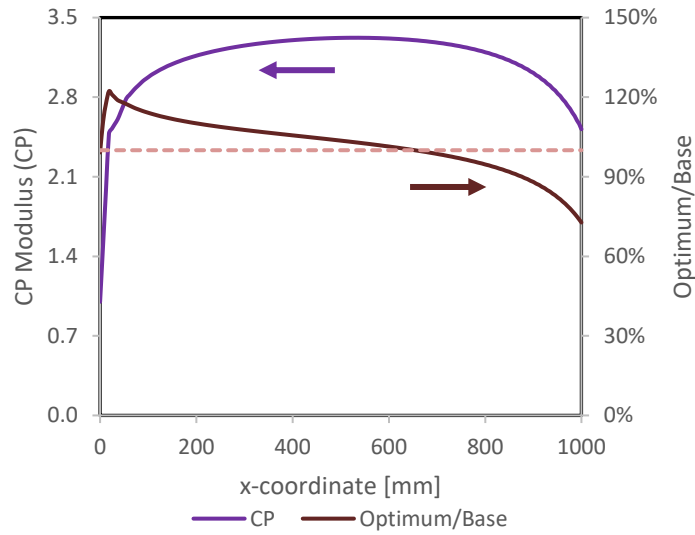


Figure 21 Concentration polarization profile (purple) along the membrane layer at optimum shape configured following Polynomial third-order wall function. The ratio between salt concentrations at this optimum shape relative to the original base shape (red)

4.1.4 Comparison of Numerical Outcomes

The optimization study revealed that the maximum profitability is achieved by narrowing feed channel geometry. Among the tested configurations, the shape defined by the Polynomial function produced the highest profitability rate, followed by the Logistics and Gompertz functions, respectively. This ranking was also consistent with the total integrated permeate water production. Although the Polynomial function ranked the highest in total dissipation losses followed by the Logistics function, there is a substantial gap between the dissipation results reported by these two models. Figure 22 illustrates the hydraulic pressure distribution along the horizontal axis for all models, where feed pressure is at $x = 0$ mm and outlet pressure is at $x = 1000$ mm. The pressure gradient in the Polynomial model demonstrates a stark contrast between the inlet and outlet regions. Near the inlet boundary, the average pressure gradient is -2 kPa/m, whereas near the outlet boundary, it increased dramatically to -397 kPa/m. This pronounced increase in pressure drop magnitude is attributed to the sharp rise in water velocity as the feed channel narrows toward the outlet. The resulting acceleration requires a significant conversion of potential energy into kinetic energy, thereby increasing the feed pressure demand. In contrast, the Logistic and Gompertz models maintained pressure losses within two orders of magnitude throughout the channel, indicating a more moderate and uniform energy requirement across the flow domain.

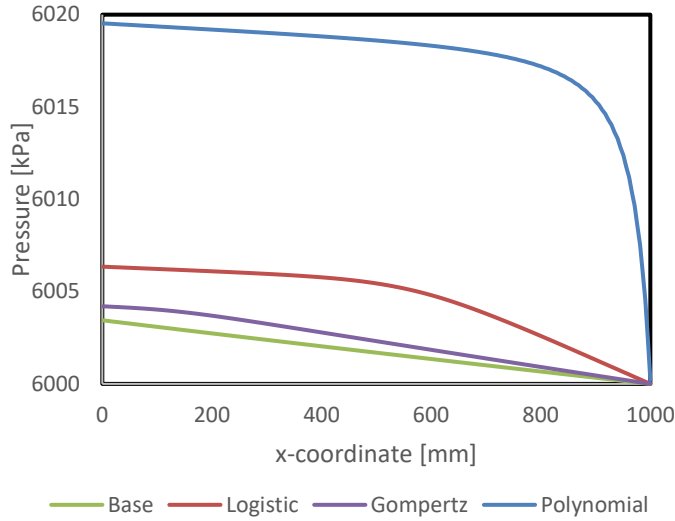


Figure 22 The hydraulic pressure losses plotted for the adopted models in constructing the feed channel. The highest losses were by the Polynomial function, followed by the Logistics, and then by Gompertz. The feed pressures in all models are higher than the conventional baseline model.

The concentration polarization profile by the Polynomial function was dropping near the channel end. This behavior can be attributed to the steep increment in shear rate, which creates hydrodynamic condition diminishing the effect of salt accumulation. This observation is aligned with experimental work performed by Bian et al., 2000 [46]. It should be noted that the results are dependent upon the feed channel length. This is apparent from studying the figures of water flux across the three models. In this study, using a standard feed channel length of one meter, the most favorable outcome was obtained with Logistics wall function. Compared to Gompertz wall function, the Logistics wall function yields higher profitability rate. Conversely, the optimum configuration with the polynomial wall function exhibited unstable hydrodynamic conditions, leading to the unsteady water flux and concentration polarization. Additionally, the overall steepness of the curvature across the membrane presents manufacturing challenges. These factors position the model

with the Logistics wall function as the most promising structure. Figure (23) presents the optimum channel shape design incorporating the Logistics function model.

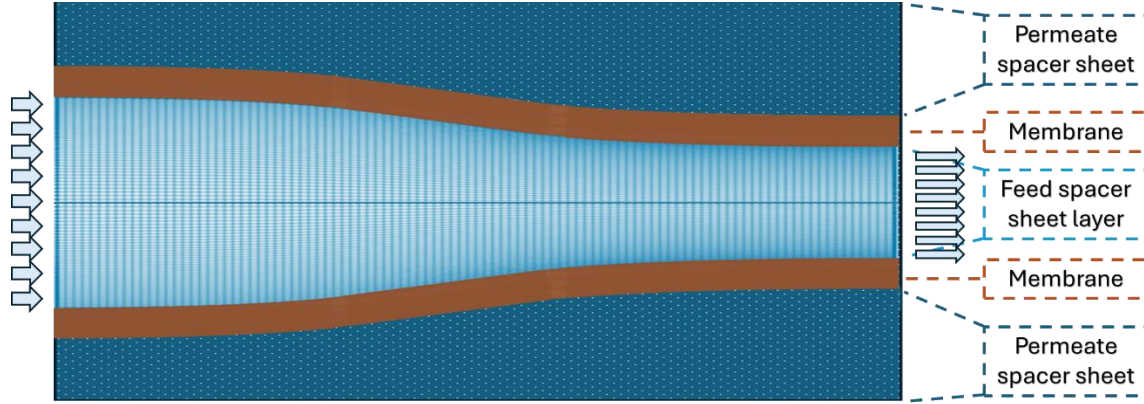


Figure 23 The novel design of RO sheet layers reflecting the optimum configuration for feed channel

4.2 Sensitivity Analysis

Additional efforts were made to perform a sensitivity analysis. Two variables were adjusted, which are Permeate value (w) and Reynolds number (Re). The permeate water value is selected to assess the significance of economic position in shaping the feed channel. Similarly, Reynolds number reflects feed water inlet to channel, which affects both water flux and viscous dissipation pressure losses. In both analyses, a new variable is introduced to demonstrate optimum membrane curvature deviation from the baseline of a horizontal profile. This variable is introduced as the channel integral depth, $|\overline{\sigma}|$, defined by equation (4.1).

$$|\overline{\sigma}| = \frac{1}{L} \int_0^L |s(x)| dx \quad (4.1)$$

For Logistics wall function, above equation becomes.

$$\overline{|\sigma|} = \frac{1}{L} \int_0^L |\beta_0 + \beta_1/[1 + \beta_2 \exp(-\beta_3 x)]| dx \quad (4.2)$$

Figure 24 demonstrates the relationship between the optimum channel integral depth, $\overline{|\sigma|}^*$, and the water permeate value, w . It reveals that the optimum channel integral depth saturates at a maximum for high permeate water values, whereas it reaches zero at low permeate water values. At low permeate values, energy costs dominate the reverse osmosis process, necessitating a uniformly horizontal channel to minimize energy expenses. In contrast, at high permeate values, a curved channel shape is preferred since it maximizes permeate flux due to water value outweighing energy costs. In addition, the same analysis was revisited for additional channel lengths of 300-mm and 2000-mm. It was revealed that the channel integral depth is proportional to the feed channel length. This is because an increment in channel length demands consistent degree of curvature, thus higher channel integral depth.

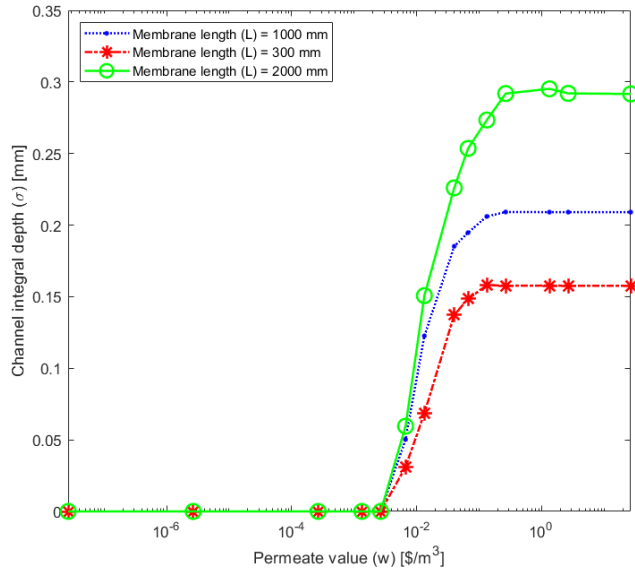


Figure 24 Optimum channel integral depth as a function of permeate water value (w) and channel length (L)

Figure 25 shows the channel integral depth for the optimal shape in relation to the feed Reynolds number (Re) and water product value (w). Reynolds number is a measure of feed flow to the channel. As per Figure 25, the channel integral depth tends to increase to a critical point, then drops and approaches a value of zero. This behavior can be attributed to impact of feed velocity over both water flux and viscous dissipation losses. Feed velocity is proportional to water flux and dissipation losses. Since the profitability rate favors high water flux and low dissipation losses, there exists a critical velocity at which curvature deviation can be maximized to generate the highest profitability rate. Increasing Reynolds number prior to the critical point implies that the increment in revenue due to water flux outweighs the operational costs, thereby a feed channel with a higher degree of curvature is desired. In contrast, the channel integral depth drops significantly as Reynolds number is increased beyond the critical point. This is because the hydraulic dissipation losses tend to dominate the profitability rate equation, thus, a uniform shape with minimal hydraulic losses is favored. As the water product value increases, the critical point shifts towards higher Reynolds number. Subsequently, the model has a higher capability to modulate the channel to achieve higher curvature.

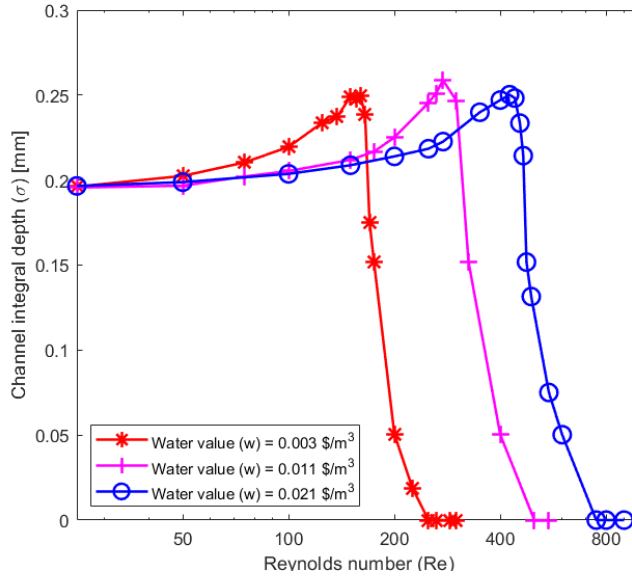


Figure 25 Optimum channel integral depth behavior with respect to Reynolds number (Re) and product water value (w)

The change in feedwater temperature inside the feed channel is assumed as minimal since the generated shear rates will be absorbed to dissipate the accumulated salts over the membrane wall. Nevertheless, variation in water temperature was explored in this work. Feedwater temperature plays a significant, albeit complex, role in the performance of seawater reverse osmosis (SWRO) systems. Dimitriou et al., 2025 [47] investigated the influence of temperature on several key performance indicators, including water flux, water permeability, salt rejection, membrane recovery, and specific energy consumption. Their study found that both water flux and water permeability exhibit a positive correlation with feedwater temperature. This is primarily due to reduction in dynamic viscosity and the enhancement of the salt diffusivity coefficient at elevated temperature, which collectively facilitate improved mass transport through the membrane.

However, further increases in temperature may negatively impact RO performance due to material limitations of spiral-wound membrane elements. Camacho Espino et al., 2025 [48] conducted a series of experiments in a small-scale SWRO system, exploring feedwater temperatures ranging from 5°C to 45°C. Their findings indicated a diminishing return in water permeate flux with increasing temperature. Specifically, water flux increased by 8.92% when the feedwater temperature rose from 5°C to 20°C, but only by an additional 2.34% as the temperature was further elevated to 45°C. In general, higher feedwater temperatures lead to an increase in permeate flow and a reduction in the required driving pressure, suggesting that operational profitability tends to favor elevated feedwater temperatures.

To reflect the influence of operating temperature on feedwater properties, thermophysical parameters were updated for the temperature range of 20°C to 45°C. These include dynamic viscosity and the salt diffusivity coefficient, while changes in density were neglected due to their minimal impact. The temperature dependence of dynamic viscosity was modeled using the correlation proposed by Isdale et al., 1972 [49].

$$\log_{10} \left(\frac{\mu_{20}}{\mu_T} \right) = \left(\frac{T-20}{T+109} \right) (A[1 + a_1S + a_2S^2] + B[1 + b_1S + b_2S^2][T - 20]) \quad (4.3)$$

Where μ_{20} and μ_T are dynamic viscosities [kg/m-s] at 20°C and target temperature, T is target temperature [°C], S is salinity [g/kg], while the other terms are empirical constants.

In addition, salt diffusivity was interpolated based on the Stokes-Einstein theory [50], which states that the diffusivity coefficient is directly proportional to temperature and inversely proportional to dynamic viscosity. Figures (26-b) depict the variation of dynamic

viscosity and salt diffusivity coefficient with respect to salt concentration at two operating temperatures, highlighting the temperature sensitivity of these parameters.

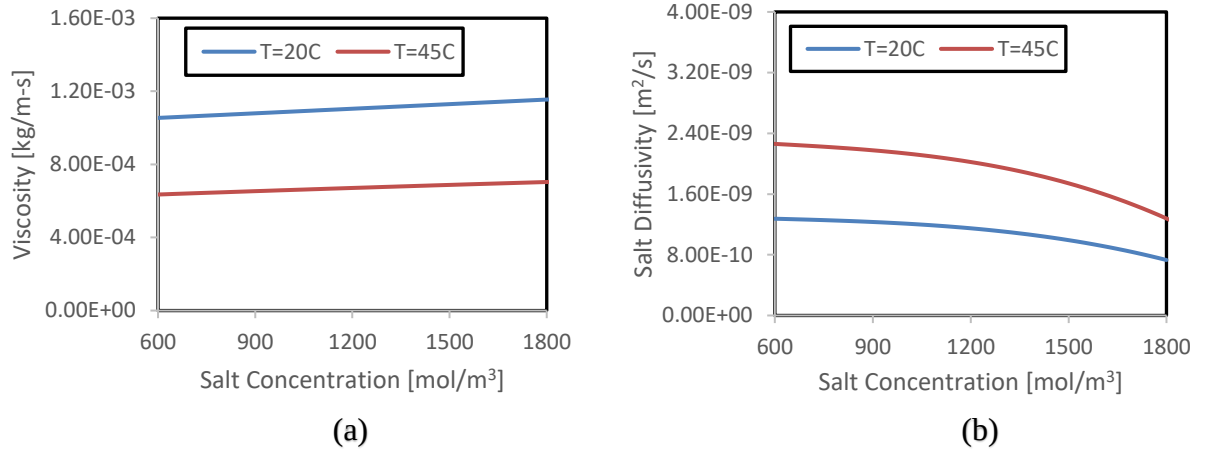


Figure 26 Thermophysical properties of (a) water dynamic viscosity and (b) salt diffusivity coefficient with respect to salt concentration are plotted at two operating temperatures, 20°C and 45°C, to showcase temperature sensitivity by these parameters.

The water permeability coefficient (A_w) increases with operating temperature, exhibiting a trend like that of the diffusivity coefficient. Sivertsen et al., 2018 [51] predicted that the water permeability coefficient is directly proportional to temperature and inversely proportional to dynamic viscosity. This relationship reflects the thermally enhanced transport properties of water molecules across the membrane. An alternative approach to account for the enhanced water permeability coefficient is by using the temperature correction factor (TCF) as proposed by Al-Obaidi et al., 2018 [52].

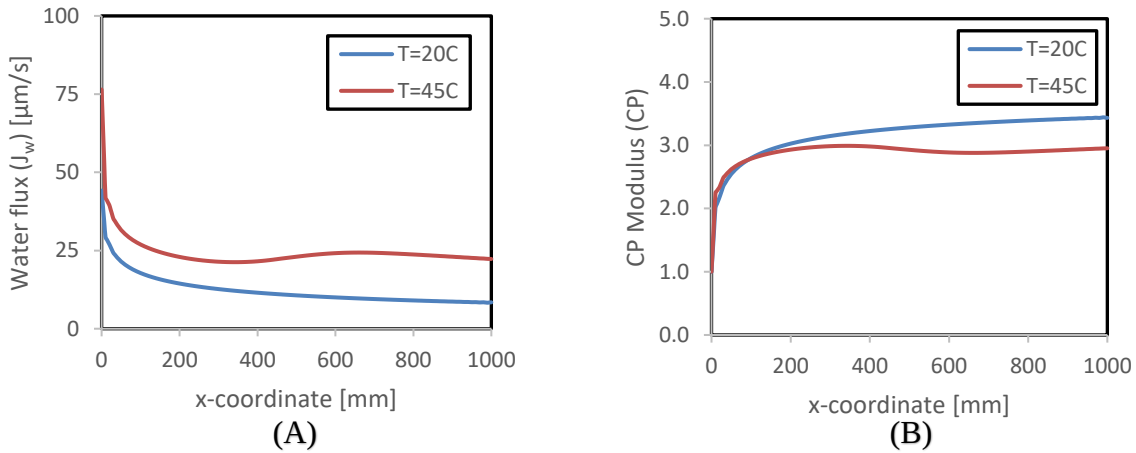
$$A_w(T) = A_w(25^\circ\text{C}) * TCF * F_f \quad (4.4a)$$

$$TCF = \exp[0.0307 (T - 25)], \text{ if } T > 25^\circ\text{C} \quad (4.4b)$$

$$TCF = \exp[0.0343 (T - 25)], \text{ if } T < 25^\circ\text{C} \quad (4.4c)$$

Where $A_w(T)$ is water permeability coefficient at target temperature, $A_w(25^\circ\text{C})$ is water permeability coefficient at a temperature of 25°C , T is the target temperature, F_f is a friction factor, and TCF is the temperature correction factor.

Figures (27a-c) illustrate the predicted impacts of raising the feedwater temperature to 45°C . on three key performance indicators: water recovery, concentration polarization, and hydraulic losses. A significant increase in water recovery was observed, accompanied by a noticeable reduction in concentration polarization. Conversely, hydraulic losses showed a slight increase. The reasoning is because the optimum shape for a channel operating at 45°C favors higher curvature and variation from the conventional baseline. Consequently, although high temperature requires lower feed pressure for a baseline shape design, shape reconfiguration causes an increase in feed pressure, thus exceeding the model operating at a temperature of 20°C .



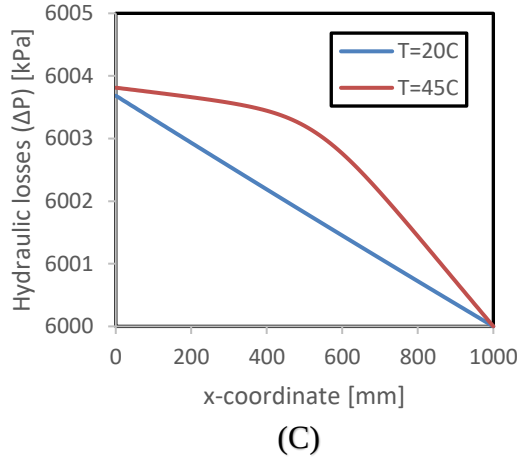


Figure 27 Comparison between two optimum feed channel designs, which are adopting Logistics function, operating at two temperatures, 20°C and 45°C. This comparison presents (A) water flux, (B) concentration polarization, and (C) hydraulic losses along the x-coordinate. These plots demonstrate the superiority exhibited by the higher operating temperature.

4.3 Assumptions Validation

Throughout this work, a series of assumptions were created to reduce numerical computations and facilitate the numerical simulation. Two assumptions will be highlighted and dissected in this section.

4.3.1 Zero Salt Transport at the Membrane

To assess the validity of the zero-salt transport assumption across the membrane boundary layer, simulation results were compared with literature data on salt rejection performance. Salt rejection in reverse osmosis systems is known to vary with feed concentration. Abdulmuttaleb et al., 2014 [53] reported a decline in salt rejection from 88% to 65% as the feed salt concentration increased from 5000 ppm to 35,000 ppm. To validate the simulation model, the lower salt rejection value of 65% is adopted as a conservative case.

Under this scenario, water flux is expected to increase due to the reduced osmotic pressure gradient across the membrane, which serves as a resistive driving force. To account for salt rejection in the water flux model, equation (3.18) is modified as follows:

$$\Delta\pi = RT(c_m - c_p) = RT(c_m - c_0(1 - SR)) \quad (4.5)$$

$$J_w = A * (\Delta P - RT(c_m - c_0(1 - SR))) \quad (4.6)$$

Where π is osmotic pressure, R is ideal gas constant, T is temperature, c is salt concentration, SR is salt rejection, J_w is water flux, P is pressure, and A is water permeability coefficient, while subscripts “m”, “p”, and “0”, reflect membrane wall, permeate, and feed, respectively.

Figures (28) presents a comparison of water recovery for the optimal membrane channel shape under two conditions. While the first considers zero-salt flux, the second incorporates the 65% salt rejection. The results indicate an 8.0% increase in permeate water flow. Additionally, the channel integral depth (σ) was recalculated for the updated model and showed a marginal increase of 0.98%. These findings suggest that the inclusion of salt passage has a negligible effect on the overall optimal design geometry.

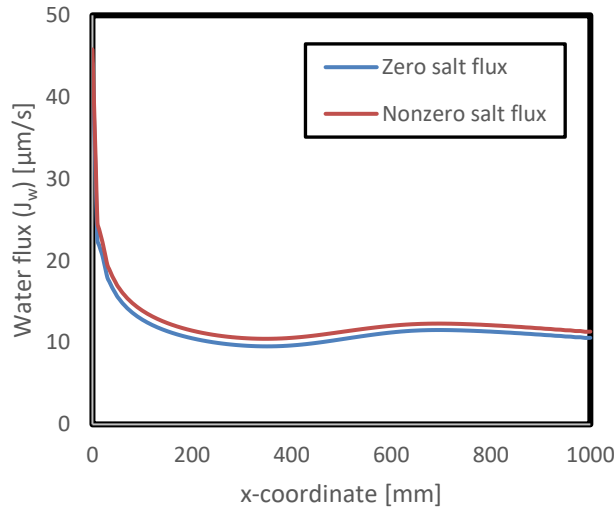


Figure 28 Comparison of water flux profile along the membrane boundary between 100% salt rejection and 65% salt rejection conditions.

4.3.2 Single Salt Species (NaCl)

According to ASTM D1141-98 [54], the concentration of sodium chloride (NaCl) in standard synthetic seawater is 24,530 ppm, accounting for approximately 68.1% of the total dissolved salts. The standard concentrations of other major constituents include 4,090 ppm for sodium sulfate (Na_2SO_4) and 1,160 ppm for calcium chloride (CaCl_2).

Figures (29a-c) present a comparative analysis of NaCl as a single salt species against three-salt mixture with respect to three physical parameters: density, dynamic viscosity, and salt diffusivity coefficient. This comparison highlights the degree to which single salt species NaCl can approximate the behavior of the seawater mixture composition for transport and fluid modeling.

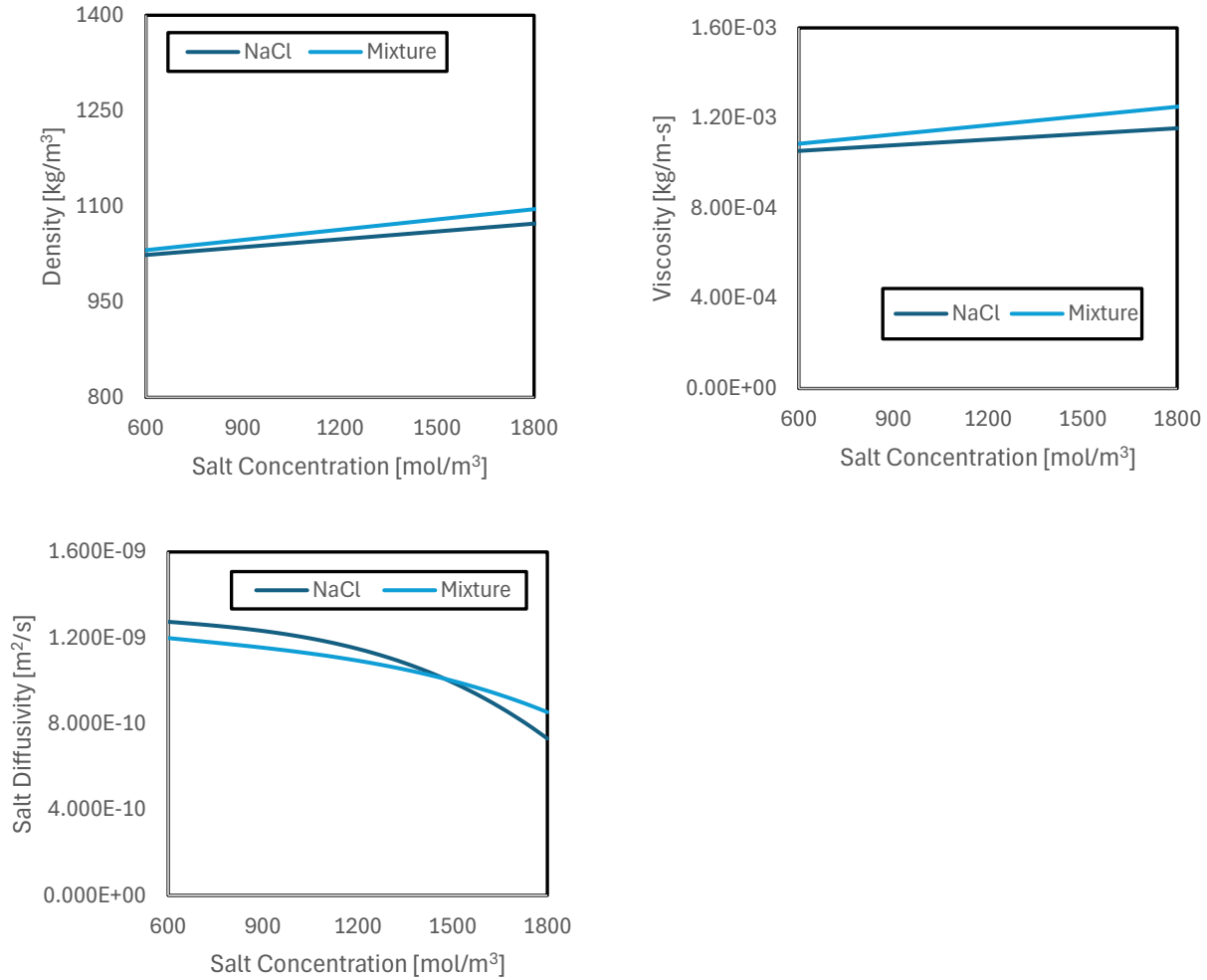


Figure 29 Thermophysical properties of (a) density, (b) viscosity, and (c) salt diffusivity coefficient are plotted showing negligible changes between single-salt species and salt species mixture.

As illustrated, the variations in density, dynamic viscosity, and diffusivity between the single-salt model and the full salt mixture are negligible. However, the most significant deviation arising from the single-salt assumption is expected in the calculation of osmotic pressure. The fundamental thermodynamic relationship for osmotic pressure is given in equation (4.7).

$$\int_p^{p+\pi} v_w dp = -RT \ln (x_w \gamma_w) \quad (4.7)$$

This expression relates osmotic pressure to the activity of water, where v_w is the partial molar volume of water, R is the ideal gas constant, T is temperature, x_w is the mole fraction of water, and γ_w is the water activity coefficient.

The commonly assumed linear relationship between osmotic pressure and solute concentration relies on the approximation that water behaves ideally, i.e., $\gamma_w \approx 1$. However, additional salt species such as Na_2SO_4 and CaCl_2 introduce stronger electrostatic interactions, forming hydration shells that bind water molecules more tightly and reduce water activity. This deviation from ideality can lead to underestimation of osmotic pressure when only NaCl is considered.

To maintain simplicity in the current modeling framework, this study adopts a single-salt NaCl approximation. Nonetheless, the influence of multicomponent interactions on water activity and osmotic pressure presents an important area for future investigation.

CHAPTER 5

CONCLUSION

This paper discussed a novel approach towards maximizing the profitability rate of the reverse osmosis process by manipulating the membrane curvature within the feed channel. Three numerical functions were used to reshape the membrane boundary throughout the optimization trials. These functions were employed for the membrane boundary modulation, comprising the following: Logistics, Gompertz, and third-order Polynomial functions. It was observed that an ascending membrane wall leading to a contracting feed channel increases both water flux and pressure losses. The optimal shape requires control over curvature such that it produces high water flux while minimizing viscous dissipation losses.

The Logistic wall function produced the most satisfactory performance; yielding a high profitability rate with stable hydrodynamic condition across the feed channel. At base water and energy unit costs of $1.96 \text{ \$/m}^3$ and $0.05 \text{ \$/kWh}$, the maximum profitability rate reached $\$ 746/\text{year}$, which is 12.2% higher than the baseline channel with uniform depth. Sensitivity analyses were performed to assess the impact of water value and feed Reynolds number. A transition point exists for the water value of $0.003 \text{ \$/m}^3$, while energy unit is $0.05 \text{ \$/kWh}$, at which that optimum shape shifts from a channel with a uniform depth to one with curvature along the membrane wall. Additionally, feed Reynolds number significantly impacts the optimum shape of the feed channel. Since both total integrated water flow and viscous dissipation losses are proportional to Reynolds number, there is a

specific velocity point at which the channel integral depth reaches a maximum, generating a relatively high-profitability rate. The critical Reynolds number is 150, while the corresponding maximum channel integral depth is 0.25 mm given that the original channel height is 1.0 mm.

Future work should focus on advancing the numerical algorithm for shape optimization by incorporating gradient-based solvers. COMSOL Multiphysics version 6.1 software does not support gradient-based techniques for this purpose because the geometric changes introduced during the optimization trials lead to variations in the finite element mesh, which results in multiple discretization errors in the objective function. These superimposed noises limit the software's computational capability to deliver the optimum shape design via a stepwise manner. In contrast, the gradient-free solvers used in this study require massive number of iterations across the study range before selecting the optimal control variables, which limits the overall computational efficiency.

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