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IN THE NAME OF ALLAH,

THE MOST GRACIOUS,

THE MOST MERCIFUL

Prophet Muhammad, peace be upon him.

Abstract

This Ph.D. thesis delves into the intricate realm of Desalination, focusing on Direct Contact Membrane Distillation (DCMD) and its optimization through various algorithmic approaches. The research navigates through the genesis of desalination, exploring both thermal and membrane methodologies, and subsequently dives into the membrane characterization techniques and materials.

A modeling design of DCMD is presented, highlighting its configuration, properties, and inherent challenges in its modeling, such as temperature polarization. The thesis further explores optimization in DCMD, introducing novel approaches like the Bonobo Optimizer (BO) and Particle Swarm Optimization (PSO) algorithms, providing a mathematical model for each, and discussing their applicability in DCMD systems.

Through simulation, the research elucidates the effects of various operating parameters on the total cross-membrane flux. It presents a comparative analysis of operating conditions on DCMD performance. The thesis encapsulates single and multi-objective optimization using BO and PSO, providing a comprehensive view into the optimization in DCMD performance, thereby contributing to the field by addressing technological and algorithmic advancements in desalination processes.

Keywords: DCMD, operating parameters, desalination process, permeate flux, optimization.

Résumé

Cette thèse de doctorat explore le domaine complexe du déssalement, en se concentrant sur la distillation en contact direct avec membrane (DCMD) et son optimisation à travers diverses approches algorithmiques. La recherche parcourt l'origine du déssalement, explorant à la fois les méthodologies thermiques et membranaires, puis plonge dans les techniques de caractérisation des membranes et des matériaux.

Une conception de modélisation de la DCMD est présentée, mettant en évidence sa configuration, ses propriétés et les défis inhérents à sa modélisation, tels que la polarisation de température. La thèse explore également l'optimisation en DCMD, en introduisant de nouvelles approches telles que l'optimiseur bonobo (BO) et l'optimisation par essaim de particules (PSO), en fournissant un modèle mathématique pour chacun et en discutant de leur applicabilité dans les systèmes DCMD.

À travers des simulations, la recherche élucide les effets de divers paramètres de fonctionnement sur le flux total à travers la membrane. Elle présente une analyse comparative des conditions de fonctionnement sur les performances de la DCMD. La thèse encapsule l'optimisation mono et multi-objectif à l'aide de BO et PSO, offrant ainsi une vision complète de l'optimisation des performances de la DCMD, contribuant ainsi au domaine en abordant les avancées technologiques et algorithmiques dans les procédés de désalinisation**.**

Mots clés : DCMD, paramètres opératoires, procédé de dessalement, flux de perméat, optimisation.

ملخص :

تتعمق هذه الاطروحة في عالم التحلية ، مع التركيز على تقنية التقطير بالغشاء بالاتصال المباشر (DCMD) وتحسينها من خلال مقاربات خوارزمية مختلفة. تتنقل البحث في تطور التحلية، مستكشفة الأساليب الحرارية والغشائية على حد سواء، ثم تنغمس في تقنيات ومواد توصيف الغشاء.

يتم تقديم تصميم نمذجة لـ DCMD، مسلطًا الضوء على تكوينها وخصائصها والتحديات الجوهرية في نمذجتها، مثل التأقلم الحراري. تستكشف الرسالة أيضًا التحسين في التقطير بالغشاء بالاتصال المباشر، وتقدم مقاربات جديدة مثل محسن البونوبو (BO) وخوارزميات تحسين تجمع الجسيمات (PSO)، وتوفر نموذجًا رياضيًا لكل منها، وتناقش تطبيقها في أنظمة DCMD.

من خلال المحاكاة، يوضح البحث تأثير معلمات التشغيل المختلفة على تدفق الغشاء العابر الكلي. يقدم تحليل مقارن لظروف التشغيل على أداء ال DCMD. يجمع البحث بين التحسين الموجه نحو هدف واحد ومتعدد الأهداف باستخدام BO و PSO، مما يوفر رؤية شاملة للتحسين في أداء DCMD، وبالتالي يسهم في المجال من خلال التطورات التكنولوجية والخوارزمية في عمليات التحلية.

الكلمات المفتاحية: DCMD، معلمات التشغيل، عملية التحلية،التدفق المتخلل، تحسين الأداء.

Preface

The research presented in this doctoral thesis was conducted at the Smart Structure Laboratory, located at the University of Ain-Temouchent in Algeria.
The thesis incorporates a collection of publications, including the following:

- **Journal Papers:**

1. **Bekraoui, H**., Nehari, D., Baki, T., & Bousmaha, M. (2023). The Effect of Operating Parameters on Total Cross-membrane Flux in a PVDF Flat Sheet Membrane. Periodica Polytechnica Chemical Engineering, 67(3), 490-503.
2. **Future perspectives**: journal papers are currently being prepared for publication and are part of the thesis work.

- **Conference papers**

1. **H. Bekraoui**, D. Nehari, A. Remlaoui, M. Sandid Abdelfatah. Numerical simulation and theoretical investigation of direct contact membrane distillation. International Conference on Renewable Energy and Energy Conversion ICREEC'2019. November 2019, USTO-MB Oran, Algeria
2. A. Remlaoui, D. Nehari, **H. Bekraoui**, M. Sandid Abdelfatah, Modelling a forced circulation solar water heater system (SWH) by TRNSYS Dynamique simulation. The International Conference on Materials Science and Engineering and their Impact on the Environment (ICMSE@2019). November 2019, Sidi Bel Abbes, Algeria.
3. M. Sandid Abdelfatah, D. Nehari, I. Ait Yala, A. Remlaoui, **H. Bekraoui**, Performance of the thermal system for membrane distillation using photovoltaic system panels and flat plate collector. The International Conference on Materials Science and Engineering and their Impact on the Environment (ICMSE@2019). November 2019, Sidi Bel Abbes, Algeria.
4. A. Elmeriah, D. Nehari, A. Remlaoui, I. Ait Yala, **H.Bekraoui**, A. Marni. Numerical investigation of a flow inside a medium thermal energy storage density unit. 2nd Day of Structures and Sustainable Development, El Wancharissi University Center in Tissemsilt. t, 11 April 2019.
5. A. Remlaoui, D. Nehari, I. Ait Yala, M. Sandid Abdelfatah, **H. Bekraoui**, A. Elmeriah. Solar forced circulation water heating systems using flat plate collector: A TRNSYS Dynamic Simulation.International Conference on Renewable Energy and Energy Conversion ICREEC'2019. November 2019, USTO-MB Oran, Algeria.
6. M. Sandid Abdelfatah, D. Nehari, I. Ait Yala, A. Remlaoui, **H. Bekraoui**, A. Elmeriah. Cooling system for membrane distillation using photovoltaic system panels in the weather of Ain-Temouchent International Conference on Renewable Energy and Energy Conversion ICREEC'2019. November 2019, USTO-MB Oran, Algeria.

Dedicated to

My beloved Dad, Muhammad El Mortada,

and cherished Mum

As well as my siblings,

Also, to my entire family and my friends,

Your support and affection mean the world to me.

Thank you all.

Special dedication to my second beloved mother,

Lala Zahra Muslim

May her soul rest in peace. Wherever you are,

I hope you are proud of me.

Hafsa Bekraoui

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Hafsa Bekraoui

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Nomenclature

Symbols	Units	Definition
Abbreviations		
A	m^2	The cross-sectional area of the membrane
a_w	-	Water activity
C_m	kg/m^2. Pa. s	Membrane mass transfer coefficient
C_p	J/kg.K	Specific heat capacity of the fluid
D_h	m^2	Hydraulic diameter
H	m	Membrane module hight
h	W/m^2 .K	Convective heat transfer coefficient
h_f	W/m^2 .K	Feed convective heat transfer coefficient
h_p	W/m^2 .K	Permeate convective heat transfer coefficient
J_w	kg/m^2.h	Permeate flux through the membrane
K_g	W/m. K	Thermal conductivity of gas in membrane pores
K_m	W/m. K	Effective thermal conductivity of the membrane
K_s	W/m. K	Thermal conductivity of solid in membrane pores
Nu	-	Nusselt number
P_{fm}^{sat}	Pa	saturation vapor pressure at the feed-membrane interface
P_{pm}^{sat}	Pa	saturation vapor pressure at the permeate-membrane interface
P_{w}^{sat}	Pa	Water vapor pressure feed-membrane / permeate-membrane interfaces
Q_c	W	Heat transfer by conduction through membrane material
Q_f	W	Heat transfer by convection through the feed boundary layer
Q_m	W	Heat transfer through membrane
Q_p	W	Heat transfer by convection through the permeate boundary layer
q_f	kg/s	Feed flow rate
Re	-	Reynolds number
T	K	The mean temperature in the pores
T_{fb}	K	Feed bulk temperature
T_{pb}	K	Permeate bulk temperature
T_{fm}	K	Feed temperature at the membrane surface
T_{pm}	K	Permeate temperature at membrane surface
Pr	-	Prandtl number
v	m/s	velocity
U	W/m^2K	overall heat coefficient
x_{NaCl}	g/kg	The NaCl mole fraction in water solution
ΔH_v	kJ/kg	Enthalpy of water vaporization
Greek Letters		
δ	m	Membrane thickness
ε	%	Membrane porosity
μ	Pa.s	Fluid viscosity
ρ	kg/m^3	Fluid density
Subscript		

b	Bulk
f	Feed
g	Gas
m	Membrane
P	Permeate
s	Solid
w	Water
	Acronyms
MD	Membrane distillation
MSF	Multi-stage Flash Distillation
MED	Multiple Effect Distillation
VCD	Vapor Compression Distillation
MVC	Mechanical Vapor Compression
TVC	Thermal Vapor Compression
ED	Electrodialysis
EDR	Electrodialysis Reversal
UF	Ultrafiltration
MF	Microfiltration
NF	Nanofiltration
RO	Reverse osmosis
FO	Forward osmosis
DCMD	Direct contact membrane distillation
AGMD	Air gap membrane distillation
VMD	Vacuum membrane distillation
SGMD	Sweeping gas membrane distillation
PTFE	Polytetrafluoroethylene
PVDF	Polyvinylidene difluoride
PP	Polypropylene
PA	Polyamide
PES	Polyether sulfone
PSU	Polysulfide
CA	Cellulose acetate
PE	Polyethylene
PVC	Polyvinyl chloride
PI	Polyimide
TPC	Temperature polarization coefficient
LEP	Liquid entry pressure
BO	Bonobo Optimization
PSO	Particle Swarm Optimization

General Introduction

General introduction

Background and Motivation

Water, an essential element in nature, is a vital resource for our society and is crucial for our survival and maintaining ecosystem balance. However, human actions have caused various environmental disruptions [1]. The consequences of climate change, such as rising temperatures, sea-level rise, reduced precipitation, and droughts, are becoming increasingly apparent.

Water scarcity is steadily increasing, and ensuring an adequate supply of both quantity and quality for human consumption is essential, emphasizing the need for effective planning, management, and exploration of sustainable water sources [2]. Saline water constitutes around 97.5% of Earth's total water, with only 2.5% remaining as freshwater. Within this limited portion, polar ice and glaciers hold approximately 70%. Consequently, lakes, rivers, and reservoirs store only 0.26% of the world's freshwater [3]. Even more significantly, only 0.014% of the planet's water supply is accessible and usable by humans [4].

The supply and management of water play a significant role in societal development and the well-being of citizens, with the need for revised water management practices, including the adoption of advanced technologies and alternative water resources, to address growing environmental and health issues [5]. It is not just about meeting human consumption needs but also fulfilling the demands of agriculture and industry, which often require substantial water resources. [6].

Desalination has emerged as a significant and practical solution for addressing water scarcity in regions facing water stress. There are two primary types of desalination projects: seawater and brackish water. Around 16,000 operational desalination plants are spread across 177 countries, producing approximately 95 million cubic meters of freshwater per day [7]. It involves extracting fresh water from saline sources such as seawater [8] and utilizing thermal distillation and membrane-based separation processes. [9],[10]

Recent advancements in desalination technology have played a crucial role in reducing costs and enhancing the quality of desalted water, aligning with stringent regulatory standards.

General introduction

Moreover, there is a growing emphasis on integrating desalination techniques with renewable energy sources, ensuring environmentally friendly operations. [11],[12].

In industrial applications, Membrane Distillation effectively adapts water desalination or treatment. A difference in partial pressure serves as the driving force, and the presence of a hydrophobic membrane ensures high water quality regardless of feedstock parameters [13]. However, addressing several issues is necessary before fully deploying this technology commercially.

Thesis Objectives and Scope

This thesis centers around the theme of desalination, with a specific focus on membrane distillation techniques, particularly Direct Contact Membrane Distillation (DCMD). The study delves into multiple facets of desalination and membrane distillation, including different desalination methods, techniques for membrane characterization, and an overview of the current advancements in membrane distillation.

The primary objective of this study is to enhance the thermohydraulic understanding of membrane distillation in the context of drinking water to subsequently improve the thermal and hydraulic performance of the DCMD unit. The specific objectives of this study are as follows:

- Conducting a comprehensive thermohydraulic analysis of the DCMD unit.
- Investigating the performance of the DCMD unit and performing simulation using the MATLAB program.
- Evaluating the performance of flat sheet membrane in the DCMD system across various conditions.
- Evaluating and analyzing various operating parameters to understand their impact on the permeate flux.
- Optimizing the performance of the DCMD system in terms of operating parameters and membrane geometric characteristics aims to enhance drinking water production by maximizing both the permeate flux and the thermal efficiency.
- Utilizing a simulation in MATLAB, the aim is to optimize and design a more efficient water distillation system based on the DCMD concept.
- The insights, conclusions, and optimization outcomes will provide valuable guidance for developing an optimal DCMD system design.

Thesis Outline

The thesis comprises three main chapters and dedicated sections for Introduction and Conclusions (refer to Figure A).

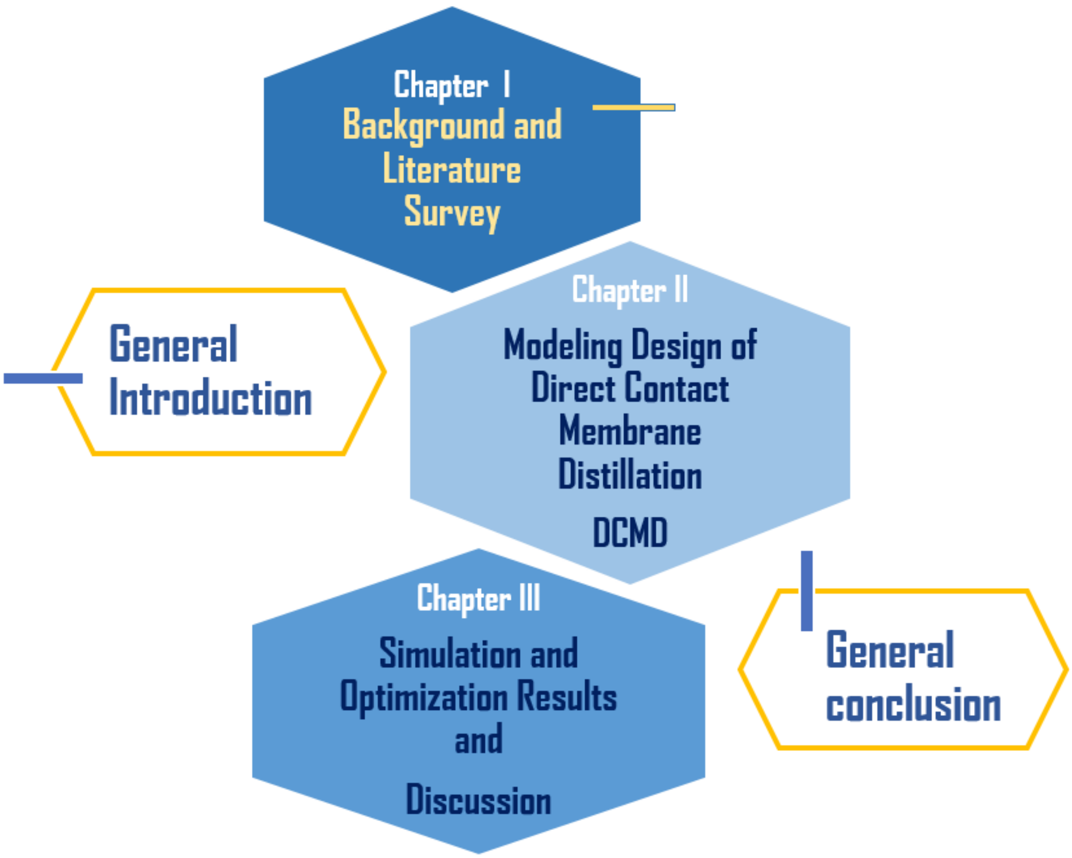


Figure A: Thesis Outline

Chapter I provides a general introduction to the topic, highlighting the genesis of desalination as an innovative solution born out of necessity. It discusses two main categories of desalination methods: thermal desalination and membrane desalination. Within thermal desalination, it covers Multi-stage Flash Distillation (MSF), Multiple Effect Distillation (MED), and Vapor Compression Distillation (VCD) techniques. The chapter also delves into membrane distillation, including Direct Contact Membrane Distillation (DCMD), Air gap Membrane Distillation (AGMD), Vacuum Membrane Distillation (VMD), and Sweeping Gas Membrane Distillation (SGMD). Additionally, it explores membrane characterization techniques and different membrane materials, focusing on organic membranes. The chapter concludes with an overview of the state of the art in membrane distillation.

Chapter II examines Direct Contact Membrane Distillation (DCMD) in depth. It centers on various aspects of DCMD, including its configuration, the potential challenges associated with DCMD membranes, and the structure of the DCMD module. The chapter delves into the properties of membranes used in DCMD and the modeling techniques employed for DCMD systems. Additionally, it highlights the significance of optimization in enhancing DCMD performance, discusses diverse optimization approaches applicable to DCMD, including Bonobo Optimization (BO) and Particle Swarm Optimization (PSO), and identifies the optimization variables and constraints relevant to DCMD systems. The chapter also addresses optimization objectives in DCMD while delving into the challenges and potential advancements in optimization techniques tailored explicitly for DCMD systems.

Chapter III builds upon the investigation of the specific DCMD system and presents two notable contributions. The first contribution explores the impact of various operating parameters on the total cross-membrane flux in DCMD, encompassing factors such as feed inlet temperature, permeate inlet temperature, feed and permeate flow rates, and feed inlet NaCl concentration. The second contribution of this study focuses on the optimization of DCMD. It emphasizes the Optimization method's significance in enhancing the performance of DCMD systems. The chapter discusses the importance of BO and identifies the optimization variables involved. Additionally, it includes a comparative analysis between two optimization methods, Bonobo Optimizer (BO) and Particle Swarm Optimization (PSO), in terms of their impact on optimizing permeate flux and thermal efficiency within DCMD systems.

This thesis provides a comprehensive overview of desalination and membrane distillation techniques, explicitly focusing on Direct Contact Membrane Distillation (DCMD). The thesis covers various desalination methods, membrane characterization studies, and optimization approaches to advance the understanding and development of membrane distillation technology.

Chapter I

Background and Literature Survey

INTRODUCTION

This chapter provides a comprehensive and detailed exploration of various desalination methods, focusing on membrane desalination (MD) as a thermal desalination technique. The main objective is to offer a thorough understanding of the technologies employed in producing safe drinking water. To facilitate comprehension, **Figure I. 1** presents a schematic chart illustrating the commonly utilized technologies in water desalination.

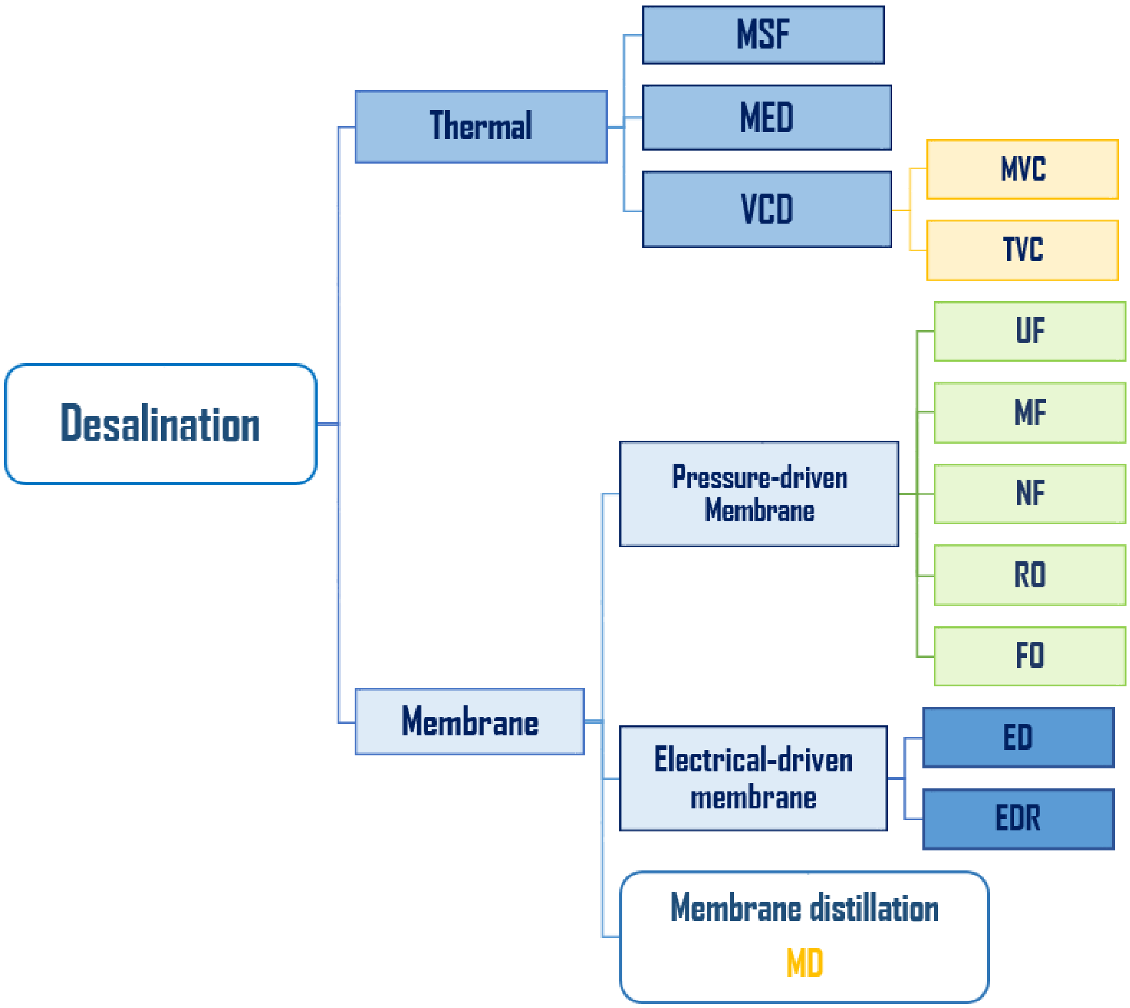


Figure I. 1: Desalination processes chart

The initial section of the chapter delves into the definition of desalination, aiming to establish a clear and comprehensive understanding of the concept while distinguishing it from other related processes. By establishing a solid foundation of knowledge, readers can better grasp the nuances and complexities of different desalination procedures.

In recent years, membrane technology has emerged as a formidable contender to conventional separation methods in desalination. Among the various pressure-driven and isothermal membrane processes, membrane distillation (MD) has gained significant attention due to its ability to address the associated challenges [14]. MD operates by utilizing water as the primary substance on the feed side, allowing only water vapor to permeate through the pores of a hydrophobic membrane. This selective permeation mechanism efficiently separates salt and other impurities, producing high-quality drinking water. The advantages and unique characteristics of MD make it a promising approach in the field of desalination.

By thoroughly exploring the principles and applications of MD, this chapter aims to provide a comprehensive understanding of its potential and limitations in water desalination. Additionally, the discussion will cover various aspects related to membrane selection, process optimization, and technological advancements in MD, providing insights into the ongoing research and developments in this field. The ultimate goal is to contribute to advancing desalination technologies and facilitate the widespread production of safe and accessible drinking water for populations worldwide.

1.1 The Desalination Genesis: Innovation Breeds from Necessity

Desalination involves the purification of seawater or brackish water by eliminating salt and other contaminants to make it suitable for consumption and various applications. The practice of desalination dates back to ancient times, when sailors and travelers employed rudimentary methods to convert seawater into potable water during their voyages. However, desalination's systematic and efficient development commenced in the latter half of the 20th century [15].

Desalination can be a solution for addressing water scarcity issues in areas facing water stress. Given the growth of populations and the depletion of natural freshwater resources caused by usage, wastage, and contamination, while saline water sources remain virtually limitless, desalination has become a hopeful solution to ensure a constant water supply. It has emerged as a vital, safe, and clean approach to tackling water scarcity [15].

There are several methods used in desalination, including distillation and membrane filtration. The distillation method involves heating seawater, causing the water vapor to rise and then condensing as freshwater, salt, and contaminants left behind. On the other hand, membrane filtration relies on semi-permeable membranes to separate salt and impurities from salt water, resulting in purified water. The increasing use of desalination brings up several economic and environmental considerations [16].

In areas where water is scarce, desalination plants provide a sustainable way of increasing water supply, reducing the dependence on unpredictable rainfall or depleting freshwater resources. This water source can promote agricultural productivity, facilitate industrial expansion, and meet the needs of a growing population [17].

However, it is crucial to recognize the environmental consequences connected to desalination. Proper management is required to dispose of the concentrated brine, a by-product of the process, and prevent any negative impact on marine ecosystems [18],[19]. Furthermore, the energy-intensive nature of desalination reinforces the need to explore renewable energy integration to decrease the carbon footprint associated with this process [20],[21].

I.1.1 Thermal desalination

Thermal desalination, an ancient approach that entails the processes of boiling, evaporating, and subsequent condensation, is a process used to remove salt and other impurities from saline water, such as seawater or brackish water, by utilizing heat energy to evaporate the water and condensing the vapor to produce fresh water [22]. This method involves the application of heat to create a phase change where water evaporates, leaving behind salts and contaminants. The resulting water vapor is then cooled and condensed back into liquid form, yielding purified fresh water. The transformation of water vapor serves as the foundation for the most commonly employed thermal desalination processes, namely multi-stage flash distillation (MSF), multiple-effect distillation (MED), and Vapor Compression Distillation (VCD) [23].

I.1.1.1 Multi-stage Flash Distillation (MSF)

Multi-stage Flash Distillation (MSF) is a widely used thermal desalination process that converts seawater into freshwater using evaporation and condensation principles. It is considered one of the oldest and most established desalination technologies [24].

In the MSF process, seawater is heated under high pressure and passed through a series of stages or chambers called "flashes." Each flash operates at a progressively lower pressure than the previous one. The high-pressure seawater is rapidly flashed into steam as it enters each stage, leaving behind a concentrated brine solution. The steam generated in each flash is then condensed to produce fresh water [25].

The flashes produce steam that heats the seawater in the next stage, maximizing energy efficiency. Moreover, the process utilizes multiple stages to achieve a higher freshwater production rate and improved overall efficiency. If necessary, the condensed fresh water is collected and treated to meet the required quality standards [8].

MSF desalination plants are known for their scalability and ability to handle large water capacities. Regions with abundant energy resources, such as oil-rich countries, commonly utilize them, as they power the process with waste heat from power generation or industrial processes [24]. Figure I. 2. shows a schematic of the MSF.

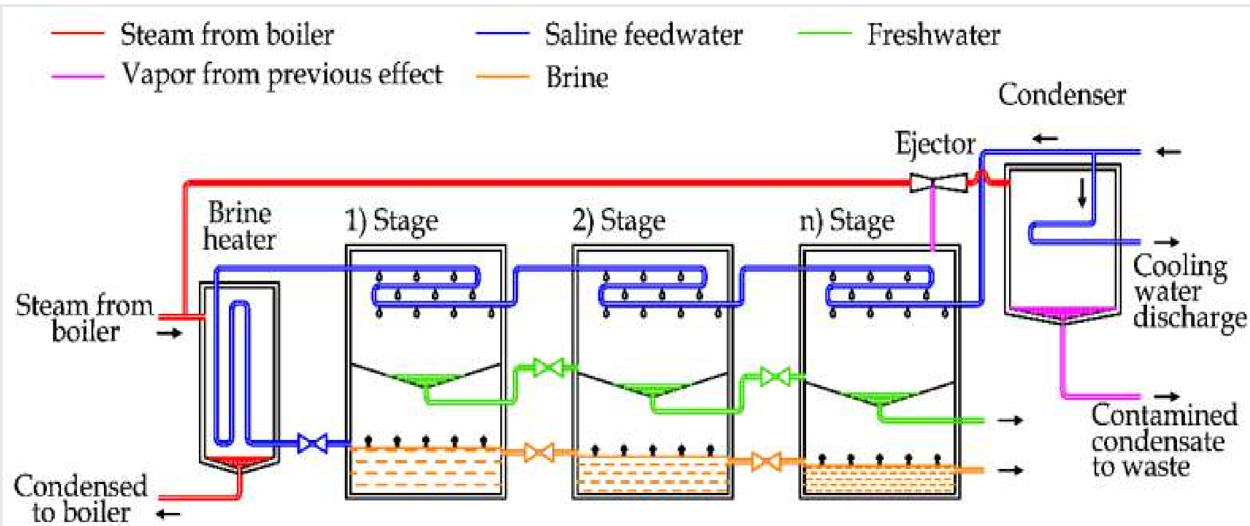


Figure I. 2: schematic of Multi-stage Flash Distillation (MSF) [10].

I.1.1.2 Multiple Effect Distillation (MED)

Multi-effect distillation (MED) is a thermal desalination process that converts seawater or brackish water into fresh water. It operates on the principle of evaporation and condensation, similar to other thermal desalination methods.

The first MED plant was realized in Kuwait in the 1950s [10], marking a significant milestone in developing and applying this technology. Since then, various parts of the world have adopted MED for large-scale desalination projects.

The Multi-Effect Distillation process utilizes multiple stages or effects to evaporate and condense the water sequentially. Each effect comprises a heat exchanger, an evaporator, and a condenser. The process typically operates at low pressure, allowing water to boil at lower temperatures [26].

The feedwater (seawater) is heated in the first effect using a heat source such as steam, solar energy, or waste heat. As the feedwater boils, it produces steam, which flows to the following effect, condensing on the surface of cooler tubes or plates [27]. The latent heat released during condensation actively contributes to the evaporation of more feedwater in the subsequent effect. Each effect repeats this process, where the vapor in each stage serves as the heating source for the subsequent stage.

The condensed fresh water is collected and separated from the concentrated brine. The brine containing the residual salts and impurities is discharged or treated for disposal [28]. The condensation process typically yields high-purity freshwater; however, meeting specific quality standards may require additional treatment.

Multi-effect distillation utilizes the heat from the condensation process to drive evaporation in subsequent stages, resulting in its renowned energy efficiency [8]. This feature renders it suitable for waste heat or low-grade thermal energy applications processes, power plants and large-scale desalination plants commonly employ it.

Overall, Multi-Effect Distillation is a well-established desalination technology that produces fresh water from seawater or brackish water, particularly in areas where thermal energy sources are readily available. Figure I.3 shows a schematic of the MED.

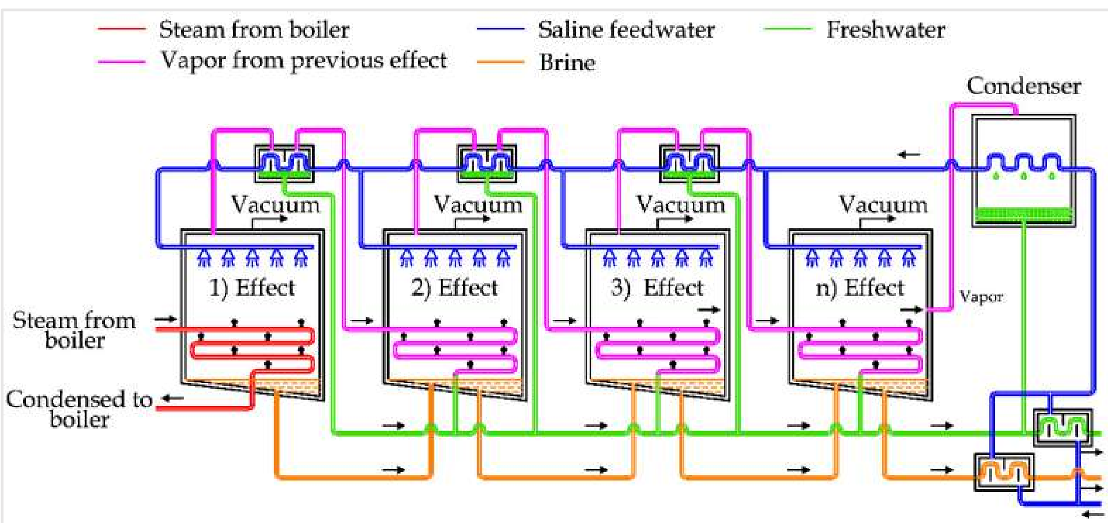


Figure I. 3: Schematic of Multi-effect distillation (MED) [10].

1.1.1.3 Vapor Compression Distillation (VCD)

Vapor Compression Distillation (VCD) evaporates contaminated saline water, harnessing the latent heat released by compressed vapor. The process involves using a compressor to increase the temperature and pressure of the vapor. As a result, the condensation process efficiently utilizes the released latent heat to generate additional vapor [22]. In VCD, the heating of the feedwater actively generates vapor, which the system subsequently compresses using a vapor compressor. The vapor compressor then condenses the compressed vapor to produce fresh water while discharging the remaining brine. Vapor compression enhances feedwater evaporation by elevating temperature and pressure. Combining it with other techniques like MED or MSF optimizes desalination [29]. Smaller units, with around 3000 m^3/day capacities, are suited for applications like hotels and industries. Mechanical Vapor Compression (MVC) and Thermal Vapor Compression (TVC) are subtypes of VCD that differ in the method used to achieve vapor compression. MVC utilizes a mechanical compressor power.

Electricity powers vapor compression, as shown in Figure I. 4, while TVC uses a steam jet ejector or thermal compressor to create a vacuum and enhance the evaporation process available [22], as shown in Figure I. 5.

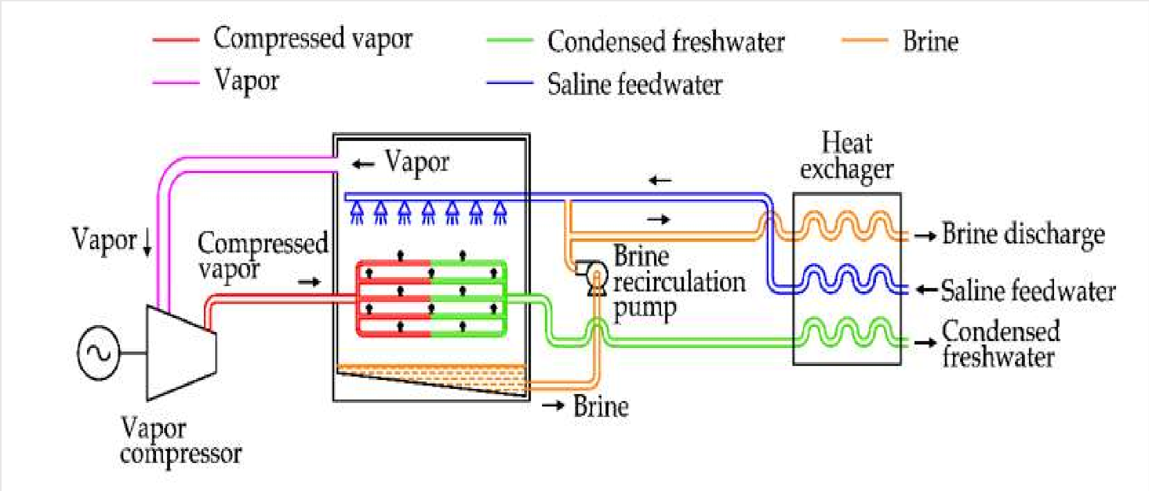


Figure I. 4: Schematic of Mechanical Vapor Compression (MVC) [10].

1.1.2 Membrane desalination

Membrane technologies are significant in various industrial processes, including water treatment and purification. These technologies fall into two main types:

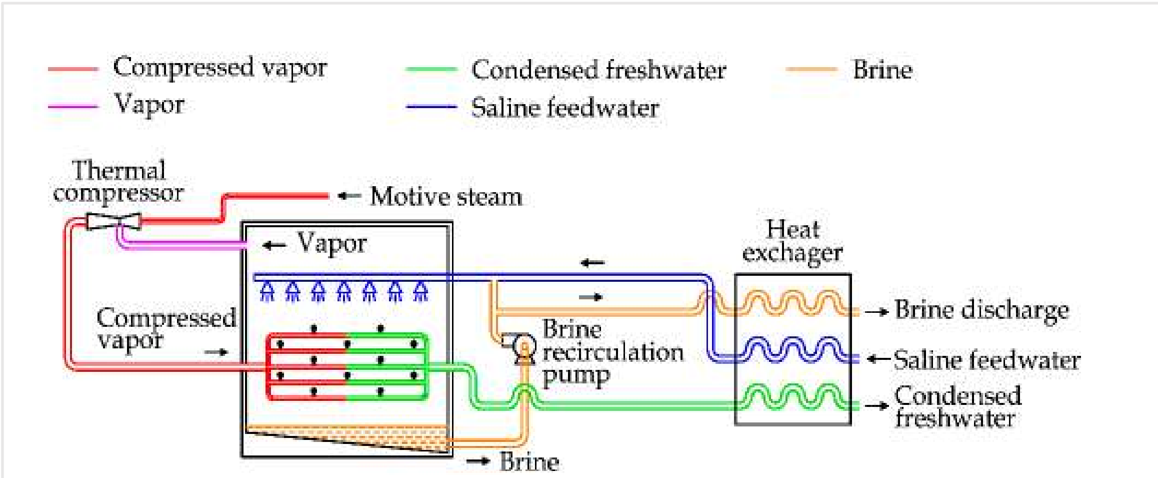


Figure I. 5: Schematic of Thermal Vapor Compression (TVC) [10].

I.1.2.1. Pressure-Driven Processes:

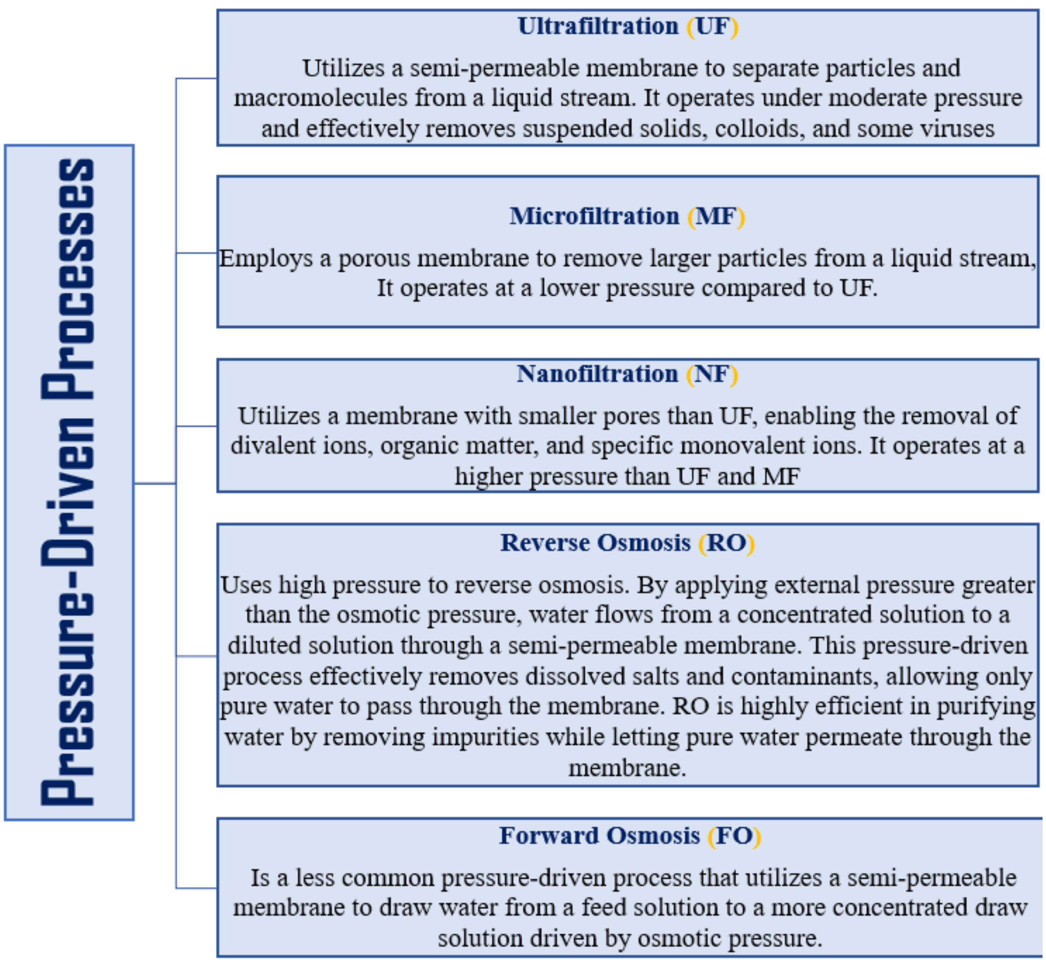


Figure I. 6: Schematic of the Pressure-Driven Processes

I.1.2.2. Electrical-Driven Processes:

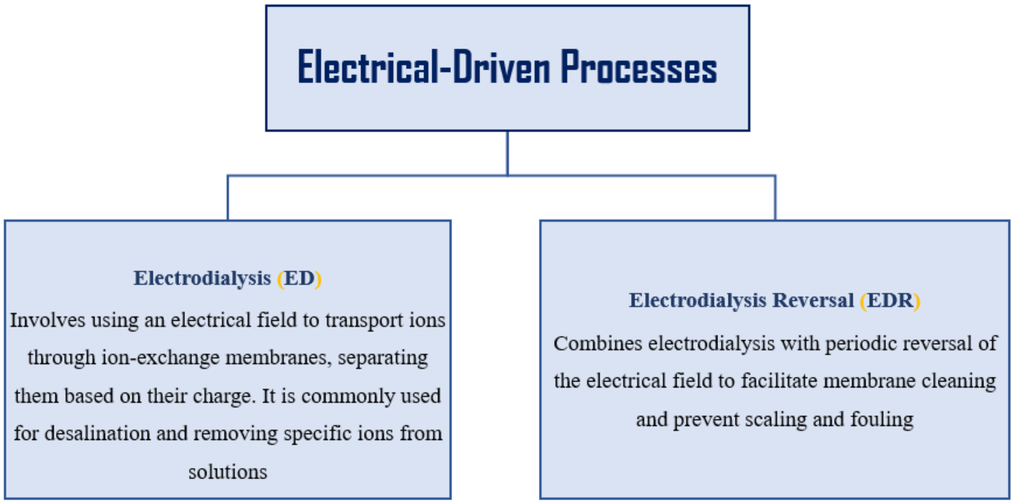


Figure I. 7: Schematic of Electrical-Driven Processes

Distinct advantages characterize pressure-driven and electrical-driven membrane processes, leading to their employment in various applications based on specific treatment requirements. They provide efficient and sustainable solutions for water purification, desalination, wastewater treatment, and many other industrial processes.

Table I.1 represents the main benefits and drawbacks of the different desalination processes

Table I. 1: Main benefits and drawbacks of the different desalination processes

Process	Benefits	drawbacks
MSF	• The potentiality for high-quality water rates. • The technology is well-established and proven in practice. • Less prone to membrane fouling issues due to its thermal process. • Can treat saltwater up to 70000 mg/L. • Construction and operation of the plants are relatively quick. • It can remain partially operational during equipment cleaning or replacement, minimizing downtime. • It has minimal pre-treatment requirements. • It does not generate waste from backwashing pre-treatment filters.	• The significant energy requirement makes it less energy-efficient than other methods. • Adding stages increases capital costs and operational complexity due to increased total surface area. • A significant contribution to air pollution, such as the increased carbon emissions, is due to the high energy consumption. • Experiences a high occurrence of scaling in tubes. • Sluggish response to fluctuation in water demand and feedwater quality sensitivity may require additional pre-treatment steps.

		• Cannot operate below 60% of its capacity
MED	• The operating temperature is lower than 70°C, mitigating the risk of corrosion and scale formation on tube surfaces. • Less expenses associated with pre-treatment and operation. • Producing potable water efficiently, exhibiting lower power consumption than MSF. • The capital costs decreased noticeably. • The flexibility to operate between 0% and 100% of its total capacity. • The effectiveness of combination with intermittent renewable energy sources.	• Significant thermal energy consumption. • Limited scalability plants can be challenging and require significant system design modifications. • Susceptibility to scaling and fouling, reducing efficiency over time. • Requiring regular maintenance and cleaning to ensure optimal performance. • Sensitivity to feedwater quality, which may require proper disposal or additional pre-treatment steps.
VCD	• more cost-effective, particularly for small-scale desalination units, as it requires fewer complex components • Operated with lower energy consumption. • It is particularly suitable for small-scale desalination units, allowing for flexible implementation based on varying water demand and resource availability. • The process can handle a wide range of feedwater salinity levels, making it adaptable to different water sources and conditions. • Have a lower environmental impact, including reduced brine discharge and lower energy requirements.	• Unsuitable for large-scale desalination projects due to its limited capacity. Commonly used for smaller-scale applications. • Dependence on electrical power to drive the compression and evaporation cycles. • Higher operating costs due to energy consumption • Limitations in removing specific contaminants or impurities from the feedwater. • Necessary Pre-treatment steps for desired water quality
UF	• Effective removal of large particles, colloids, and macromolecules. • Enhanced bacteria removal. • High permeate flow rates. • Moderate operating pressure.	• Limited removal of small dissolved solutes. • Moderate rejection of divalent ions. • It may require pretreatment to prevent fouling. • Energy-intensive process.
MF	• Efficient removal of suspended solids, bacteria, and larger particulates. • Low operating pressure. • Minimal fouling and clogging.	• Limited ability to remove dissolved solutes • Low rejection of small particles • Not suitable for desalination

NF	• Enhanced removal of divalent ions, organic matter, and selected salts. • Partial desalination capabilities. • High rejection of larger solutes. • Moderate operating pressure.	• Limited rejection of monovalent ions. • Lower rejection of small dissolved solutes compared to reverse osmosis. • It may require pretreatment to prevent fouling.
RO	• Highest level of desalination and solute removal. • High rejection of salts, minerals, and organic compounds. • Low operating pressure for brackish water desalination. • Wide range of applications.	• Energy-intensive process. • Requires high operating pressure for seawater desalination. • Potential fouling and scaling issues. • Limited removal of certain uncharged or small organic compounds.
FO	• Low operating pressure • Minimal fouling and scaling potential. • Can utilize lower-quality feed water. • Energy potential recovery.	• Lower water recovery compared to RO. • Limited membrane options and commercial availability. • Osmotic agent regeneration is required. • Moderate rejection of solutes.
ED	• Selective removal of ions. • Continuous operation without fouling. • Energy-efficient process. • Suitable for desalination and salt removal.	• Limited removal of uncharged solutes. • Requires electricity for operation. • Scaling and fouling potential in high-concentration environments. • Requires complex system setup.
EDR	• Efficient removal of ions and salts. • Continuous operation with self-cleaning capability. • Suitable for desalination and water treatment. • Energy-efficient process.	• Limited removal of uncharged solutes. • Requires electricity for operation. • Scaling and fouling potential in high-concentration environments • Higher capital and operational costs compared to ED.

I.1.3. Membrane distillation

Membrane distillation (MD) is a promising technology with many applications, including desalination and wastewater treatment. MD harnesses the vapor pressure differences across a hydrophobic membrane to efficiently separate components in a liquid mixture. Unlike conventional distillation methods that rely on heat transfer, MD relies on the vapor pressure discrepancy of the membrane to drive the separation process. The membrane acts as a selective barrier, preventing liquid water, dissolved salts, and non-volatile substances from passing through while allowing water vapor to permeate through its pores. The feed side of the membrane comes into direct contact with a hot saline solution, while the permeate side remains cool, resulting in a temperature contrast. This temperature difference creates a vapor pressure gradient, facilitating the passage of water vapor through the membrane's pores [30].

The initial exploration of the MD process occurred in Europe during the late 1960s when Haute and Hendeyckx conducted notable research in this field [31]. However, the development of MD experienced setbacks. It was not until June 3, 1963, that Bruce R. Bodell [32] achieved a significant milestone by obtaining the first US patent for an apparatus designed to allow the passage of water vapor molecules while impermeable to liquid water, thus producing potable water. Bodell's innovative device utilized a resilient silicon rubber membrane capable of withstanding high temperatures, creating a drier environment within the membrane [33]. Figure I. 8 presents a schematic representation of the apparatus: Non-potable water is heated by a Bunsen burner (12) in an evaporator (10) operating under partial vacuum conditions.

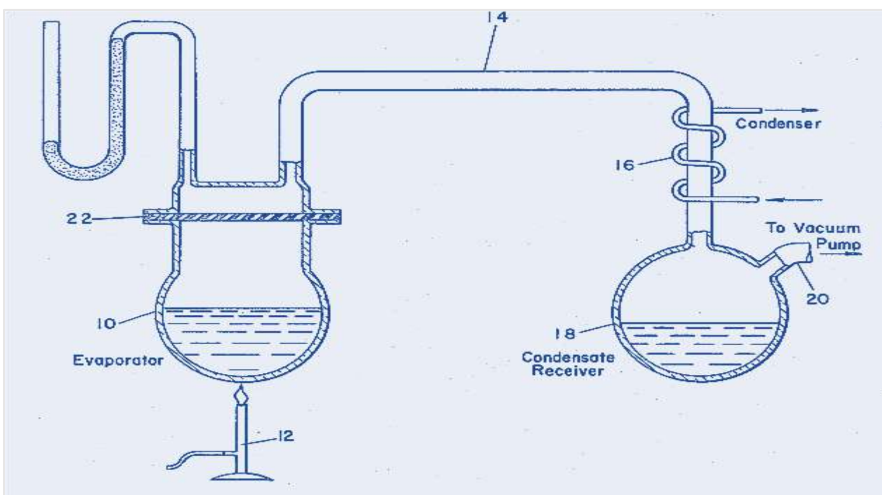


Figure I. 8: Schematic representative of Bedell's apparatus [36]

As the water evaporates, it permeates the porous silicon rubber membrane (22) and is transported to a condenser (16) through a connecting tube (14), eventually collecting in the condensate receiver (18). The condensate receiver is connected to a vacuum pump via another tube (20). The system operates at sub-atmospheric pressures ranging between 40-50 mmHg in the heating and condensing zones.

Notable advancements in membrane distillation (MD) have been documented, including the work of Weyl, who introduced a novel concept patented on September 5, 1967 (filed on May 14, 1964). Weyl's approach involved using an air-filled, porous hydrophobic membrane made from polytetrafluoroethylene (PTFE) [37]. The membrane had an average pore size of 9 microns and a porosity of approximately 42%.Weyl's work aimed to enhance the efficiency of membrane desalination. In his research, Weyl explored various materials suitable for hydrophobic membranes, including polyethylene (PE), polypropylene (PP), polyvinyl chloride (PVC), and hydrophobic ceramic compositions) [34]. Additionally, he considered the possibility of creating a hydrophilic membrane with a hydrophobic surface layer supported by a porous structure.

These advancements in membrane materials and designs have contributed to improving the efficiency and performance of MD systems, enabling better separation and the production of high-quality water. Ongoing research and development in membrane technology continue to explore new materials, surface modifications, and system configurations to enhance MD efficiency further and expand its applications.

In 1967, Findley made a notable contribution to the membrane distillation (MD) field by publishing the first paper on the topic in the journal "Industrial & Engineering Chemistry Process Design Development [35]. Using a direct contact membrane distillation (DCMD) setup, Findley conducted experiments investigating heat and mass transfer phenomena [35]. He examined various membrane materials, including gumwood, aluminum foil, cellophane, glass fibers, and glass paper. Findley also introduced silicone, water-repellent, and Teflon suspensions to enhance the hydrophobicity of the membranes, aiming to prevent the infiltration of liquids and non-volatile constituents.

Based on his experimental findings, Findley emphasized critical factors for effective mass transfer, including minimizing heat flow through conduction, achieving an adequate membrane thickness, utilizing hydrophobic pores with small dimensions, reducing moisture absorption, and ensuring uniformity in porosity and thermal conductivity.

From the 1970s to the 1980s, reverse osmosis (RO) experienced significant technological advancements and gained prominence due to its higher productivity rates than membrane distillation (MD). In contrast, MD progressed gradually in research and remained somewhat overshadowed. This phase, characterized by lower flow productivity rates and limited capacity of small-scale MD facilities, has been referred to as a period of slow development [28].

From the early 1980s to the 1990s, there was a notable resurgence of interest and activity in membrane distillation (MD) [32]. During this phase, researchers enthusiastically dedicated their efforts to optimizing the MD process, developing suitable membranes, and exploring various applications. This period, commonly called the "reawakening," was marked by a renewed focus on advancing MD technology.

In particular, researchers conducted numerous studies focused on modeling and testing MD processes to improve the MD flux, which is the water vapor transport rate through the membranes. However, it is worth mentioning that there was relatively limited interest in pilot-scale research during this time. The emphasis was primarily on laboratory-scale investigations to understand the fundamental principles and refine the MD process.

The phase of growth that followed in the 1990s and continues to the present day further solidified the position of MD as a promising technology [32]. Researchers have continued to explore and refine MD processes, develop novel membrane materials, and expand the range of applications. This ongoing effort reflects the sustained interest and potential for further advancements in MD technology.

Membrane distillation is implemented in various configurations, including Direct Contact Membrane Distillation (DCMD), Air Gap Membrane Distillation (AGMD), Sweep Gas Membrane Distillation (SGMD), and Vacuum Membrane Distillation (VMD). Each configuration utilizes different methods on the permeate side to collect the distillate. DCMD and AGMD are well-suited for desalination applications, focusing on water as the permeate. SGMD and VMD, on the other hand, are commonly used to remove volatile organic compounds or dissolved gases from aqueous solutions.

Among these configurations, DCMD is characterized by a straightforward arrangement where the hot saline feed water and the cold distillate stream directly interact with the membrane, leading to vapor condensation within the module's permeate side. In comparison, AGMD exhibits commendable thermal efficiency but with a relatively reduced flux. VMD offers a notable high flux while effectively minimizing conductive heat loss, although it faces increased vulnerability to potential membrane pore risks. Lastly, SGMD boasts elevated thermal efficiency but requires a substantial condensation capacity for optimal operational effectiveness [36].

I.1.3.1 Direct Contact Membrane Distillation DCMD

DCMD is a membrane distillation process that involves direct contact between the feed solution and the membrane surface. In DCMD, a hydrophobic membrane is used, which allows only water vapor molecules to pass through while preventing the passage of liquid water [37].

DCMD process operates based on the principle of vapor pressure difference. The feed solution, typically a saline or contaminated water source, is heated, and the resulting vapor is brought into contact with one side of the hydrophobic membrane. A cold condensation surface or coolant is on the other side of the membrane. As the water vapor molecules pass through the membrane, they condense on the cold surface, forming purified liquid water, commonly known as distillate. However, it requires a significant temperature difference between the feed and coolant to drive the vapor pressure difference and maintain the distillation process.

The hydrophobic nature of the membrane ensures that liquid water does not cross the membrane, allowing only water vapor to permeate. This prevents the mixing of the feed solution and distillate, resulting in the separation of contaminants and impurities from the desired purified water. Additionally, the hydrophobic membrane used in DCMD must be carefully selected and maintained to ensure its long-term performance and prevent fouling or degradation.

I.1.3.2 Air gap Membrane Distillation AGMD

AGMD is a membrane distillation process involving an air gap between the feed solution and the membrane surface. In AGMD, a hydrophobic membrane is utilized, which allows only water vapor molecules to pass through while preventing the passage of liquid water.

AGMD process operates based on the principle of vapor pressure difference. The feed solution, typically a saline or contaminated water source, is heated, and the resulting water vapor is brought into contact with one side of the hydrophobic membrane. There is an air gap on the other side of the membrane [38]. This air gap acts as an insulating layer, preventing direct contact between the feed solution and the membrane. As the water vapor molecules pass through the hydrophobic membrane, they diffuse through the air gap and reach a cold condensation surface or coolant. On this cold surface, the water vapor condenses, forming purified liquid water known as distillate. The air gap acts as a barrier, ensuring the separation of the feed solution and distillate, thus allowing the removal of contaminants and impurities.

The hydrophobic membrane used in AGMD must be carefully selected and maintained to ensure its long-term performance and prevent fouling or degradation. Additionally, the design of AGMD systems needs to consider the management of the air gap and any potential limitations associated with its thickness and stability.

I.1.3.3 Vacuum Membrane Distillation VMD

VMD is a membrane distillation process that utilizes a vacuum on the permeate side of the membrane to facilitate vapor transport. In VMD, a hydrophobic membrane is employed, allowing only water vapor molecules to pass through while blocking the passage of liquid water.

VMD process operates based on the principle of vapor pressure difference and the application of a vacuum. The feed solution, typically a saline or contaminated water source, is heated, and the resulting water vapor is brought into contact with one side of the hydrophobic membrane [39]. On the other side of the membrane, a vacuum is applied. This vacuum lowers the pressure on the permeate side, creating a vapor pressure difference across the membrane. As a result of the vapor pressure difference, water vapor molecules pass through the hydrophobic membrane from the feed side to the permeate side. The membrane permeate side is maintained at a lower pressure due to the vacuum, causing the water vapor to condense on a cold surface or coolant [40]. This condensation leads to the formation of purified liquid water known as distillate.

I.1.3.4 Sweeping Gas Membrane Distillation SGMD

SGMD is a membrane distillation process using a gas stream to enhance vapor separation from the liquid feed. In SGMD, a hydrophobic membrane is employed, allowing only water vapor molecules to pass through while blocking the passage of liquid water.

SGMD process operates by introducing a sweep gas, typically air or an inert gas, on the permeate side of the membrane. The sweep gas flows parallel to the membrane surface, creating a concentration gradient that helps remove the vapor molecules from the permeate side, thereby increasing the driving force for vapor transport [41].

As the feed solution, a saline or contaminated water source is often heated, and water vapor is generated and brought into contact with one side of the hydrophobic membrane. The sweep gas flow on the permeate side of the membrane carries away the vapor molecules, reducing their partial pressure and maintaining a concentration gradient across the membrane. This differential in vapor concentration facilitates water vapor diffusion through the hydrophobic membrane.

On the other side of the membrane, a cold surface or coolant is provided to condense the water vapor carried by the sweep gas. This condensation results in the formation of purified liquid water known as distillate.

In SGMD, introducing a sweep gas helps enhance vapor removal and minimizes the risk of concentration polarization on the membrane surface. However, carefully controlling the sweep gas flow rate and temperature is necessary to optimize the process and maintain efficient vapor transport. Selecting and maintaining an appropriate hydrophobic membrane ensures long-term performance and prevents fouling or degradation. Additionally, the design and operation of SGMD systems must consider factors such as the sweep gas composition, flow dynamics, and energy requirements to achieve optimal distillation performance [42].

To comprehensively understand each configuration's unique mechanisms, application domains, advantages, and limitations, please refer to **Figure I.9** and **Table I. 2**. Upon reviewing the table, it becomes evident that among the various membrane distillation (MD) configurations, DCMD stands out as the most straightforward design. AGMD showcases commendable thermal efficiency, and VMD demonstrates a notable high flux with reduced conductive heat loss but increased pore risks. SGMD exhibits elevated thermal efficiency with a need for substantial condensation capacity.

Various new configurations have been developed to enhance thermal efficiency and permeate flux in membrane distillation processes [42] :

1. Material-gap MD (MGMD): This configuration is considered an advanced version of AGMD and is currently under development. It aims to improve the performance of AGMD by optimizing the material properties and gap design.
2. Permeate-gap MD (PGMD): PGMD is a hybrid configuration combining DCMD and AGMD elements. By incorporating a permeate gap, it seeks to benefit from the advantages of both configurations and enhance the overall efficiency and flux.

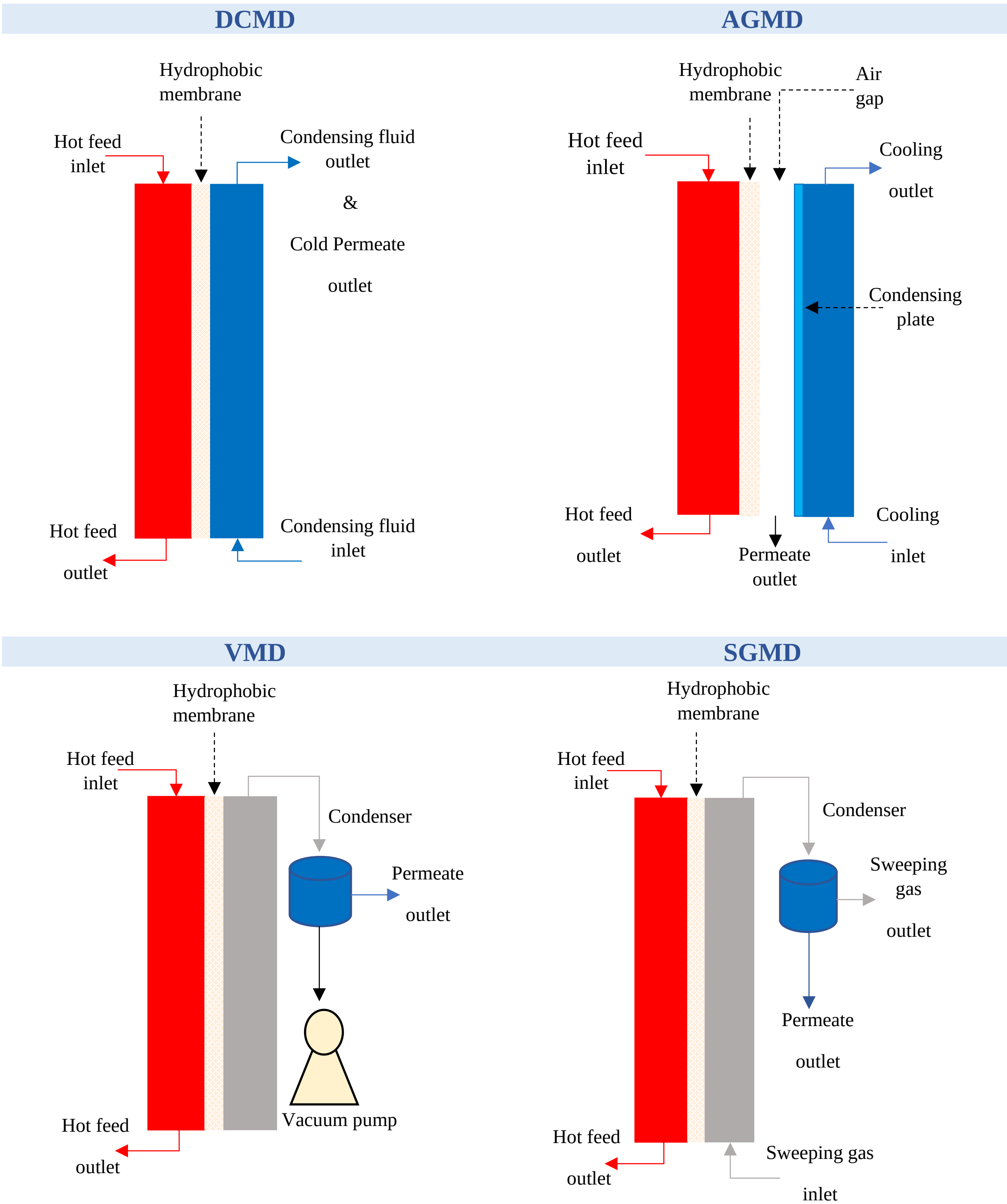


Figure I. 9: Schematic representative of Membrane desalination configurations.

3. Multi-effect MD (MEMD): MEMD is based on recovering internal heat within the AGMD module. It leverages multiple stages or effects to improve energy utilization and increase the overall efficiency of the distillation process.

4. Vacuum multi-effect MD (VMEMD): integrates the multi-effect concept into the VMD form. Using vacuum conditions and multiple effects, it aims to optimize energy consumption further and enhance the performance of the distillation process.

Table I. 2: Configuration's unique mechanisms, benefits, and drawbacks

DCMD	**MECHANISM** • Beginning with evaporating the feed solution. • The temperature difference induces pressure difference (driving force), which forces volatile molecules to evaporate, diffuse through the membrane, and condense at the permeate side. • The evaporated hot feed and condensing fluid are in direct contact with the membrane surface on the permeate side. • The condensing fluid used to condense water vapor is often freshwater.
	BENEFITS • High permeate flux is more stable than VMD due to its facility, mass, and heat transfer. • High separation efficiency. • Low fouling potential • Operate at low pressures. • The most straightforward kind of MD categories (Simple design). • Most straightforward setup on a laboratory scale. • No need for an external condenser. • Most appropriate for the water-based application. • The lowest cost option is solar thermal energy.
	DRAWBACKS • Huge conductive heat loss due to conduction via a membrane from the hot feed side to the cold distillate stream. • Highest temperature polarization.
AGMD	**MECHANISM** • In this process, a thin stagnant air layer (air gap) is introduced between the membrane surface on the permeate side and the condensing plate. • After feed solution evaporation, volatile components across both membrane and air gap condense over the condensing plate.
	BENEFITS • The most versatile MD categories. • The most resistant to membrane wetting. • Low conductive heat loss compared to DCMD due to the less thermal air conductivity.

	• Low-temperature rate polarization phenomena. • No need for an external condenser. • Less fouling. **DRAWBACKS** • The lowest permeate flux. • The air layer creates additional resistance to mass transfer. • The most expensive cost option is using solar thermal energy.
VMD	**MECHANISM** • The water vapor is transferred from the membrane module to the outside condenser under a vacuum. • The vacuum pressure must be less than the saturation pressure of volatile components in the feed solution to provide a necessary force for the condensation. • The vacuum is applied on the permeate side by installing the pump. **BENEFITS** • High permeate flux. • No conductive heat loss. • Remove the air in the membrane pore (improving the mass transfer) **DRAWBACKS** • High risk of wetting the membrane. • Requiring the external condenser. • Requiring the vacuum pump. • Electricity consumption by the pump. • Limited thermal energy recovery.
SGMD	**MECHANISM** • A cold, inert gas is pushed into the condensation chamber to carry the vapor molecules. • After the vapor molecules are collected, the sweeping gas takes them out of the membrane module to be condensed. **BENEFITS** • Improve mass transfer. • Less conductive heat loss. • High Thermal efficiency. **DRAWBACKS** • Drop-in driving force due to an increase in the temperature of gas swept along the membrane surface. • Gas transport requires more electrical energy (additional cost). • Difficult to recover the vaporization heat. • A small volume of the vapor diffuses in a large volume of sweeping gas, requiring a sizeable external condenser.

I.2. Membrane Characterization Techniques

Membrane characterization holds significant importance at various stages of a membrane's lifecycle. During the research and development phase, it is a critical element within the iterative design-synthesize-test-evaluate process. By characterizing membranes, researchers can gain valuable insights into their structural and functional properties, enabling them to optimize the design and synthesis of membranes for specific applications. This characterization evaluates pore size, surface chemistry, porosity, and mechanical strength.

As membranes transition to the operational phase, the focus of membrane characterization shifts. At this stage, the characterization becomes more limited in scope and primarily revolves around assessing the membrane's condition to determine if cleaning, regeneration, or replacement is necessary. This characterization typically involves monitoring parameters such as fouling, scaling, and loss of permeability or selectivity over time [43]. Operators can make informed decisions regarding maintenance activities by conducting such assessments and ensuring the membrane system operates optimally. Membrane characterization serves different purposes throughout the membrane's lifecycle. During research and development, it aids in fine-tuning membrane properties, while during operation, it helps in assessing membrane conditions and determining maintenance requirements for sustained performance. There are three types of membrane characterization [43].

I.2.1 Characterization of Composition:

Characterizing a membrane's composition involves determining the membrane material's chemical components and molecular structure [44]. This characterization helps understand the membrane's chemical compatibility, stability, and potential interactions with the substances it comes into contact with. Techniques such as Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), and elemental analysis are commonly used to identify and quantify the chemical composition of membranes.

I.2.1.1 Characterization of Morphology and Structure:

Characterizing membrane morphology and structure provides insights into the membrane's physical properties and internal structure. This characterization includes parameters such as pore size, pore distribution, surface roughness, and membrane thickness [43]. Techniques such as scanning electron microscopy (SEM), atomic force microscopy (AFM), and porosity measurements are employed to analyze the membrane's surface topography, pore structure, and overall morphology [50]. These analyses help understand the membrane's transport properties, separation efficiency, and mechanical strength.

In membrane characterization, "membrane morphology" refers to the membrane material's physical structure and arrangement, including its pores' distribution and characteristics [45]. Pores are openings within the membrane that allow the passage of certain substances while retaining others. These pores' size, shape, and distribution significantly determine the membrane's separation properties [45].

Estimating the pore size and pore size distribution is one way to gain insights into the membrane morphology. By knowing the size range of the pores, one can infer the structural characteristics of the membrane, such as the average pore size, pore size distribution, and the presence of any distinct pore types. This information helps to understand how the membrane will perform regarding selectivity (ability to separate specific molecules or particles) and permeability (ability to allow the passage of substances). Techniques such as the bubble point technique, capillary flow Porometry, mercury intrusion porosimetry, and scanning electron microscopy are commonly used to estimate the pore size and the pore size distribution [46]. These techniques provide valuable information about the membrane's morphology by measuring the dimensions and characteristics of the pores.

However, it is essential to note that membrane morphology is a more comprehensive term encompassing other aspects beyond pore size. For example, membrane thickness, surface roughness, surface charge, and any surface modifications or coatings contribute to the overall membrane morphology. Therefore, although pore size estimation plays a crucial role in assessing membrane morphology, it is typically complemented by other techniques to comprehensively understand the membrane's structure, morphology, and performance attributes [47]. These additional methods provide valuable insights into the membrane's morphology by measuring pore dimensions and characteristics. Other characterization techniques are summarized in Table I. 3.

I.2.1.2 Characterization of Performance:

Characterizing the performance of a membrane involves evaluating its functional properties and effectiveness in specific applications. This characterization focuses on permeability, selectivity, fouling resistance, and mechanical stability. Permeability refers to the membrane's ability to allow the passage of certain substances, while selectivity measures its ability to separate specific components or contaminants. Performance characterization involves conducting filtration tests, flux measurements, rejection tests, and assessing the membrane's resistance to fouling or scaling. These tests help assess the membrane's performance and suitability for different applications.

Membrane characterization techniques refer to methods used to evaluate and analyze the properties and performance of membranes [43, 48]. These techniques provide valuable insights into membranes' structural, morphological, chemical, and transport properties, enabling researchers and engineers to understand and optimize their behavior in various applications.

Researchers and operators can comprehensively understand a membrane's composition, morphology, structure, and performance by combining characterization techniques from these three categories. This knowledge aids in developing, optimizing, and operating membranes for various industrial, environmental, and biomedical applications.

Table I. 3: Characterization techniques of membrane

Techniques	characteristics
Scanning Electron Microscopy (SEM)	• Examine surface morphology and structure of membranes. • Provides high-resolution images for observing pore size, shape, and distribution.
Atomic Force Microscopy (AFM)	• Map surface topography at the nanoscale. • Provide information on surface roughness, pore size, and membrane thickness.
Fourier Transform Infrared Spectroscopy (FTIR)	• Analyze the chemical composition and functional groups in membrane materials. • Identifies specific components, detects impurities, and assesses membrane stability.
X-ray Diffraction (XRD)	• Provide information on the crystalline structure and orientation of membrane materials. • Determine the degree of crystallinity and phase composition for understanding physical properties.
	• Measure the permeability of specific gases through membranes.

Gas Permeation Testing	• Evaluate the membrane's transport properties, selectivity, diffusion coefficient, and permeability coefficients.
Liquid Permeability Testing	• Assess flux and rejection capabilities of membranes for liquid solutions. • Evaluate the membrane's separation efficiency and performance.
Pore Size Distribution Analysis	• Determine the distribution of pore sizes within a membrane. • Utilize techniques like bubble point, capillary flow porosimetry, or mercury intrusion porosimetry.
Contact Angle Measurement	• Assesses wetting properties of membranes • Provide information on the membrane's hydrophobic or hydrophilic nature and fouling potential.
Bubble Point	• Measure the minimum pressure to force liquid or gas through the largest pore.
Capillary Flow Pyrometry	• Measure the pore size distribution by measuring the pressure required to force a liquid through the porous sample.
Mercury Intrusion Porosimetry (MIP)	• Determine the pore size distribution by measuring mercury intrusion into the pores.

I.3 Membrane materials

Membrane materials are at the forefront of numerous separation processes and applications, acting as fundamental components that enable precise control over the transport of substances. These materials are carefully engineered to possess the unique ability to selectively permit the passage of specific molecules or particles while effectively hindering the transit of others based on factors such as their size, charge, polarity, or other distinct properties. By harnessing this selective permeability, membranes facilitate the separation, purification, and concentration of target components from complex mixtures, making them indispensable in various industries and scientific disciplines.

The selective nature of membrane materials arises from their inherent structural characteristics and composition [49]. Membranes are crafts from diverse materials, including [50]:

I.3.1. Inorganic Membranes

Inorganic membranes, such as ceramic or metal membranes, excel in extreme operating conditions, showcasing exceptional chemical resistance, thermal stability, and selectivity for particular gases or compounds.

I.3.1.1 Ceramic Membrane

Ceramic membranes are known for their excellent chemical and thermal stability, making them suitable for harsh operating conditions [51]. Typically, this membrane comprises inorganic materials such as alumina, zirconia, titania, or silica. Ceramic membrane fabrics are dense or porous structures used in gas separation, liquid filtration, and catalysis applications [51]:

a. **Porous Ceramic Membrane**: Porous ceramic membrane has a well-defined pore structure and high mechanical strength. It is commonly employed in microfiltration (MF), ultrafiltration (NF), and gas separation processes.

b. **Dense Ceramic Membrane:** A dense ceramic membrane has a non-porous structure, and it is used in applications requiring high selectivity, such as molecular separation and membrane reactors.

I.3.1.2 Inorganic Membrane

Inorganic membrane encompasses many materials, including metals, metal oxides, and glass. They offer advantages such as high chemical resistance, high-temperature tolerance, and excellent thermal stability. This inorganic membrane is used in gas separation, hydrogen purification, and high-temperature catalysis applications [52]:

a. **Metal Membrane:** Metal membranes, such as palladium (Pd) and silver (Ag) membranes, exhibit high selectivity for specific gases, such as hydrogen and helium. They find applications in hydrogen separation and purification.
b. **Metal Oxide Membrane:** Metal oxide membranes, such as zeolites, alumina, and silica membranes, are used in gas separation, liquid filtration, and pervaporation.

I.3.2. Organic membrane

I.3.2.1 Polymeric Membrane

Polymeric membrane is the most common type of membrane used in various applications. It is made from synthetic or natural polymers that form a porous structure [44]. Polymeric membranes are classified into different types based on the nature of the polymer used [53], including:

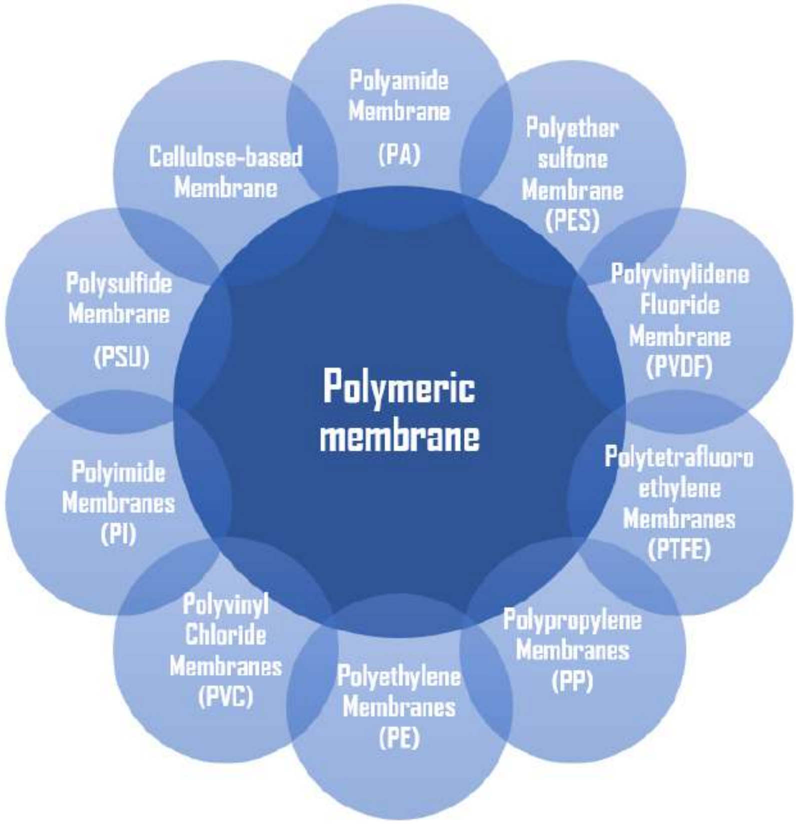


Figure I. 10: Schematic of Polymeric Membrane

a. **Polyamide (PA) Membrane:** PA membranes, such as thin-film composite (TFC) membranes, are widely used in reverse osmosis (RO) and nanofiltration (NF) applications. They exhibit excellent salt rejection and high-water permeability.
b. **Polyether sulfone (PES) Membrane**: known for its excellent chemical resistance and high thermal stability. Commonly used in ultrafiltration (UF) and microfiltration (MF) processes.
c. **Polyvinylidene Fluoride (PVDF) Membrane**: PVDF membrane is marked by hydrophobic and hydrophilic characteristics and possesses good mechanical strength, chemical resistance, and thermal stability. The PVDF membrane finds applications in gas separation, water treatment, and biomedical fields.
d. **Polytetrafluoroethylene (PTFE) Membranes:** PTFE membrane possesses excellent chemical resistance, high-temperature resistance, and low friction properties. They are hydrophobic, which makes them suitable for applications where liquid repellency is desired. PTFE membranes find application in filtration processes for chemicals, solvents, and aggressive fluids, as well as in air and gas filtration.

e. **Polypropylene (PP) Membranes:** PP membranes are cost-effective and widely used for microfiltration applications. They have good chemical compatibility and mechanical strength. PP membranes find applications in water treatment, food and beverage processing, and pharmaceutical applications.

f. **Polyethylene (PE) Membranes**: PE membranes are cost-effective and have good chemical resistance. They find applications in water purification, industrial processes, and gas separation.

g. **Polyvinyl Chloride (PVC) Membranes:** PVC membranes are used in various applications, including water treatment and gas separation. PVC membranes offer good chemical resistance and are relatively easy to process.

h. **Polyimide (PI) Membranes:** PI membranes have high thermal stability and excellent chemical resistance. PI membranes find applications in gas separation, fuel cells, and high-temperature processes.

i. **Polysulfide (PSU) Membrane**: PSU membrane exhibits high resistance to fouling and is used in various water and wastewater treatment processes.

j. **Cellulose-based Membrane**: Cellulose-based membranes, such as cellulose acetate (CA) and regenerated cellulose (RC), are biocompatible and widely used in medical applications, as well as in (RO) and (UF) processes.

I.3.3. Composite Membranes:

Composite membranes are fabricated using different materials to enhance their performance and selectivity. They often consist of a thin selective layer deposited on a porous support [54]. The selective layer can be made of polymers, ceramics, or inorganic materials, while the support layer provides mechanical strength and structural integrity. Composite membranes offer a combination of the desired properties of different materials and are used in various applications, including NF, RO, and forward osmosis (FO) processes.

Other emerging membrane materials, such as carbon-based membranes, graphene oxide membranes, and bio-inspired membranes, are also being researched and developed.

It is worth noting that selecting the appropriate membrane material depends on the specific separation requirements, operating conditions, and target applications. Factors such as pore size, chemical compatibility, fouling resistance, mechanical strength, and cost must be considered when choosing the most suitable membrane material for a particular process [55]. Scientists and engineers can harness their unique properties to accomplish myriad separation objectives by strategically selecting and designing membrane materials. Membrane processes encompass many applications, including water purification, desalination, gas separation, pharmaceutical production, food and beverage processing, and environmental remediation.

As research and development in membrane science continue to advance, exploring novel materials, innovative fabrication techniques, and advanced membrane architectures is expanding the possibilities for even more efficient and specialized separations.

Membrane materials are becoming increasingly important for various industries to maintain environmental sustainability and drive advancements, particularly in the field of water management as follows [55]:

- **Water management:**

Membrane materials play a crucial role in water treatment and desalination by enabling the selective separation of contaminants and solutes from water. The key ways in which membrane materials are instrumental in this process are as follows:

1. **Selectivity**: Membrane materials are designed to have specific pore sizes or molecular structures that allow them to separate different components in water selectively. For example, membranes with smaller pore sizes can effectively remove suspended solids and bacteria, while membranes with larger pore sizes are suitable for removing larger particles and macromolecules. The material properties of membranes determine their selectivity towards specific contaminants and solutes.
2. **Permeability**: Membrane materials are engineered to have appropriate permeability characteristics, allowing the passage of water molecules while retaining dissolved solutes, salts, and other contaminants. The permeability of a membrane material determines its ability to facilitate the desired separation process efficiently. Materials with high water and low solute permeability are preferred for desalination processes.
3. **Fouling Resistance**: Membrane materials are designed to resist fouling and accumulating unwanted substances on the membrane surface. Fouling can negatively impact the performance and lifespan of membranes. By selecting appropriate membrane materials with specific surface

properties, such as hydrophobicity or charge characteristics, fouling can be minimized, and the operational efficiency of the water treatment process can be maintained.

4. **Chemical Compatibility:** Membrane materials must be chemically compatible with the treated water and any chemicals or cleaning agents used. They should resist chemical degradation and be capable of withstanding the concentrations and pH levels commonly encountered in water treatment and desalination operations. Different materials have varying levels of chemical compatibility, allowing their use in specific applications.

5. **Mechanical Strength:** Membrane materials must possess sufficient mechanical strength to withstand the operating conditions and pressures involved in water treatment and desalination processes. They should withstand physical stress, temperature differentials, and pressure differentials without undergoing deformation or damage.

By carefully selecting and engineering membrane materials, water treatment, and desalination processes, we can achieve efficient separation and high-water recovery rates with high product quality.

- **Environmental sustainability:**

Advancements in membrane technology focus on developing sustainable membrane materials. Membrane materials contribute to environmental sustainability, including using eco-friendly polymers and biodegradable materials and recycling or reusing membranes. The exploration of bio-based materials and incorporation of renewable resources into membrane fabrication lead to reducing the environmental footprint of membrane production and disposal [56].

1.3.4 Benefits and drawbacks of membrane materials:

Table 4 provides a clear overview of the benefits and drawbacks associated with using organic, inorganic, and composite membranes in separation processes:

Table I. 4: The benefits and drawbacks associated with membrane materials

Membrane material	Benefits	Drawbacks
	• Versatility in design and customization: Can be tailored to meet specific separation requirements. • Cost-effectiveness production and installation: More affordable compared to other membrane types	• Limited temperature and chemical tolerance. • Susceptible to fouling and degradation. • Lower mechanical strength compared to some inorganic membranes. • Limited thermal and chemical stability: May degrade under extreme conditions

Polymeric (Organic)	• Ease of fabrication: Can be easily manufactured using various techniques • High flux rates: Offers efficient mass transfer and high productivity • Chemical compatibility: Can be designed to be compatible with a wide range of substances	• Susceptibility to fouling and degradation: Requires pre-treatment or regular cleaning • Poor solvent resistance: Not compatible with certain solvents or organic compounds • Narrow pH range: Limited stability in highly acidic or alkaline environments • Limited selectivity: Relatively lower selectivity compared to other membrane types.
Ceramic (Inorganic)	• Excellent chemical and thermal stability. • High mechanical strength and durability. • Suitable for high-temperature applications. • Wide range of pore size options • High resistance to fouling and scaling	• Higher cost compared to polymeric membranes. • Brittle nature and susceptibility to cracking. • High manufacturing and installation costs compared to polymeric membranes. • Brittle nature and susceptibility to cracking • Limited flexibility and adaptability
Metal (Inorganic)	• High-temperature and chemical resistance. • Excellent mechanical strength and durability. • Suitable for aggressive environments. • Low fouling propensity.	• Limited flexibility and adaptability. • Higher cost compared to polymeric membranes. • Limited pore size options.
Composite	• Combines advantages of polymeric and ceramic membranes. • Enhanced mechanical strength and durability. • Improved chemical and thermal stability. • Tailored properties for specific applications.	• Higher cost compared to single-component membranes. • Complexity in manufacturing and design. • Potential interfacial issues in composite layers.

1.3.5 Limitations and challenges in membrane materials:

Inorganic membrane offers unique advantages regarding chemical resistance, thermal stability, and selectivity but also have limitations and challenges. Some key considerations are [54]:

- **Cost:** Inorganic membranes, especially those made from precious metals or rare materials, can be expensive. The high cost of materials and manufacturing processes can limit their widespread adoption, particularly in large-scale industrial applications.
- **Brittle Nature:** Inorganic membranes, particularly ceramics and glass-based membranes, tend to be brittle compared to polymeric membranes. This brittleness can make them more susceptible to

mechanical damage or cracking, especially under high-pressure or dynamic operating conditions. Handling and installing inorganic membranes must be adequately taken to avoid structural failure.

- **Fouling:** Inorganic membranes can be prone to fouling, accumulating unwanted substances on the membrane surface or within its pores. Fouling can reduce membrane performance, decrease flux rates, and increase the frequency of cleaning or replacement. Developing effective fouling mitigation strategies, such as surface modifications or pre-treatment processes, is crucial when using inorganic membranes.
- **Limited Pore Size Range:** Inorganic membranes often have a narrower range of pore sizes than polymeric membranes. While they excel in fine separations, they may not be as versatile in applications requiring a broader range of molecular size cut-offs. This limitation may restrict their suitability in specific separation processes.
- **Fabrication Complexity:** Manufacturing inorganic membranes can be technically challenging and require specialized equipment and expertise. Processes such as sintering, deposition, or etching may be involved, which adds complexity and cost to the production. Achieving uniform pore structures or selective layers can be demanding regarding process control and quality assurance.
- **Scaling-up Difficulties:** Scaling up the production of inorganic membranes from lab-scale to industrial-scale can be complex. Maintaining consistent performance, reproducibility, and quality control across larger membrane modules or systems poses challenges. Transitioning from small-scale prototypes to commercially viable products requires careful optimization and validation.
- **Limited Flexibility:** Inorganic membranes, particularly dense ceramic membranes, are often rigid and lack the flexibility of polymeric membranes. This limitation can affect their adaptability to specific operating conditions or applications that require mechanical flexibility, such as membrane modules subject to high vibrations or varying pressure conditions.

In organic membranes, when selecting and designing for specific applications, it is crucial to consider these limitations and challenges to overcome and improve performance and reliability [57]:

- **Limited temperature and chemical tolerance:** Organic membranes have lower resistance to high temperatures and certain chemicals, which restricts their use in applications that require thermal or chemical stability.

- **Susceptibility to fouling**: Organic membranes are prone to fouling, where unwanted substances accumulate on the membrane surface or within its pores. This can lead to reduced performance and increased maintenance requirements.
- **Lower mechanical strength:** Organic membranes generally have lower mechanical strength compared to inorganic membranes, making them more susceptible to damage or deformation.
- **Poor solvent resistance**: Some organic membranes may not be compatible with certain solvents or organic compounds, leading to swelling, loss of mechanical strength, or changes in separation properties.
- **Limited lifespan:** Organic membranes may have a shorter lifespan than inorganic membranes due to their susceptibility to degradation and fouling.
- **Narrow pH range:** Certain organic membranes have limited stability in highly acidic or alkaline environments, affecting their performance and durability.
- **Selectivity challenges:** Due to organic membranes' separation mechanisms, achieving high selectivity with organic membranes can be challenging compared to other membrane types, such as inorganic or composite membranes.

1.2.5.6 Manufacturing limitations in membrane materials:

The manufacturing limitations associated with membrane production consider efforts directed towards several crucial areas, including [58, 59]:

- **Improving scalability:** One challenge is scaling up membrane production from laboratory-scale to industrial-scale without compromising quality or performance. Researchers are exploring efficient and cost-effective manufacturing processes that scale up quickly for large-scale production.
- **Enhancing reproducibility:** Consistency and reproducibility are crucial in membrane manufacturing. Consistency in membrane manufacturing refers to the stability of membrane properties across production runs. For instance, if a particular type of membrane is intended to have specific attributes like thickness, pore size, and surface texture, these traits must remain uniform from one batch to the next. This ensures the membrane's performance is dependable and can be anticipated reliably. Reproducibility pertains to consistently replicating a specific manufacturing process to yield consistent outcomes. Essentially, if researchers devise a particular method for producing membranes

with specific characteristics, they should be able to employ that method consistently to generate membranes with identical properties.

- **Controlling membrane morphology**: The morphology of the membrane, including its structure and surface characteristics, plays a significant role in separation performance. Researchers are investigating methods to control and optimize the membrane morphology during manufacturing processes to enhance selectivity, permeability, and fouling resistance.
- **Minimizing defects:** Defects in membranes, such as cracks, pinholes, or non-uniform pore distribution, can compromise performance. Researchers are developing strategies to minimize defects and improve the integrity and reliability of the membranes during manufacturing.
- **Exploring new materials and fabrication techniques:** Novel materials and fabrication techniques have been explored to expand the range of membrane options available. This includes exploring advanced polymers, nanomaterials, composites, and innovative fabrication methods to create membranes with improved properties, such as higher selectivity, enhanced stability, and reduced fouling.

Addressing these manufacturing limitations aims to develop more efficient, cost-effective, and suitable membranes for various separation processes across different industries. Ongoing research and development efforts focus on optimizing manufacturing processes and exploring innovative approaches to overcome these limitations and advance membrane production.

1.3.6 Innovative Fabrication Methods

Several innovative fabrication methods have been explored to enhance membrane production. Some of these methods include [60]:

- **Electrospinning:** involves using an electric field to create ultrafine fibers from a polymer solution or melt. This technique can produce membranes with high surface area, small pore sizes, and controlled pore distribution.
- **Layer-by-layer assembly:** involves the sequential deposition of alternating layers of different materials, such as polymers or nanoparticles, to create a membrane with desired properties. This technique allows for precise control over membrane structure and functionality.

- **Self-assembly:** utilizes the inherent properties of certain materials to arrange themselves into ordered structures spontaneously. By carefully designing the molecular interactions, researchers can create membranes with controlled pore sizes and structures through self-assembly.
- **Template-based synthesis:** In this method, a sacrificial template, such as colloidal particles or nanofibers, is used to create a porous structure. The template is subsequently removed, leaving behind a membrane with well-defined pores. This technique enables the fabrication of membranes with precise control over pore sizes and distribution.
- **3D printing:** 3D printing, or additive manufacturing, allows for the precise layer-by-layer deposition of materials to create complex structures. Researchers are exploring 3D printing techniques to fabricate membranes with tailored architectures, including hierarchical structures and interconnected pore networks.
- **Sol-gel processing** involves the conversion of a sol, a dispersion of inorganic or organic precursors, into a gel-like material. This method enables the fabrication of thin films or coatings with controlled porosity and surface chemistry, which can be used as membranes in various applications.
- **Molecular self-assembly:** involves the spontaneous organization of molecules into ordered structures based on intermolecular interactions. Researchers are exploring using self-assembled monolayers and molecular scaffolds to create membranes with specific functionalities and high selectivity.

These innovative fabrication methods offer opportunities to tailor membrane properties, such as pore size, surface chemistry, and structural characteristics, to meet specific application requirements. Continued research and development in these areas are expected to contribute to the advancement of membrane technology.

1.3.7 Choice of appropriate material (organic membrane)

The appropriate polymeric membrane depends on the application and the desired performance criteria. Different membranes excel in different areas, and the choice of the best membrane will vary based on the separation requirements, operating conditions, and cost considerations. Some factors to consider when evaluating the suitability of a polymeric membrane are [61]:

- **Separation Performance:** The primary consideration is the membrane's ability to achieve the desired separation or filtration goals. Factors such as pore size, selectivity, and rejection efficiency determine the membrane's performance.
- **Chemical Compatibility:** The membrane should be compatible with the chemical environment it will be exposed to. Different polymers have varying degrees of resistance to different chemicals, so selecting a membrane that can withstand the specific chemical constituents present in the process is essential.
- **Mechanical Strength and Durability:** The membrane should possess adequate mechanical strength to withstand the operating conditions, including pressure differentials and physical stresses. Durability is essential to ensure a longer membrane lifespan and reduce the need for frequent replacements.
- **Fouling Resistance:** Membrane fouling can impact performance, where particles or contaminants accumulate on the membrane surface. Membranes with anti-fouling properties or surface modifications that inhibit fouling can be advantageous in applications where fouling is a concern.
- **Cost and Availability:** The cost of the membrane, including its production, installation, and maintenance, is an important consideration. Availability and scalability of the membrane material are also crucial factors, as some specialized membranes may have limited availability or higher costs.

Rather than identifying a single appropriate polymeric membrane, it is more appropriate to evaluate the suitability of a membrane based on these factors about the specific application requirements. Conducting pilot tests, consulting membrane manufacturers, and considering real-world case studies can help select the most suitable membrane for a given application.

1.3.8 General comparison between PTFE, PVDF, and PP

The most commonly employed polymeric membranes in membrane distillation (MD) include PTFE, PVDF, and PP. Choosing the most appropriate membrane among them depends on the application requirements [62]. Making a definitive recommendation without detailed information about the specific application is challenging. Each membrane has its strengths and limitations.

Moreover, PTFE may suit membranes with excellent chemical resistance and hydrophobicity. It is often used in applications involving aggressive chemicals and where liquid repellency is desired.

Additionally, PVDF can be a suitable option for a versatile membrane with good chemical resistance, mechanical strength, and the ability to perform microfiltration and ultrafiltration. It is commonly used in various industrial applications.

Furthermore, PP is commonly employed for its high salt rejection capabilities for membranes commercially available and widely used in various filtration and separation applications, including MD, especially for desalination and water purification.

For making a definitive choice, it is crucial to consider the application's specific requirements, such as the desired separation performance, chemical compatibility, temperature resistance, and other factors. Conducting pilot tests or consulting with membrane manufacturers can help to make an informed decision based on the specific needs. Table I.5 provides a comparison view between PTFE, PVDF, and PP.

Table I. 5: Comparison between PTFE, PVDF, and PP [62].

Factors	PTFE	PVDF	PP
Separation performance	• Excellent separation performance due to its tight molecular structure, • well-suited for membrane distillation due to its exceptional hydrophobicity and high vapor permeability. • Efficient water vapor transport • effectively prevents liquid water intrusion.	• Good separation performance in membrane distillation for a wide range of solutes, including organic compounds and oils. • Low liquid entry pressure and high hydrophobicity. • Good separation performance	• Hydrophobic nature. • Excellent vapor permeability. • Effective separation of larger particles and solids • It may have limited performance in separating small molecules
Chemical compatibility	• Highly inert and resistant to most chemicals, acids, bases, and solvents. • Exceptionally suitable for	• Highly resistant to various chemicals, acids, bases, and solvents. • Suitable for applications	• Resistant to most chemicals, acids, and bases, making it suitable for a broad range of chemical environments.

	chemically aggressive environments.	involving aggressive chemicals. • withstand exposure to various chemicals and solvents encountered in membrane distillation operations	• It may not be compatible with potent oxidizing agents. • Maybe less resistant to certain aggressive chemicals compared to PVDF.
Mechanical strength and durability	• excellent mechanical strength and durability. • Can withstand high-pressure differentials and physical stress, ensuring long-term performance • Highly suitable for membrane distillation. • Can withstand high-pressure differentials and physical stress.	• Exhibits good mechanical strength and durability. • Can withstand moderate pressure differentials and physical stress.	• Offers good mechanical strength and durability. • Can withstand pressure differentials and maintain their integrity during operation
Fouling resistance	• Excellent fouling resistance in MD. • Smooth surfaces and low surface energy make them highly resistant to fouling by most substances. • Ensuring stable performance and longer operation intervals between cleanings.	• Exhibit good fouling resistance in MD due to their hydrophobic nature. • Less prone to fouling by organic matter and biological growth. • Can resist the deposition of scales and particulates, thereby minimizing performance decline.	• Have moderate fouling resistance in membrane distillation. • Susceptible to fouling by contaminants, oils, greases, and certain organic compounds present in the feedwater. • Periodic cleaning may be required to maintain performance.
Cost and availability	• are available in different configurations and sizes. • Slightly more limited availability compared to PP	• Widely available in the market in various forms, including flat sheets and hollow fibers. • Suitable for MD applications	• Cost-effective and readily available. • Commonly used in various water treatment applications due to their affordability and availability.

It is worth noting that the performance and properties of membranes in MD are influenced by factors such as membrane thickness, surface modifications, pore size, membrane configuration, manufacturing processes, and module design.

1.4. State of the Art in Membrane Distillation

The membrane distillation process has been widely studied, particularly in desalination. Many research papers have focused on this method, significantly gaining theoretical studies and research attention. In the next section, we will explore the history of membrane technology in this field and discuss recent advancements.

Woo-Ju Kim et al. [63] studied membrane distillation (MD) for wastewater treatment and desalination. They explored direct contact membrane distillation (DCMD) using different membranes and feed solutions. They examined membrane characteristics, fouling behavior, and energy consumption. Simulations were conducted to optimize energy efficiency and maximize permeate flux. One study focused on recovering cleaning agents from CIP wastewater using a membrane system combining nanofiltration and DCMD. Heat-stretching treatment of PVDF hollow fiber membranes improved stability and flux by reducing pore size and increasing liquid entry pressure.

Haneen Wadi Abdelrazeq et al. [64] prepared porous membranes by blending PPO/PS using the NIPS method. The membranes underwent characterization using various techniques, including FESEM, ATR-FTIR, AFM, and zeta potential analysis. Their performance was evaluated in a DCMD experimental setup, measuring permeate flux at different feed concentrations and temperatures. The increase in the feed temperature led to higher permeate flux while altering the feed concentration resulted in reduced permeate flux. The prepared membranes exhibited high rejection rates in all DCMD tests. They also demonstrated anti-scaling properties when CaCl2 and Na2SO4 were introduced to the feed solution. Fouling caused by HA in the feed solution caused a reduction in flux, but the rejection was still maintained. However, when SDS and CTAB surfactants were added as foulant agents, rejection was decreased, accompanied by a slight decrease in permeate flux.

Zare and Kargari [65] focus on the computational fluid dynamics (CFD) simulation and optimization of a DCMD desalination system using a counter-current flow mode. They adopt a two-step approach and utilize response surface methodology (RSM) to optimize the system and maximize the permeate flux.

Rahimnia and Pakizeh [66] focused on preparing and evaluating PPO/PS blend membranes in a DCMD setup.

Hou et al. [67] introduced a heat-stretching treatment method to improve the structure and stability of PVDF hollow fiber membranes in MD.

Additionally, Liu et al. [68] developed an omniphobic membrane designed explicitly for MD applications with exceptional anti-wetting performance.

Kovanich et al. [69] studied the effects of three different antiscalants, namely PBTCA, DTPMPA, and HPMA, on the scaling of polytetrafluoroethylene (PTFE) membranes during the treatment of synthetic brackish water

Anjos et al. [70] investigated heat recovery in DCMD systems and found that coupling a heat exchanger to recover energy from the distillate stream can improve energy efficiency.

De Sampaio [71] developed a computational model to simulate the performance of a DCMD plant with heat recovery and validated it with experimental data.

Okati et al. [72] conducted a comprehensive analysis of the performance of a DCMD unit, including energy, exergy, economic, and environmental aspects.

Yan et al. [73] studied the effect of membrane properties on membrane flux and desalination performance in DCMD and found that membrane porosity is critical.

Chang et al. [74] Conducted a study to improve membrane stability and reduce the temperature polarization effect in membrane distillation. The study focused on enhancing heat and mass transmission to prevent vibrations and achieved a 61.7% increase in flow by implementing a countercurrent flow configuration.

Many studies prioritize optimizing system configurations for maximum energy efficiency rather than membrane design.

Lijo et al. [75] investigated modified and innovative membrane distillation configurations, emphasizing upscaling impacts, pilot-scale research, heat loss reduction, and improved mass transmission.

Francois et al. [76] developed a mathematical model to predict distillate flux in direct contact membrane distillation (DCMD) in the presence of an inorganic fouling layer formed by salt deposition.

Malikhatul et al. [77] fabricated a Polysulfone-nano zinc oxide (ZnO) membrane with enhanced stability and permeate flux by incorporating nano ZnO and a polyvinyl alcohol (PVA) coating.

Khalifa et al. [78] experimentally and analytically assessed the effect of various parameters on the performance of a DCMD system, including feed temperature, permeate temperature, and flow rate.

Alwatban et al. [79] analyzed the influence of properties and operational parameters on a three-dimensional DCMD system using a computational fluid dynamics (CFD) model and implemented a net-type spacer to reduce polarization effects.

Laqbaqbi et al. [80] investigated fouling issues in textile dye treatment using PVDF flat sheet membranes.

Al-Salmi et al. [81] explored DCMD for water generation in an oil field using a polypropylene (PP) membrane.

Li et al. [82] fluorinated a ZnO-blend PVDF membrane to create a super-hydrophobic nanofibrous composite membrane with improved performance.

Foureaux et al. [83] tested PTFE and PVDF membranes for water reclamation using DCMD.

Wanke et al. [84] electrospun a layer of PVP-co-PMMA over a hydrophobic PVDF microfiltration membrane, quadrupling the permeate flux.

Niknejad et al. [85] used an electro-blowing method to fabricate a superhydrophobic nanofibrous PMMA membrane with superior performance compared to commercial membranes.

Bandar et al. [86] evaluated a modified membrane's performance with well water as the feed stream, achieving an average permeate flux of 13.10 kg/m2h and a salt rejection of 98.96%.

Fortunato et al. [87] compared DCMD's efficiency in treating a synthetic textile dye solution to other research studies.

Sousa Silva et al. [88] examined the influence of operating parameters on DCMD performance in synthetic effluents containing reactive and dispersed dyes, achieving high dye rejection and permeate flux for both reactive and dispersed dyes.

Zhu et al. [89] present a novel poly-generation system that integrates a proton exchange membrane fuel cell (PEMFC), DCMD, and a heat pump. This system aims to enhance energy efficiency while simultaneously generating power and fresh water.

Furthermore, Direct Contact Membrane Distillation (DCMD) has gained significant attention as a well-studied configuration in membrane distillation due to its simplicity of installation and operation in laboratory settings.

Park et al. [90] conducted CFD simulations and experimental studies to investigate the impact of screen spacers on DCMD, highlighting the enhancement of convective heat transfer. This study aimed to develop a one-dimensional semi-empirical model to analyze downstream variables and assess the significance of localized heat generation or the use of a directly heated concept on DCMD performance, particularly in the presence of considerable downstream alterations.

Guo et al. [91] presented two Model Predictive Control (MPC) strategies for enhancing the water production rate in DCMD systems. The first scheme focused on tracking an optimal set-point, while the second scheme, Economic Model Predictive Control (EMPC), aimed to maximize the flux of distilled water. Simulations demonstrated that operating the DCMD process under the EMPC scheme resulted in higher distilled water production than in the MPC scheme.

Lou et al. [92] utilized computational fluid dynamics (CFD) simulations to analyze downstream flow properties.

Lopez et al. [93] investigated the impact of various factors on DCMD for seawater desalination, including hydrodynamic conditions, antiscalants, feed temperature, and membrane thickness. Adding an antiscalant improved DCMD performance by dispersing salts, significantly increasing water vapor flux. The study highlighted the importance of antiscalant selection and concentration for enhancing the process efficiency without adverse effects.

Elrasheedy et al. [94] studied the effects of incorporating multi-walled carbon nanotubes (MWCNTs) into polystyrene (PS) during the fabrication of nanofibrous membranes for DCMD. The numerical evaluation showed significant improvements in the hydrophobicity and porosity of the PS/MWCNTs composite membrane compared to the blank membrane. Simulation results indicated superiority.

Ameen et al. [95] developed a MATLAB software model to analyze the DCMD process. They employed a system of nonlinear equations to evaluate the performance of a poly-tetra-fluoroethylene (PTFE) membrane for treating saline water under various operating conditions. The simulation results agreed with experimental findings, demonstrating high salt rejection (greater than 99.9%) across all tested scenarios. The study also provided insights into the temperature polarization coefficient, gain output ratio, and thermal efficiency of the DCMD system.

1.5 Conclusion

In conclusion, this chapter presented a comprehensive literature survey of membrane distillation (MD) in various fields, including traditional to advanced desalination processes, membrane characterization techniques, and membrane materials.

The survey revealed that MD has emerged as a promising technology for desalination, offering advantages such as low energy consumption, high salt rejection, and the ability to handle a wide range of feedwater salinities. The chapter highlighted the historical progression of desalination processes, from traditional thermal-based methods to advanced membrane-based techniques, with MD being a notable contender in the latter category.

The chapter also discussed the importance of membrane characterization techniques in understanding and optimizing MD processes. Various characterization methods, such as scanning electron microscopy (SEM), atomic force microscopy (AFM), contact angle measurements, and porosity analysis, were highlighted as valuable tools for evaluating membrane morphology, surface properties, pore size distribution, and wetting behavior. These techniques aid in assessing membrane performance, identifying fouling mechanisms, and guiding membrane design and optimization.

A key focus of the literature survey was on membrane materials utilized in MD. Various membrane types, including polymeric, inorganic, and composite membranes, were explored for their suitability in MD applications. The advancements in membrane material development aimed to achieve improved selectivity, permeability, fouling resistance, and thermal stability. To enhance MD performance, noteworthy efforts were observed in exploring hydrophobic and nanostructured membranes, surface modifications, and functionalization techniques.

Overall, this literature survey highlights the significant progress made in membrane distillation (MD), underscoring its

potential as an efficient and sustainable desalination technology. These advancements in membrane materials and characterization techniques pave the way for future research and development in MD. By adopting the configuration of an MD system presented in the next chapter, researchers can further optimize the design and operation of MD processes. This will facilitate the broader adoption of MD as a viable desalination solution, addressing the growing global demand for freshwater while promoting sustainability and efficient resource utilization.

Chapter II

Modeling Design of Direct Contact Membrane Distillation DCMD

II.1 Introduction

The increasing demand for freshwater resources and the growing challenges of water scarcity have driven the exploration of innovative technologies for seawater desalination. Seawater desalination has emerged as a practical and essential solution to address the pressing need for a reliable freshwater supply in coastal communities worldwide. Among these technologies, membrane distillation (MD) has emerged as a promising solution with unique advantages over traditional methods such as reverse osmosis (RO). With the increasing global water scarcity and a growing population, traditional freshwater sources are becoming insufficient to meet the demand. Seawater covers 71% of the Earth's surface and offers a vast potential resource for clean drinking water [96].

Traditional desalination technologies, such as reverse osmosis (RO), multi-stage flash (MSF) distillation, and multi-effect distillation (MED), have proven to be effective for large-scale seawater desalination projects [97]. However, these methods are often unsuitable for small-scale applications with limited access to a consistent power supply and technical support.

Reverse osmosis, the most widely used desalination method, requires extensive pre-treatment, high-pressure pumps, and costly components, making it less viable for small-scale operations [98]. Thermal distillation methods, while effective, are energy-intensive and have large physical footprints, limiting their practicality for smaller communities [98].

Recognizing the critical need for water security in these coastal areas, researchers have explored alternative technologies. Among these, membrane distillation (MD) has emerged as a promising technology platform for small-scale, stand-alone, and off-grid seawater desalination projects [99]. MD utilizes a hydrophobic membrane, allowing only water vapor to pass through while rejecting salts and impurities. This process harnesses the vapor pressure gradient to separate pure and saline water.

Seawater desalination projects often involve pre-treatment processes to remove suspended solids and contaminants, ensuring the longevity and efficiency of the desalination equipment [20]. The choice of desalination technology depends on factors such as energy consumption, cost, efficiency, and environmental impact [100].

While seawater desalination offers a valuable solution, it is essential to consider the energy requirements and environmental implications associated with the process. Efforts are being made to improve energy efficiency, explore renewable energy integration, and develop sustainable disposal methods for the concentrated brine by-product.

MD is a thermally driven membrane separation process that operates on the principle of selective vapor transport through a hydrophobic membrane [41]. Unlike RO, MD does not rely on high hydraulic pressure for mass transfer, resulting in significant cost savings during system construction and maintenance [101]. The use of inexpensive plastic materials in MD systems makes them more accessible and affordable, particularly for small-scale applications [56].

In MD, a hydrophobic membrane is a barrier between the hot feed solution and the cold coolant stream. The feed solution, typically saline or brackish water, is heated to create a vapor pressure gradient. The hot feed solution vaporizes, and the water vapor molecules pass through the membrane, leaving behind the dissolved salts and impurities [102].

On the other side of the membrane, a cold coolant stream is maintained at a lower temperature, which condenses the water vapor and collects it as fresh water. Since the driving force in MD is the vapor pressure difference rather than the osmotic pressure, MD can effectively handle highly saline feedwater with elevated salt concentrations. This ability to handle more saline water sets MD apart from other desalination processes like RO, which have limitations on the feedwater salinity they can effectively treat.

Moreover, MD's reliance on vapor pressure difference allows for a larger volume of freshwater production. The absence of osmotic pressure limitations means that MD can achieve higher process water recovery rates than RO. With MD, a significant portion of the feedwater can be converted into freshwater, resulting in a higher overall water yield.

Overall, MD's reliance on the vapor pressure difference and elimination of osmotic pressure limitations make it a promising technology for handling highly saline feedwater and producing a larger volume of freshwater. This characteristic is particularly advantageous in regions facing water scarcity or where the available water sources have high salinity levels [103].

MD also offers benefits in terms of reduced pre-treatment requirements. Its hydrophobic membrane is less susceptible to fouling from organic and colloidal substances, minimizing the need for intensive pre-treatment processes. This characteristic simplifies the overall system design and operation, contributing to cost savings and improved system efficiency.

Additionally, MD operates within a temperature range of 40 to 80 ºC, allowing it to utilize waste heat and solar thermal energy sources [103]. By harnessing these heat sources, MD can significantly reduce energy consumption and enhance sustainability. It is suitable for off-grid or remote applications with limited access to a consistent power supply.

By examining its operating conditions, material compatibility, cost-effectiveness, and integration with renewable energy sources, we can gain insights into the potential of MD as a reliable and efficient technology for addressing water scarcity challenges and ensuring a sustainable freshwater supply in coastal regions.

Within the broad field of membrane distillation (MD), one particular configuration that stands out is direct contact membrane distillation (DCMD). While MD offers unique advantages in seawater desalination and water treatment, DCMD takes this technology further. In DCMD, the feedwater and coolant streams come into direct contact on opposite sides of a hydrophobic membrane [104]. This direct contact enhances the heat transfer efficiency and enables a higher driving force for vapor transport. As a result, DCMD exhibits superior flux production rates and improved energy efficiency compared to other MD configurations [105]. The direct contact between the streams also facilitates better thermal management and effective heat recovery [106]. These characteristics make DCMD an attractive option for applications that require high flux rates, enhanced energy efficiency, and optimal thermal performance.

II.2. Direct Contact Membrane Distillation Configuration

Membrane distillation (MD) is characterized by four distinct configurations, which are differentiated based on the arrangement of permeate flux and the techniques used for its collection [107]. Although the feed side remains unchanged across all four systems, the variations primarily arise from the methods employed to handle and collect the permeate flux, as discussed in Chapter I. These configurations include:

1. Direct Contact Membrane Distillation (DCMD).
2. Air Gap Membrane Distillation (AGMD).
3. Vacuum Membrane Distillation (VMD).
4. Sweeping Gas Membrane Distillation (SGMD).

The choice of which configuration is most studied can depend on several factors, including research interests, available resources, application requirements, and specific research goals. Other configurations of membrane distillation, such as Air Gap Membrane Distillation (AGMD), Vacuum Membrane Distillation (VMD), and Sweeping Gas Membrane Distillation (SGMD), have also received significant attention and research focus.

Among this configuration of membrane distillation, the light will be on the Direct Contact Membrane Distillation (DCMD), known for its simplicity and ease of operation. The simplicity of installation and operation in laboratories is one aspect that makes DCMD attractive for research purposes. Its straightforward setup and ease of use make it accessible for experimental investigations and feasibility studies in laboratory settings. Additionally, the simplicity of DCMD can facilitate the evaluation of critical parameters and optimization of the process. In DCMD, the feed solutions, such as seawater and the coolant, flow in direct contact with each other on opposite sides of a hydrophobic membrane.

The basic setup of a DCMD system involves a module consisting of a flat sheet or hollow fiber membrane. The feed solution is heated to create a vapor pressure gradient, which causes the water to vaporize and diffuse through the membrane. On the other side of the membrane, a cold coolant is circulated to condense the water vapor and collect it as purified water.

Direct contact membrane distillation (DCMD) performance in flux production, membrane lifetime, and environmental impacts is a multifaceted subject that depends on various factors [108]. DCMD, a membrane-based desalination process, offers great potential to address water scarcity challenges and provide a sustainable freshwater supply. However, to maximize its efficiency and effectiveness, it is crucial to understand and optimize the factors that influence its performance.

One of the critical factors impacting DCMD performance is the characteristics of the membrane itself. Factors such as the membrane material, pore size, thickness, and surface properties significantly determine the vapor permeation rate, salt rejection, and propensity for membrane fouling [109]. The selection of an appropriate membrane is crucial for achieving desirable DCMD outcomes.

The properties of the feedwater being treated also directly impact DCMD performance. The salinity, temperature, and presence of impurities in the feedwater can influence flux production, salt rejection, and fouling potential [110].

The temperature difference or gradient between the hot feedwater and the cold coolant stream is another critical factor that affects DCMD performance. This temperature difference is the driving force for vapor transport and influences flux production. Finding the optimal temperature difference is essential for balancing flux rates and minimizing energy consumption.

The conditions of the coolant stream, including its temperature and flow rate, also play a vital role in DCMD performance. These factors affect vapor condensation, heat transfer, and overall system efficiency. Proper management of the coolant conditions is necessary to maintain the desired temperature difference and optimize DCMD operation.

Furthermore, membrane fouling and scaling pose challenges to DCMD performance and longevity. Organic fouling, inorganic scaling, and biofouling can occur due to impurities in the feedwater [111]. Effective pre-treatment, cleaning protocols, and periodic maintenance are essential to mitigate fouling and scaling issues and maintain optimal DCMD performance [112].

Moreover, temperature polarization and concentration polarization are two main phenomena that can reduce the transmembrane vapor flux if operating conditions remain constant [113]. However, most studies have focused primarily on temperature polarization, with minimal discussion on the adverse effects of concentration polarization on DCMD performance [113].

II.2.1 The DCMD module

A membrane module is a device or assembly containing one or more membranes designed to facilitate the separation or filtration. The module serves as a structural unit that holds the membranes in place, creates flow channels for the feed solution, and allows for the collection of permeate or concentrate. Membrane modules are crucial in various applications, including desalination. In the context of MD with DCMD, a membrane module is a crucial component that enables the separation process and facilitates the transfer of vapor or distillate through the membrane. Here is an overview of membrane modules in DCMD:

1. **Membrane Configuration:** In DCMD, the membrane module typically consists of flat sheets or hollow fiber membranes. The configuration choice depends on the specific DCMD system design and application requirements.
2. **Feed and Permeate Channels:** The membrane module includes separate feed and permeate channels. The feed solution, referred to as the "hot" or "concentrate" stream, comes into direct contact with one side of the membrane, while the permeate vapor or distillate is generated on the other side.
3. **Module Housing:** The module housing encloses the membranes and provides structural support. It ensures proper alignment of the membranes, maintains the separation barrier, and prevents leakage of the feed and permeate streams.

4. **Feed and Permeate Connections:** The module has inlet and outlet connections for the feed and permeate streams. The feed solution enters the module through an inlet port and flows over the membrane surface in direct contact. The vapor or distillate is collected and removed through the permeate outlet port.
5. **Spacers:** Spacer structures may be used in DCMD modules to create flow channels on the feed side of the membrane. These spacers help maintain a uniform gap between the membrane surface and enhance the mixing of the feed solution, promoting mass transfer and preventing concentration polarization.
6. **Scalability and Array Configuration**: DCMD membrane modules can be designed to be scalable, allowing for the integration of multiple modules in parallel or series arrangements to achieve the desired processing capacity. The array configuration can vary depending on system requirements and available space.

II.2.3 The arrangement of DCMD membrane

In DCMD, different arrangements or configurations can be used to set up the membrane modules, including flat sheet, spiral-wound, tubular, plate-and-frame, and customized configurations. Table II.1 provides the DCMD's arrangement with descriptions. Each configuration has its advantages and considerations in terms of scalability, pressure drop, module packing density, and ease of maintenance. The selection of a particular configuration depends on factors such as the desired flux, membrane material, feedwater characteristics, and system design considerations.

Table II.1 The DCMD 's arrangements

Arrangement	Description
Flat Sheet Configuration	• In this arrangement, flat sheet membranes are used. • The feed solution flows over one side of the membrane. • The distillate is collected on the other side. • It is straightforward and relatively simple to implement
Spiral-Wound Configuration	• This arrangement involves winding a flat sheet membrane into a spiral shape. • The feed solution flows along the membrane surface • The distillate is collected in the center tube. • It provides a compact design with a large, effective membrane area.
Tubular Configuration	• The membrane is in the form of a tube. • The feed solution flows through the tube. • The distillate is collected inside the tube.

	• It is commonly used when dealing with high fouling or solids content in the feed solution.
Plate-and-Frame Configuration	• This arrangement involves using a series of plates and membranes stacked together. • The feed solution is introduced between the plates. • The distillate is collected on the other side of the membranes. • It is versatile and allows for easy replacement of the membranes.
Customized Configurations	• It is designed based on the specific requirements of the separation process. • It tailoring the configuration to meet the application's unique needs. • Hybrid configurations can be utilized, combining different types of membrane modules, such as flat sheets and tubular membranes. • By incorporating hybrid configurations, the performance of the DCMD system can be optimized to achieve the desired separation efficiency and productivity.

II.2.4 Membrane property

Membrane properties directly impact the membrane distillation process. The four main membrane properties in membrane distillation are presented in the following table:

Table II.2. The membrane property

Membrane Property	Description
Thickness	• Affects mass transfer resistance and heat transfer efficiency. • Thinner membranes exhibit lower resistance and higher flux.
Porosity	• Refers to pores in the membrane structure. • Higher porosity increases permeability and flux by providing more pathways for vapor transport.
Tortuosity	• Represents convoluted pathways within the membrane that fluid molecules must traverse. • Higher tortuosity leads to longer diffusion paths and potential mass transfer resistance.
pore Size	• Refers to the size of individual pores in the membrane. • Determines membrane selectivity, allowing water vapor passage while rejecting liquid water and solutes.

II.3. Modeling of direct contact membrane distillation DCMD

II.3.1 Heat and mass transfer DCMD under Study

Heat and mass transfer are crucial in operating Membrane Distillation (MD) systems. Heat transfer and mass transfer are fundamental concepts in membrane distillation (MD), playing a crucial role in its operation. It is often regarded as the rate-controlling mechanism [114]. Heat and mass flow in an MD system occur in the same direction, facilitating simultaneous transfer processes. In this context, it is essential to understand the mechanisms of heat and mass transfer. Detailed heat and mass transfer explanations will be provided for the flat sheet membranes. A cross-sectional view of a DCMD, Figure II.1, is considered to examine the heat and mass transfer mechanism.

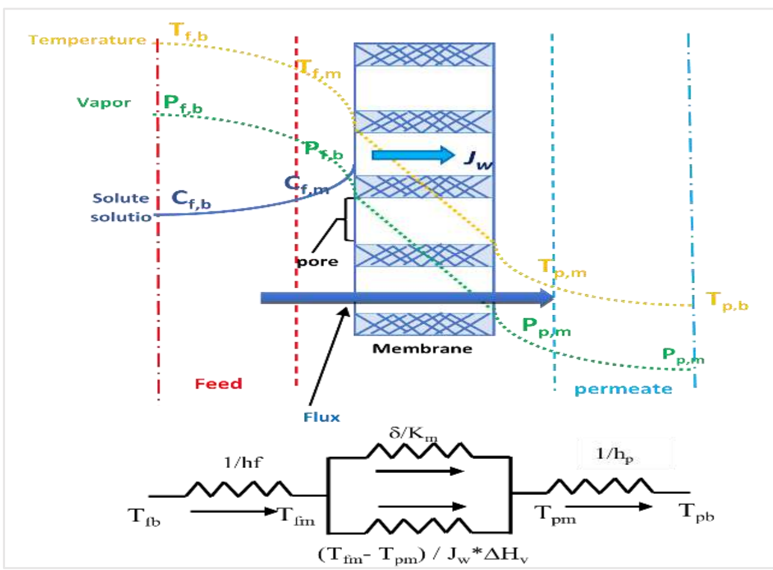


Figure II. 1: Schematic of heat and mass transfer in DCMD.

II.3.1.1 Heat transfer (Flat sheet membrane)

Heat transfer in membrane distillation (MD) involves the transfer of thermal energy between two objects or systems due to a temperature difference. Heat flows from regions of higher temperature to regions of lower temperature. The heat transfer follows three steps, as will explained below:

II.3.1.1.1 Heat transfer by Convection through feed boundary layer (Q_f)

In this step, the hot feed solution, with an initial temperature of T_{fb}, is brought into contact with the membrane surfaces. As the hot feed solution flows near the membrane, its temperature gradually decreases until it reaches the temperature T_{fm} of the membrane. This temperature decrease occurs due to the convective heat transfer process within the feed boundary layer.

Convection is crucial in this step, where the temperature difference between the hot feed solution and the membrane drives the heat transfer. The convective heat transfer coefficient $\mathbf{h_f}$ determines heat transfer efficiency through the feed boundary layer. Maximizing the convective heat transfer coefficient and promoting turbulent flow patterns can minimize temperature polarization effects.

The heat transfer in the feed boundary layer (Q_f) is quantified by the equation (1) [76]:

$$Q_f = h_f * \left(T_{fb} - T_{fm}\right) \tag{1}$$

Here, Q_f represents the heat transfer in the feed boundary layer in (W), T_{fb} is the initial temperature (bulk) of the hot feed solution in (K), and T_{fm} is the temperature of the membrane surface in (K). H_f is the convective heat transfer coefficient (W/m^2K). This equation calculates the amount of heat transferred through convection in the feed boundary layer.

Overall, the heat transfer by convection through the feed boundary layer in membrane distillation involves the gradual decrease in temperature of the hot feed solution as it approaches the membrane surface. This temperature difference drives the convective heat transfer, and maximizing this heat transfer, for example, through turbulent flow, can help mitigate temperature polarization effects and improve the overall performance of the membrane distillation system.

II.3.1.1.2 The heat transfer through the membrane occurs via conduction (Q_m)

The thermal energy from the hot feed solution is conducted through the membrane to the permeate side, facilitating water vapor transport. Heat transfer occurs through the membrane, comprising the combined effects of the latent heat of vaporization (Q_v) and the conductive heat transfer through the membrane material and pores (Q_c). When the feed solution is heated, the heated feed solution comes into contact with the hydrophobic membrane, leading to the conduction of thermal energy across the membrane to the permeate side. This conduction process enables the transportation of water vapor contacts the hydrophobic membrane, allowing thermal energy to conduct through the membrane via equation (2):

$$Q_m = Q_c + Q_v \tag{2}$$

In this equation, Q_m represents the total heat transfer across the membrane in (W). Q_c accounts for the conductive heat transfer through the membrane material and pores in (W). It can be calculated using Equation (3):

$$Q_c = A * h_m * \left(T_{fm} - T_{pm}\right) = \frac{A * K_m}{\delta} * \left(T_{fm} - T_{pm}\right) \tag{3}$$

The thickness of the membrane (δ) is measured in (m), T_{fm} and T_{pm} are the temperatures on either side of the membrane surface in (K), and the effective thermal conductivity of the membrane K_m is expressed in (W/m.K). K_m can be determined by utilizing the data of the membrane material as represented in equation (4):

$$K_m = \left(1 - \varepsilon\right) K_s + \varepsilon K_g \tag{4}$$

The porosity (ε) represents the pores fraction, while K_s and K_g denote the thermal conductivity (W/m.K) of solids and gas within the pores.

The second component involves the transfer of heat through evaporation Q_v in (W), which is the heat associated with the latent heat of vaporization, calculated using Equation (5):

$$Q_v = J_w * \Delta H_v \tag{5}$$

Here, J_w is the vapor mass flux in (kg/m^{2}h), and ΔH_v is the enthalpy of water vaporization in (kJ/kg), which depends on the feed membrane surface temperature T_{fm} in (K) and is determined by Equation (6) [78]:

$$\Delta H_v = 1.75535 * T_{fm} + 2024.3 \tag{6}$$

II.3.1.1.3 The heat transfer by Convection through permeate boundary layer (Q_p)

Heat transfer in the permeate boundary layer occurs through convection on the permeate side. The cooled water vapor releases its thermal energy to the surrounding fluid or environment, condensing water vapor. The heat transfer in the permeate boundary layer can be calculated using the equation (7):

$$Q_p = h_p * \left(T_{pm} - T_{pb}\right) \quad \textbf{(7)}$$

Here, Q_p represents the heat transfer in the permeate boundary layer in (W), h_p is the convective heat transfer coefficient on the permeate side (W/m^2K), T_{pm} is the temperature of the membrane surface on the permeate side, and T_{pb} is the initial temperature (bulk) of the permeate stream in (K), respectively.

Under steady-state conditions, the heat transfer equations are balanced, as represented by equation (8), to validate the energy conservation.

$$Q_f = Q_m = Q_p \quad \textbf{(8)}$$

The equality of heat transfer equations allows for determining temperatures at the feed and permeate membrane surfaces, T_{fm} and T_{pm}, respectively, in (K), which cannot be directly measured or calculated. The resulting temperature equations are given by equations (9) and (10):

$$T_{fm} = \frac{k_m * \left(T_{pb} + \frac{h_f}{h_p} * T_{fb}\right) + \left(\left(\delta * \left(h_f * T_{fb} - J_w * \Delta H_v\right)\right)\right)}{\left(k_m\right) + \left(h_f * \left(\delta + \left(\frac{k_m}{h_p}\right)\right)\right)} \quad \textbf{(9)}$$

$$T_{pm} = \frac{k_m * \left(T_{fb} + \frac{h_p}{h_f} * T_{pb}\right) + \left(\left(\delta * \left(h_p * T_{pb} + J_w * \Delta H_v\right)\right)\right)}{\left(k_m\right) + \left(h_p * \left(\delta + \left(\frac{k_m}{h_f}\right)\right)\right)} \quad \textbf{(10)}$$

Convective heat transfer coefficients are crucial in determining the heat transfer rate within the feed and permeate boundary layers in membrane distillation. These coefficients describe the effectiveness of convective heat transfer between the membrane surface and the adjacent fluid layers.

To estimate these convective heat transfer coefficients, researchers often resort to Nusselt correlations N_u. Nusselt correlations are empirical formulas that provide a relationship between the convective heat transfer coefficient and relevant parameters such as flow conditions, fluid properties, and geometry.

These correlations are derived from experimental data and are specific to certain flow regimes and geometries. They are widely used in engineering and scientific literature to estimate convective heat transfer coefficients in various applications, including membrane distillation.

Applying the appropriate Nusselt correlation, the convective heat transfer coefficients are evaluated in the feed and permeate boundary layers. This enables them to better understand and analyze the heat transfer mechanisms within the membrane distillation process. It is important to note that selecting an appropriate Nusselt correlation depends on factors like flow regime, fluid properties, and the specific system under consideration. Researchers often validate these correlations through experimental data or numerical simulations to ensure accuracy and reliability for a given application.

The convective heat transfer coefficient, denoted as h in (W/mK), is determined through equation (11). The value of this coefficient depends on the specific operating conditions of the MD module. The calculation of the convective heat transfer coefficient is performed as follows:

$$h = \frac{Nu * k}{D_h} \quad \textbf{(11)}$$

Where k is the fluid's average thermal conductivity on both the feed and permeate sides in (W/mK), the hydraulic diameter D_h of the flow channel in (m), and Nu is the dimensionless Nusselt number, which is expressed in equation (12):

$$Nu = C * \mathrm{Pr}^a * \mathrm{Re}^b \quad \textbf{(12)}$$

A, B, and C are the constants, *Pr* is the Prandtl number, and *Re* is the Reynolds number. Equations (13) and (14) present the essential parameters required for the evaluation of Nusselt correlations:

$$\mathrm{Pr} = \frac{\mu * c_p}{k} \quad \textbf{(13)}$$

Where μ is the dynamic viscosity in (Pa· s), k is thermal conductivity, and specific heat capacity C_p of the fluid in (J/kg.K) are the relevant factors in the equation. Moreover, Reynolds number *Re* is represented in equation (14):

$$Re = \frac{v * d * \rho}{\mu} \quad \textbf{(14)}$$

Where. v is the fluid velocity in (m/s), d is the diameter in (m), ρ is the density in (kg/m^3), and μ is the viscosity in (pa.s).

The determination of the total heat transfer in the membrane, expressed in terms of the overall heat coefficient U, follows the following equation (15):

$$Q_m = U * \left(T_{fb} - T_{pb}\right) \quad \textbf{(15)}$$

The overall heat coefficient U in (W/m^{2}K), which represents the total heat transfer in the membrane, can be calculated by equation (16) as follows:

$$U = \left[\frac{1}{h_f} + \frac{1}{\left(\frac{k_m}{\delta}\right) + \frac{J_w * \Delta H_v}{\left(T_{fm} - T_{pm}\right)}} + \frac{1}{h_p}\right]^{-1} \quad \textbf{(16)}$$

II.3.1.2 Mass transfer (Flat sheet membrane)

Mass transfer in MD occurs through the vapor-phase transport of water molecules across the hydrophobic membrane. The driving force for mass transfer is the difference in vapor pressure or vapor concentration between the liquid feed and the permeate side.

Water vapor molecules evaporate from the liquid feed, diffuse through the porous structure of the membrane, and condense on the permeate side. Temperature gradient, membrane properties, and concentration difference influence mass transfer.

Mass transfer in the DCMD process involves the transfer of vapor molecules collected on the permeate side after passing through the membrane. The mass transfer in the DCMD process can be divided into three stages:

1. **Vaporization and Transfer:**

   Water molecules in the liquid feed vaporize and transition from the liquid phase to the vapor phase. As the liquid is heated, the water molecules gain enough energy to overcome the intermolecular forces and become vapor.

2. **Vapor Transport:**

   The vapor molecules from the hot side of the system transport through the membrane pores to the cold side. The vapor pressure difference across the membrane drives this movement. The higher vapor pressure on the hot than cold side drives the vapor molecules to pass through the membrane's porous structure.

3. Condensation and Transfer:

On the cold side, the vapor molecules condense and transfer from the vapor phase back to the liquid phase. The condensation occurs as the vapor molecules lose energy due to the temperature difference between the hot and cold sides.

Several factors control the mass transfer in DCMD. The vapor pressure difference across the membrane plays a crucial role in driving the movement of vapor molecules. Additionally, the membrane's permeability, influenced by its properties, such as pore size and surface characteristics, affects mass transfer efficiency.

Within the membrane pores, mass transfer occurs through various mechanisms:

- **Knudsen diffusion (K)** predominates when the membrane pore size is small, and the primary collisions occur between the molecules and the membrane wall.
- **Molecular diffusion (M)** occurs when molecules move along a concentration gradient.
- **Poiseuille flow (P)** occurs in viscous media as molecules move along a pressure gradient.
- **The transition mechanism** combines Knudsen diffusion and molecular diffusion to describe the collision process of molecules between each other and the membrane.

Understanding the intricacies of mass transfer in the DCMD process allows for identifying and quantifying concentration and temperature polarization effects on mass and heat transfer analysis.

The permeate flux, denoted as J_w in (kg/m^{2}h), in the membrane distillation process. The permeate flux expression represents the rate at which water vapor crosses the hydrophobic membrane pores. It expresses in general to capture the underlying mass transfer mechanisms in equation (17):

$$J_w = A * C_m * \left(P_{fm}^{sat} - P_{pm}^{sat} \right) \quad \textbf{(17)}$$

Where the surface area of the membrane is denoted as A in (m^2), the overall mass transfer coefficient C_m , representing the water vapor membrane permeability, measured in (kg/m^2*Pa*s), the saturation vapor pressure P_{fm}^{sat} at the feed-membrane interface in (Pa), and the vapor pressure P_{pm}^{sat} at the permeate-membrane interface also in (Pa), it is essential to note that the relationship between saturated vapor pressure and temperature for pure water vapor follows Antoine's equation (18), which expresses an exponential relationship as follow:

$$P = \exp\left(23.20 - \frac{3816.44}{T_m - 46.13}\right) \tag{18}$$

Where the vapor pressure P in (Pa) and the local temperature on the membrane surface T_m in (K) are essential factors to consider, the saturated water vapor pressure on the feed side can be represented in equation (19) as a function of the water activity coefficient a_w, which depends on temperature and solute content. Determining the water activity coefficient represented in equation (20) can be achieved through various methods, such as employing empirical equations like NRTL and VanLarr or utilizing existing experimental data by applying Raoul's law [78, 115, 116, 117]:

$$P_{fm}^{sat} = \left(1 - x_{NaCl}\right) * a_w * P_w^{sat} \tag{19}$$

$$a_w = 1 - 0.5 * x_{NaCl} - 10 * x_{NaCl}^2 \tag{20}$$

The term x_{NaCl} represents the mole fraction of NaCl in the water solution. The water activity a_w and the water vapor pressure P_w^{sat} at the feed-membrane or permeate-membrane interfaces can be determined based on this information regarding the adaptation from [118]:

$$\lg P^{sat} = A - \frac{D}{T + C} \tag{21}$$

$$p^{sat} = 133.322 * 10^{\{8.07131 - [1730.630/(T - 39.724)]\}} \tag{22}$$

The Antoine equation determines the water vapor pressure based on the mean temperature across the membrane surfaces, denoted as T_m, where:

$$T_m = \frac{T_{fm} + T_{pm}}{2} \tag{23}$$

II.3.1.3 Temperature polarization

Temperature polarization (TP) at the membrane surface is a common and significant challenge encountered in Membrane Distillation, which profoundly impacts the process's performance [119]. This phenomenon arises when the temperature of the feed solution near the membrane surface decreases, leading to a diminished driving force required for generating permeate flux. Figure II.2 illustrates the thermal boundary layer responsible for inducing temperature polarization.

The primary cause of temperature polarization can be attributed to the transfer of latent heat during the evaporation of water [120]. Consequently, the temperatures at the membrane surfaces deviate from the bulk temperatures observed on the feed and permeate sides. To assess the extent of temperature polarization and its consequences on the mass transfer and heat transfer processes in MD, the temperature polarization coefficient (TPC) is employed [74].

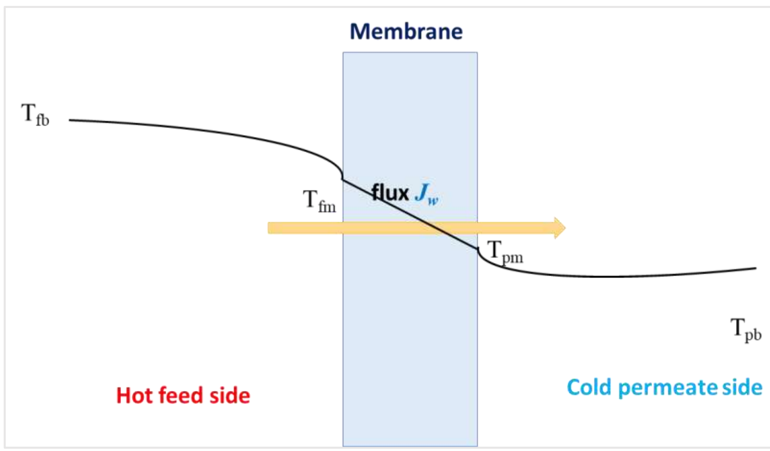


Figure II. 2: Schematic of temperature polarization.

The TPC is the ratio between the total thermal driving force ($T_{fb} - T_{pb}$) and the mass transfer driving force ($T_{fm} - T_{pm}$). This relationship is mathematically expressed by equation (24) [74]:

$$\mathrm{TPC} = \frac{T_{fm} - T_{pm}}{T_{fb} - T_{pb}} \quad \textbf{(24)}$$

In this context, T_{fm} it represents the temperature at the membrane surface on the feed side, T_{pm} denotes the temperature at the membrane surface on the permeate side, T_{fb} signifies the bulk temperature on the feed side, and T_{pb} represents the bulk temperature on the permeate side.

Understanding the TPC is crucial for accurately analyzing heat and mass transport in DCMD systems [121]. A TPC value close to zero suggests a significant boundary layer resistance controlling the system. However, in the case of DCMD, studies have shown that the TPC typically ranges between 0.4 and 0.7, as reported in research [116]. On the other hand, aiming to keep the TPC as close to unity as possible in well-designed systems is desirable. A TPC value close to unity implies that the system is limited by mass transport across the membrane rather than heat transfer from the bulk of the feed to the membrane surface. This indicates efficient membrane performance and optimal utilization of the driving force for permeation.

Regarding the relationship between temperature polarization (TP) and feed temperature, it is essential to note that TP is closely linked to latent heat. When the feed temperature increases, there is a higher rate of convective heat transport from the feed to the permeate side of the membrane. Simultaneously, the temperature at the feed side membrane surface decreases. Consequently, the TPC decreases, resulting in a reduction in permeate flux.

The TPC provides valuable insights into the mass transport behavior and helps understand the extent of the effect occurring during the membrane distillation process. Temperature polarization refers to a phenomenon that can weaken the efficiency of the MD process. It occurs when there is a slight difference between the feed membrane surface and permeate membrane surface and a slight difference between feed bulk temperature and permeate bulk temperature in the DCMD module. This temperature difference affects the mass transport phenomenon across the membrane, leading to reduced performance.

II.4.1 Introduction to Optimization in Direct Contact Membrane Desalination

II.4.1.1 Significance of optimization in improving DCMD performance

Optimization refers to the process of finding the best possible solution or set of solutions for a given problem. It involves maximizing or minimizing an objective function or a set of objective functions subject to a set of constraints or limitations. The objective function represents the quantity that needs to be optimized, while the constraints define the permissible values or conditions for the variables involved in the problem.

Optimization aims to find the optimal solutions that satisfy the given objectives while adhering to the constraints. The optimal solutions can be determined by exploring the search space of possible solutions and evaluating their fitness or objective function values. The search process typically involves iteratively improving solutions until a satisfactory or optimal solution is reached.

Optimization problems can vary widely in nature and complexity, ranging from simple mathematical functions to complex real-world systems. They can involve multiple conflicting objectives, discrete or continuous variables, and different types of constraints. Various optimization techniques, including metaheuristic algorithms, mathematical programming, evolutionary algorithms, and gradient-based methods, are employed to solve different types of optimization problems.

Metaheuristic algorithms are a type of optimization method used to solve complex problems. Metaheuristics are general-purpose search algorithms that can be applied to a wide range of optimization problems where traditional exact methods may be impractical or infeasible due to the problem's complexity or computational requirements [122].

Unlike exact methods, metaheuristics are stochastic and approximate. They are designed to explore the search space efficiently, balancing exploration and exploitation to find good-quality solutions within a reasonable amount of time [123].

Metaheuristic algorithms draw inspiration from natural or social processes such as evolution, swarm behavior, or simulated annealing [123]. They often involve maintaining a population of candidate solutions and iteratively improving them through various operators such as mutation, crossover, and selection.

Examples of metaheuristic algorithms include Genetic Algorithms (GA), Particle Swarm Optimization (PSO), Simulated Annealing (SA), Ant Colony Optimization (ACO), and Tabu Search (TS), Bonobo Optimization (BO). These algorithms exhibit robustness, flexibility, and the ability to handle complex optimization problems with multiple objectives or constraints.

Optimization is crucial in improving the performance of Direct Contact Membrane Distillation (DCMD) systems. Hence, some fundamental significances of optimization are:

- **Maximizing Permeate Flux**: One of the primary objectives in DCMD systems is to maximize the production of permeate or fresh water while maintaining acceptable product quality. This objective is essential in water-scarce regions or situations requiring high water production rates. Optimization techniques help identify the optimal operating conditions, such as feed temperature, flow rate, membrane properties, and system configuration, that maximize the permeate flux in DCMD. Optimization can significantly enhance the system's productivity by achieving the highest possible permeate production rate by finding the right combination of variables, allowing for more efficient desalination or separation processes.

- **Enhancing Thermal Efficiency**: It is possible to improve the thermal efficiency of DCMD systems through optimization. Optimization can maximize thermal energy utilization and minimize losses by adjusting variables such as feed temperature, operating pressure, and heat recovery methods, improving overall system efficiency and reducing energy consumption.
- **Minimizing Fouling and Scaling:** Optimization can help mitigate fouling and scaling issues in DCMD systems. By carefully selecting and optimizing various variables, such as flow rates, membrane materials, and feedwater pretreatment processes, it is possible to minimize fouling and scaling tendencies. This leads to a longer membrane lifespan, reduced maintenance requirements, and improved system reliability.
- **Balancing Flux and Selectivity:** Optimization allows finding the balance between permeate flux and solute selectivity in DCMD. Fine-tuning operating conditions and membrane properties makes it possible to achieve high flux rates while maintaining desired separation efficiencies. This is crucial for applications with high productivity and high-quality permeate.
- **System Cost Optimization:** Optimization techniques can also be used to optimize the cost-effectiveness of DCMD systems. By considering factors such as membrane cost, energy consumption, maintenance requirements, and system scalability, optimization can help identify the most cost-efficient design and operation strategies. This enables the implementation of economically viable DCMD systems.
- **Minimizing Energy Consumption:** Energy efficiency is crucial in DCMD systems, as desalination processes can be energy-intensive. Minimizing energy consumption is often a key optimization objective to reduce operating costs and environmental impact. The system can be designed and operated by optimizing temperature, pressure, and flow rates to minimize energy requirements while still meeting the desired permeate production rate and product quality.
- **Process Scale-up and Design Optimization:** Optimization is essential when scaling up DCMD processes from laboratory-scale to industrial-scale. It allows for optimizing various parameters to ensure smooth operation, efficient heat and mass transfer, and cost-effective system design. Optimization helps address challenges associated with scaling up, such as maintaining desired performance metrics, managing larger feed flow rates, and ensuring system reliability.

Optimization techniques also improve heat and mass transfer within the DCMD module [135]. Heat and mass transfer rates can be maximized by identifying optimal temperature profiles, flow patterns, and channel geometries. This results in higher productivity and better separation efficiency, as the system operates under conditions that enhance heat transfer and mass across the membrane.

Stability and reliability are crucial aspects of any DCMD system. Optimization is vital in achieving stable and reliable operations by identifying critical process variables and establishing control strategies [122]. Optimization minimizes process fluctuations, ensures consistent performance, and reduces the risk of system failure by maintaining optimal operating conditions. This leads to improved system stability and enhances the reliability of the DCMD process.

Finally, optimization allows for customizing DCMD systems to specific applications and feedwater characteristics [124]. Optimization techniques can be employed to tailor process parameters, membrane selection, and module design by considering each application's unique requirements and challenges. This customization ensures optimal performance, efficient operation, and effective treatment in diverse water treatment and desalination applications.

In summary, optimization is essential in improving the performance of DCMD systems. It maximizes productivity, minimizes energy consumption, enhances membrane performance, mitigates fouling and scaling, improves heat and mass transfer, enhances system stability and reliability, and allows customization for specific applications. By employing optimization techniques, DCMD systems can achieve higher efficiency, lower costs, and improved overall performance in various water treatment and desalination applications.

II.4.1.2 Optimization objectives and questions addressed in this contribution

Overall, the membrane optimization objective is to enhance the performance and longevity of membranes used in DCMD by improving system stability, reducing maintenance requirements, and extending operational cycles. This objective involves optimizing membrane characteristics such as material selection, pore size, and surface modifications.

Investigating various membrane materials, various feedwater pretreatment methods, flow velocities, and module configurations to identify the most suitable membranes seeks to improve the separation efficiency, flux, and resistance to fouling and scaling to achieve high performance and durability in DCMD applications.

Ensuring stable and reliable operation is another critical objective in DCMD optimization to minimize process fluctuations, ensure consistent performance, and reduce the risk of system failure By establishing and developing control strategies.

Lastly, In DCMD systems, the choice of optimization objectives depends on the specific goals and priorities of the system's operation. The primary objective of this contribution to DCMD optimization is to improve the process's flux productivity and thermal efficiency. This involves identifying the optimal operating parameters such as feed flow rate, feed temperature, height, and thickness.

Addressing these objectives leads to exploring specific questions such as:

- What are the optimal operating conditions for maximizing DCMD productivity?
- How can membrane characteristics be optimized to improve membrane performance?
- What optimization methods effectively enhance the permeate flux and the efficiency?
- What critical process variables must be optimized for stable and reliable DCMD operation?
- What are the appropriate ranges for each chosen variable to optimize the primary objective?

Addressing these questions contributes to advancing DCMD optimization and improving performance, efficiency, and reliability in various water treatment and desalination applications.

II.4.2 Optimization Approaches for DCMD

II.4.2.1 Overview of different optimization techniques applicable to DCMD

There are many techniques of optimization applicable to DCMD. Each technique offers distinct advantages and considerations, and selecting the most appropriate technique depends on the specific objectives, constraints, and complexity of the studied DCMD system. These optimization techniques are used to improve the performance, efficiency, and reliability of DCMD systems and contribute to the advancement of membrane-based desalination technologies, including [123]:

1. **Design of Experiments (DoE):** Design of Experiments is a statistical approach that allows for systematically exploring the parameter space in DCMD. By designing and conducting experiments based on statistical principles, DoE helps identify the optimal combination of operating parameters that maximize productivity and minimize energy consumption. This technique enables efficient

and comprehensive analysis of multiple factors and their interactions, improving process understanding and optimization, as used in [118].

2. Response Surface Methodology (RSM): RSM is an optimization technique that utilizes mathematical models to explore the relationships between process variables and performance indicators. By fitting response surfaces to experimental data, RSM allows for identifying optimal operating conditions. This technique enables researchers to analyze the impact of various factors on DCMD performance, predict optimal parameter settings, and guide decision-making for process optimization [65].

3. Genetic Algorithms (GA): Genetic Algorithms are population-based optimization algorithms inspired by the principles of natural evolution. GA involves the creation of a population of potential solutions (chromosomes) and the application of genetic operators such as selection, crossover, and mutation to mimic the process of natural selection and evolution. GA can be applied to optimize multiple parameters simultaneously and search for the global optimum in complex DCMD systems [89].

4. Particle Swarm Optimization (PSO): Particle Swarm Optimization is a population-based optimization technique that simulates the collective behavior of a swarm of particles. Each particle represents a potential solution, and they move through the search space to find the optimal solution based on the collective information. PSO has been successfully applied to optimize DCMD systems by exploring the parameter space and identifying the optimal combination of operating conditions, as used in [125].

5. Artificial Neural Networks (ANN): Artificial Neural Networks are computational models inspired by the structure and function of biological neural networks. ANNs have been used in DCMD optimization to develop predictive models that relate process parameters to performance indicators. These models can then guide optimization efforts by predicting the optimal parameter settings for achieving desired outcomes.

Optimization methods are classified into two main categories: single-objective and multi-objectives optimization, as shown in **Figure II. 3.**

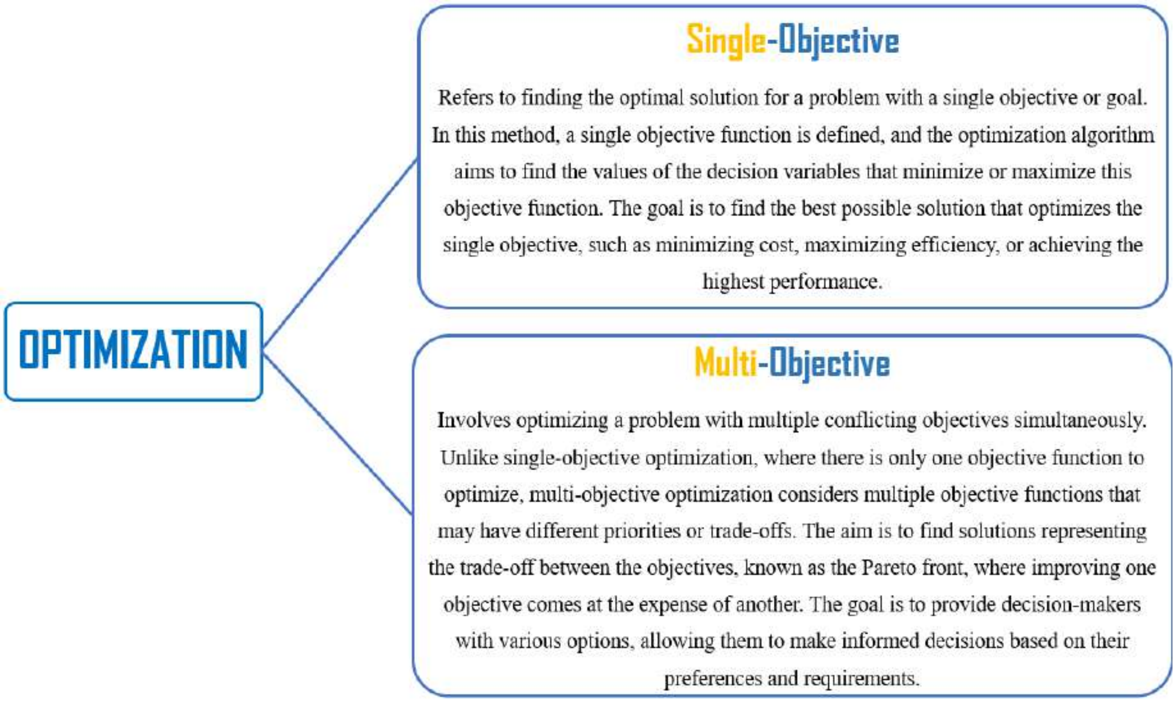


Figure II. 3: Schematic of Optimization methods categories.

II.4.3 Optimization Variables and Constraints in DCMD

II.4.3.1 Identification and selection of optimization variables in DCMD systems

When identifying and selecting optimization variables in DCMD systems, two critical variables are permeated flux and thermal efficiency. Here is a closer look at these variables:

1. **Permeate Flux** refers to the rate at which pure water passes through the membrane in a DCMD system. It is a crucial performance indicator that directly affects the productivity and efficiency of the system. Higher permeate flux indicates a greater water production rate, typically desired in desalination processes. Optimization efforts can focus on variables that influence permeate flux, like:

- **Feedwater flow rate**: Increasing the feedwater flow rate can enhance permeate flux, but it should be balanced with other considerations like membrane thickness.
- **Membrane properties**: The choice of membrane material, thickness, and surface characteristics can impact permeate flux. Optimizing these parameters can improve water permeability.
- **Temperature difference**: The temperature difference between the feed and permeate sides affects the driving force for mass transfer and can influence permeate flux.

2. Thermal Efficiency: Thermal efficiency in DCMD systems represents the effectiveness of utilizing thermal energy to drive desalination. It measures how efficiently heat is transferred from the heat source to the feedwater, contributing to the vaporization and subsequent condensation on the membrane surface. Variables that can impact thermal efficiency include:

- **Temperature difference**: The temperature difference between the system's hot and cold sides affects heat transfer efficiency. Maximizing this temperature difference while considering practical constraints can improve thermal efficiency.
- **Insulation:** Proper system insulation can minimize heat loss and improve thermal efficiency by maintaining the desired temperature gradients.
- **Membrane Properties**: The properties of the membrane, such as its thermal conductivity and thickness, can affect the overall thermal efficiency. Membranes with higher thermal conductivity can facilitate better heat transfer and potentially improve efficiency.

It is worth noting that the selection of optimization variables may also depend on other factors such as energy consumption, fouling mitigation, and system cost. A holistic approach and considering the system's constraints and objectives will help identify and select the most relevant optimization variables for DCMD systems.

II.4.3.2 Consideration of Constraints

When applying an optimization technique to Direct Contact Membrane Desalination (DCMD) systems, it is essential to consider constraints such as flow rates, temperature, and membrane characteristics:

1. **Flow Rates:** Flow rates are crucial in DCMD systems as they affect mass transfer, system efficiency, and pressure distribution. Constraints on flow rates can be imposed to ensure the system operates within safe and optimal conditions. These constraints can be based on equipment limitations, desired production rates, or avoiding excessive pressure drops. The optimization process should consider these constraints and optimize the variables accordingly while respecting the flow rate limits.
2. **Temperature**: Temperature is a significant parameter in DCMD systems as it influences the driving force for mass transfer, heat transfer, and overall system performance. Temperature constraints can be set to maintain the desired thermal conditions, prevent membrane damage, and ensure efficient operation. The optimization process should consider these temperature constraints and select variables that adhere to the specified limits while achieving the desired objectives.

3. **Membrane Characteristics:** Membrane characteristics, such as permeability, porosity, selectivity, and fouling propensity, have a significant impact on the performance and efficiency of DCMD systems. Constraints related to membrane characteristics can be incorporated into the optimization process to ensure the selected variables align with the capabilities and limitations of the chosen membrane material. For example, constraints can be set to maintain a certain level of salt rejection, avoid exceeding fouling thresholds, or consider the membrane's maximum operating pressure or temperature.II.4.4 Optimization Challenges and Future Directions.

II.4.3.3 Discussion of challenges encountered in the optimization of DCMD systems

The optimization of DCMD systems presents several challenges due to the complex nature of the process and the interplay between various factors. Some of the challenges encountered in the optimization of DCMD systems are [126]:

1. **Nonlinear Behavior**: DCMD systems exhibit nonlinear behavior due to mass transfer, heat transfer, and fluid dynamics coupling. This nonlinearity makes the optimization process more challenging, as traditional linear optimization techniques may not be applicable. Advanced optimization algorithms, such as genetic algorithms, bonobo, or particle swarm optimization, may be required to handle the nonlinear behavior and find optimal solutions.
2. **Multi-objective Optimization:** DCMD systems often involve conflicting objectives, such as maximizing permeate production while minimizing energy consumption. Balancing these objectives can be complex and may require trade-offs. Multi-objective optimization techniques must be employed to find Pareto-optimal solutions representing the best compromise between different objectives.
3. **High-Dimensional Parameter Space**: DCMD systems typically have many parameters and variables that can be optimized, such as feedwater flow rate, temperature difference, membrane properties, and operating conditions. The high-dimensional parameter space increases the complexity of the optimization process and makes it computationally intensive. Advanced optimization algorithms and techniques, such as surrogate modeling or response surface methodology, can be used to reduce the computational burden.
4. **Constraints and Uncertainties:** Optimization of DCMD systems needs to consider various constraints such as flow rates, temperature limits, pressure constraints, and membrane characteristics. Incorporating these constraints into the optimization process can be challenging,

especially when dealing with uncertainties in system parameters or variations in feedwater composition. Robust optimization techniques that account for uncertainties and variations can be employed to ensure that the optimal solutions are feasible under different operating conditions.

5. **Computational Resources**: The optimization of complex DCMD systems often requires significant computational resources and time. The optimization process involves evaluating the system's performance for different parameter combinations, which can be computationally expensive. Efficient algorithms, parallel computing, and optimization software can help overcome computational limitations and reduce the time required for optimization.
6. **System Dynamics and Transient Behavior:** DCMD systems can exhibit dynamic behavior and transient responses during startup, shutdown, or changes in operating conditions. Optimizing such systems requires considering dynamic effects and transient behavior. Time-dependent optimization techniques or model predictive control approaches can optimize the system's performance while accounting for dynamic responses.

Addressing these challenges requires a comprehensive understanding of the DCMD system, expertise in optimization techniques, and access to suitable computational tools. Optimizing DCMD systems can lead to improved performance, increased energy efficiency, and enhanced desalination capabilities by addressing these challenges.

II.4.4 Potential advancements in optimization techniques to overcome existing limitations

Advancements in optimization techniques can help overcome existing limitations in optimizing DCMD systems. Here are potential advancements that can address current limitations:

1. **Machine Learning-Based Optimization**: Integrating machine learning algorithms, such as neural networks or genetic programming, with optimization techniques can enhance the efficiency and effectiveness of DCMD system optimization. Machine learning can be used to learn complex relationships between system variables and performance metrics, enabling more accurate and faster optimization. It can also aid in handling uncertainties and nonlinearity in the system behavior [127].
2. **Surrogate Modeling and Response Surface Methodology**: Surrogate modeling techniques involve building simplified mathematical models (surrogates) that approximate the behavior of the DCMD system. These surrogates can be used in place of computationally expensive models to accelerate the optimization process. Response surface methodology is a statistical

technique used to construct and optimize surrogate models based on a limited number of system simulations or experimental data points [128].

3. **Multi-Objective Evolutionary Algorithms**: Traditional optimization techniques often struggle to handle conflicting objectives in DCMD optimization. Advanced multi-objective evolutionary algorithms, such as NSGA-II (Non-dominated Sorting Genetic Algorithm II) or MOEA/D (Multi-Objective Evolutionary Algorithm Based on Decomposition), can efficiently explore the Pareto-optimal front and help find optimal trade-off solutions between various objectives, such as permeate production and energy consumption [129].
4. **Hybrid Optimization Approaches**: Combining different optimization techniques or algorithms can leverage their respective strengths and overcome limitations. For example, combining gradient-based optimization methods and evolutionary algorithms can lead to efficient local search and global exploration. Hybrid approaches can improve convergence speed, enhance solution quality, and effectively handle complex optimization problems [130].
5. **Dynamic Optimization and Model Predictive Control:** DCMD systems often exhibit dynamic behavior and transient responses. Dynamic optimization techniques, such as dynamic programming or model predictive control (MPC), can optimize system performance while considering time-varying variables, constraints, and objectives. These approaches can account for system dynamics, anticipate changes, and optimize control actions in real-time, improving system operation [131].
6. **Uncertainty Quantification and Robust Optimization**: DCMD systems are subject to uncertainties in operating conditions, feedwater composition, and system parameters. Robust optimization techniques that explicitly account for uncertainties and variations can provide optimal solutions more resilient to uncertainties. Uncertainty quantification methods, such as Monte Carlo simulations or stochastic optimization, can be incorporated to assess the robustness and reliability of the optimized solutions [132].

By advancing these optimization techniques, researchers and engineers can overcome existing limitations in DCMD system optimization, leading to more efficient designs, improved performance, and better utilization of resources in desalination processes.

II.4.5 Overview of chaotically based-Bonobo Optimizer (BO) in DCMD systems

Bonobo Optimization is a term that refers to a specific optimization algorithm inspired by the social behavior of bonobo apes. It is a relatively new population-inspired optimization algorithm for various optimization problems.

Bonobo Optimization (BO) is based on the social behavior and foraging patterns observed in bonobo apes, known for their cooperative and peaceful nature. The algorithm mimics the social interactions and cooperation among the known chimpanzees named bonobos or pygmy chimpanzees, where the initial discovery took place in 1929 at the Belgian Colonial Museum to search for optimal solutions to optimization problems [132].

The key concept behind Bonobo Optimization is the division of the population into multiple subgroups (referred to as clans), each representing a potential solution. Within each clan, individual solutions (bonobos) communicate and share information to improve overall performance [132]. The algorithm combines exploration and exploitation strategies to search the solution space efficiently.

In the bonobo world, four different mating strategies contribute to maintaining harmony in their society. These strategies include restrictive mating, promiscuous mating, extra-group mating, and consortship mating. Each strategy aims to ensure social balance within the bonobo community [132].

The algorithm iteratively updates the solutions based on their fitness values. Bonobos within a clan communicate and exchange information, allowing them to adjust their positions in the search space accordingly. The algorithm aims to converge towards an optimal solution or a set of Pareto-optimal solutions in multi-objective optimization problems through iterations and interactions [132].

Pareto optimality, also known as Pareto efficiency or Pareto optimality, is a concept in multi-objective optimization that represents a state where no further improvements can be made to one objective without sacrificing the performance of another objective. A solution is said to be Pareto-optimal if no other feasible solution can improve one objective without worsening at least one other objective.

Bonobo Optimization offers a unique approach that leverages the principles of cooperation and social learning to explore and exploit the search space effectively.

It is important to note that Bonobo Optimization is one among many nature-inspired optimization algorithms [132], each with its strengths, weaknesses, and areas of applicability. The effectiveness of this algorithm and its performance may vary depending on the problem being solved.

II.4.5.1 Mathematical model of the Bonobo Optimizer (BO) algorithm

The BO algorithm initiates by generating a random set of solutions within the search space, as shown in Table III.1in the third chapter. The initial solutions generated randomly are used to evaluate the objective function and determine the alpha bonobo. Subsequently, during the iterative process, the positions of both the alpha bonobo and the other agents are updated. As previously mentioned, the bonobos exhibit a behavior where they form temporary subgroups before regrouping into a larger community. To model this behavior, Kumar et al. [132] introduced the concept of the maximum size of the temporary sub-group $tsgs_{\max}$ ranging between 2 and the ratio of the total population (N). Thus, the $tsgs_{\max}$ can be defined as follows:

$$tsgs_{\max} = maximum\left(2,\left(tsgs_{\text{factor}} \times N\right)\right) \quad \textbf{(25)}$$

The self-adaptive factor $tsgs_{\max}$ dynamically adjusts during the iteration process to determine the size of the temporary sub-group. The product of $tsgs_{\max}$ and N is rounded to the nearest integer value, representing the temporary sub-group size. It is important to note that based on Equation (26), the minimum value for the agents is determined to be 2. Subsequently, the sub-group agents update their locations according to the selected reproduction strategy, including restrictive mating, promiscuous mating, extra-group mating, and consortship mating [132].

The BO algorithm uses a self-adaptive phase probability (Pp) to distinguish between different mating strategies, determined by the variable rate of change in phase probability ($rcpp$). Restrictive and promiscuous mating is considered when Pp is between 0.5 and 1, while extra-group and consortship mating have higher chances when $Pp \in (0, 0.5)$. Agents adjust their positions using specific formulas based on the selected mating strategy, such as promiscuous and restrictive mating [132].

$$\text{new bonobo}_j = \text{bonobo}^i_j + r_1 \times scab \times \left(\alpha^j_{\text{bonobo}} - \text{bonobo}^i_j\right) + \left(1 - r_1\right) \times scsb \times \text{flag} \times \left(\text{bonobo}^i_j - \text{bonobo}^p_j\right) \quad \textbf{(26)}$$

The j^{th} variable of the new offspring, denoted as new bonobo_j , and the alpha bonobo, represented by α^j_{bonobo}, are involved in the equation. The range of the dimension of j varies from 1 to d, where d represents the total number of variables in the given optimization problem. The variables bonobo^i_j and bonobo^p_j represent the i^{th} and p^{th} bonobos for the j^{th} variable. The sharing factors $scab$ and $scsb$ are values between [1-2], indicating the degree of sharing between the α^j_{bonobo} and the p^{th} bonobos. The flag serves as an indicator for the type of mating, with a value of (1) representing promiscuous mating and (-1) representing restrictive mating. The random number r_1 is obtained from a uniform distribution between [0-1].

In the case of consortship mating and extra-group mating (third and fourth mating), the selection between the two types is determined by a random factor (r_3). New offspring are created if r3 is less than or equal to the probability of extra-group mating. Conversely, if r_3 is greater than the probability factor, the bonobos engage in consortship mating, following the described conditions.

- The creation of new offspring during extra-group mating involves utilizing the following equations:

$$\text{new\_bonobo}_j = \text{bonobo}^i_j + \beta_1 \times \left(\text{Var\_max}_j - \text{bonobo}^i_j\right) \; if \; (\alpha^j_{\text{bonobo}} \geq \text{bonobo}^i_j \text{ and } r_3 \leq p_d)$$

$$\text{new\_bonobo}_j = \text{bonobo}^i_j + \beta_2 \times \left(\text{bonobo}^i_j - \text{Var\_min}_j\right) \; if \; (\alpha^j_{\text{bonobo}} \geq \text{bonobo}^i_j \text{ and } r_3 \succ p_d) \quad \textbf{(27)}$$

$$\text{new\_bonobo}_j = \text{bonobo}^i_j + \beta 1 \times \left(\text{bonobo}^i_j - \text{Var\_min}_j\right) \; if \; (\alpha^j_{\text{bonobo}} \prec \text{bonobo}^i_j \text{ and } r_3 \leq p_d)$$

$$\text{new\_bonobo}_j = \text{bonobo}^i_j + \beta_2 \times \left(\text{Var\_max}_j - \text{bonobo}^i_j\right) \; if \; (\alpha^j_{\text{bonobo}} \prec \text{bonobo}^i_j \text{ and } r_3 \succ p_d)$$

$$\beta_1 = e^{\left(r_4^2 + r_4 - 2/r_4\right)}$$

$$\beta_2 = e^{\left(-r_4^2 + 2 \times r_4 - 2/r_4\right)} \quad \textbf{(28)}$$

In this context, β_1 and β_2 represent two intermediate measured values used to calculate the value of new_bonobo_j. The variable r_4 is a randomly generated number ranging from 0.0 to 1.0, where $r_4 \neq$ is 0. Var_min_j and Var_max_j refers to the lower and upper boundary values associated with the j^th^ variable, respectively.

- Creating new offspring during consortship mating involves utilizing the following equations.

$$\text{new\_bonobo}_j = \left\{ \text{bonobo}_j^i + \text{flag} \times e^{(-r_5)} \times \left(\text{bonobo}_j^i - \text{bonobo}_j^p \right), (\text{flag} = 1 \| r_6 \le p_d), \right\} \quad \text{bonobo}_j^p, \textit{otherwise} \tag{29}$$

Random values r_5 and r_6 are chosen from the interval between 0 and 1. The symbol p_d represents the directional probability used to determine the employed strategy for modifying the solutions vector. In the BO, Kumar et al. [132] updated the probability values during the iterations.

The BO algorithm can be visualized using the flowchart shown in Figure II.4, starting with an initial set of solutions and utilizing the mentioned equations to modify them iteratively. Eventually, the presented results include the best solutions corresponding to the minimum fitness function.

II.4.6 Overview of Particle Swarm Optimization (PSO) in DCMD systems

Particle Swarm Optimization (PSO) is an optimization technique proposed by J. Kennedy and R.C. Eberhart. It can be applied to improve the performance of DCMD systems. PSO is a population-based algorithm inspired by the social behavior of bird flocking or fish schooling. It operates by iteratively adjusting a set of candidate solutions called particles to search for optimal solutions in a given problem space [132].

In the context of DCMD, PSO can be used to optimize various aspects of the process, such as productivity, energy consumption, thermal efficiency, and operating conditions. Here is how PSO can be applied to DCMD systems [132] :

1**. Objective Function**: Define the objective function representing the optimization goal, such as maximizing water production and thermal efficiency or minimizing energy consumption. The objective function should capture the relationship between the process variables and the desired performance indicators.

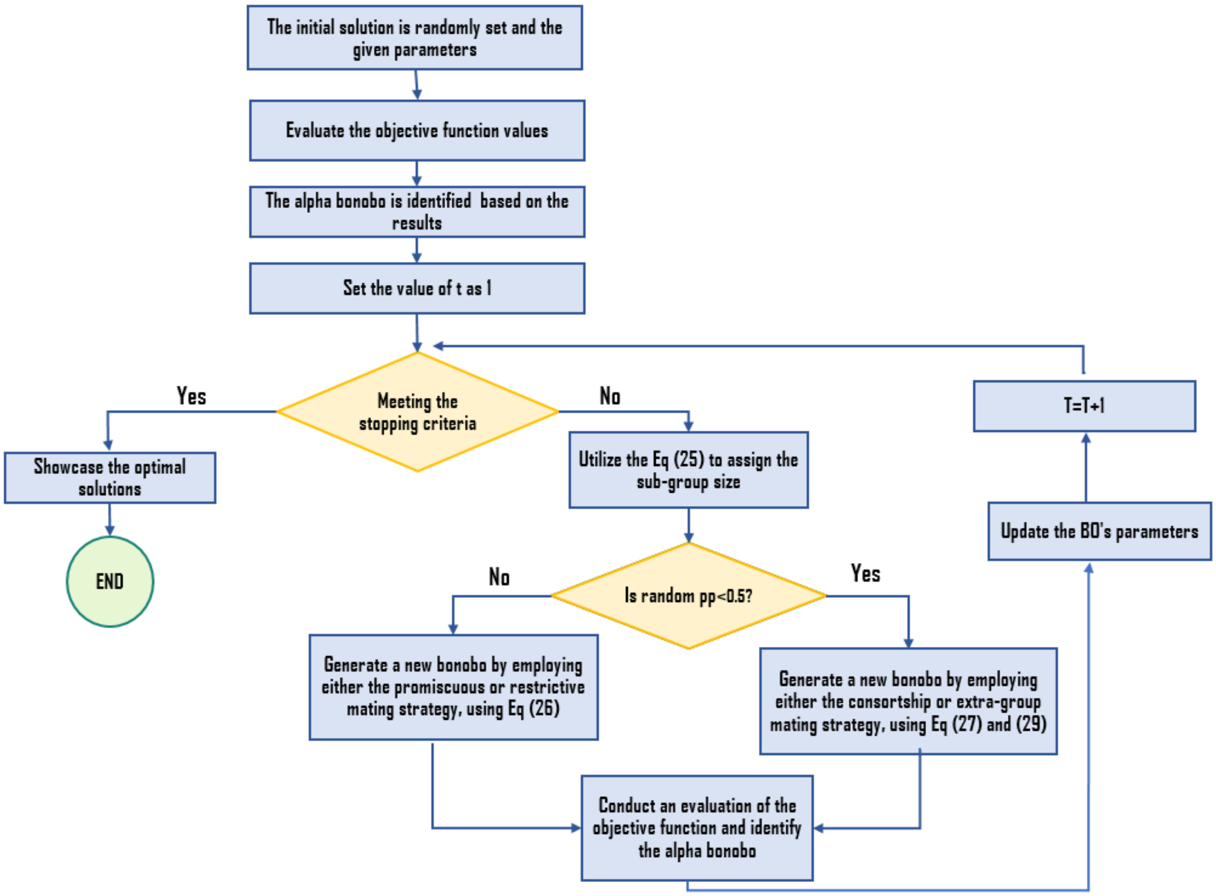


Figure II.4. Flowchart of the proposed BO algorithm.

2. Parameter Initialization: Initialize a population of particles, where each particle represents a potential solution in the parameter space. The particles are randomly distributed within the search space, corresponding to the range of feasible values for the process variables.

3. Particle Movement: Each particle in the population adjusts its position in the search space based on its current position, velocity, and the influence of its own best-known solution (personal best) and the best-known solution among all particles (global best). The particle movement is guided by optimization equations that update the velocity and position of each particle.

4. Fitness Evaluation: Evaluate the fitness of each particle by applying the objective function to the corresponding parameter values. The fitness value represents how well the particle's solution performs regarding the optimization objective.

5. Update Personal and Global Best: Update the personal best position for each particle based on its current fitness value. Additionally, update the global best position based on the best fitness value among all particles.

6. Iteration: Repeat the particle movement, fitness evaluation, and update steps for a certain number of iterations or until a convergence criterion is met. The particles gradually converge towards better solutions as they share information and explore the search space.

7. Solution Extraction: Once the PSO iterations are completed, extract the best solution corresponding to the particle with the best fitness value. This solution represents the optimized process variable set that achieves the desired objective.

By applying PSO to DCMD systems, researchers and engineers can explore the parameter space and identify optimal operating conditions that maximize productivity or achieve other desired outcomes. PSO allows for efficient and effective search of the solution space, potentially leading to improved performance, energy efficiency, and overall optimization of DCMD processes.

It is important to note that the specific implementation and customization of PSO for DCMD systems may vary based on the optimized system's unique characteristics, constraints, and objectives.

II.4.6.1 Mathematical model of the Particle Swarm Optimization (PSO) algorithm

Particle Swarm Optimization (PSO) is a population-based metaheuristic optimization algorithm that mimics the behavior of bird flocking or fish schooling. It begins by initializing a group of particles, each representing a potential solution. Particles update their positions and velocities through iterations based on their personal best and the global best solutions. This balance between exploration and exploitation helps guide the particles towards the optimal solution.

The mathematical model of PSO can be described as follows [133]:

Principle:

The essence of PSO lies in the particles "flying" through the search space with velocities adjusted based on their own experience and the experience of their neighbors. The particles are influenced by the best position they have found (cognitive component) and the best position found by their neighbors (social component). This balance between self-experience and social experience allows the swarm to explore and exploit the search space [133] efficiently.

For each particle *i* in the swarm:

- Evaluate the fitness of the particle's current position: $f(x_i)$.

- Compare the current position's fitness with the particle's personal best position: *f*(*pbesti*).
- If the current position has a better fitness than the personal best position (depending on whether it is a minimization or maximization problem), update the personal best:

For a **minimization** problem:

$$\mathrm{pbest}_i = \begin{cases} x_i & \text{if } f\left(x_i\right) < f\left(\mathrm{pbest}_i\right) \\ \mathrm{pbest}_i & \text{otherwise} \end{cases} \tag{30}$$

For a **maximization** problem:

$$\mathrm{pbest}_i = \begin{cases} x_i & \text{if } f\left(x_i\right) > f\left(\mathrm{pbest}_i\right) \\ \mathrm{pbest}_i & \text{otherwise} \end{cases} \tag{31}$$

2. Global Best (Gbest) Calculation:

After updating the personal best positions for all particles in the swarm:

- Compare the fitness of all the personal best positions:

  $f(pbest_1), f(pbest2), \ldots, f(pbest_N)$ where N is the number of particles.

- The position with the best fitness among all the personal best positions becomes the global best position:

  For a **minimization** problem:

$$\mathrm{gbest} = argmin_i \; f\left(\mathrm{pbest}_i\right) \tag{32}$$

For a **maximization** problem:

$$\mathrm{gbest} = argmax_i \; f\left(\mathrm{pbest}_i\right) \tag{33}$$

- The fitness function *f* is problem-specific and determines how good a solution (or position) is.
- The *pbest* values are stored for each particle and are updated in each iteration based on the current positions of the particles.

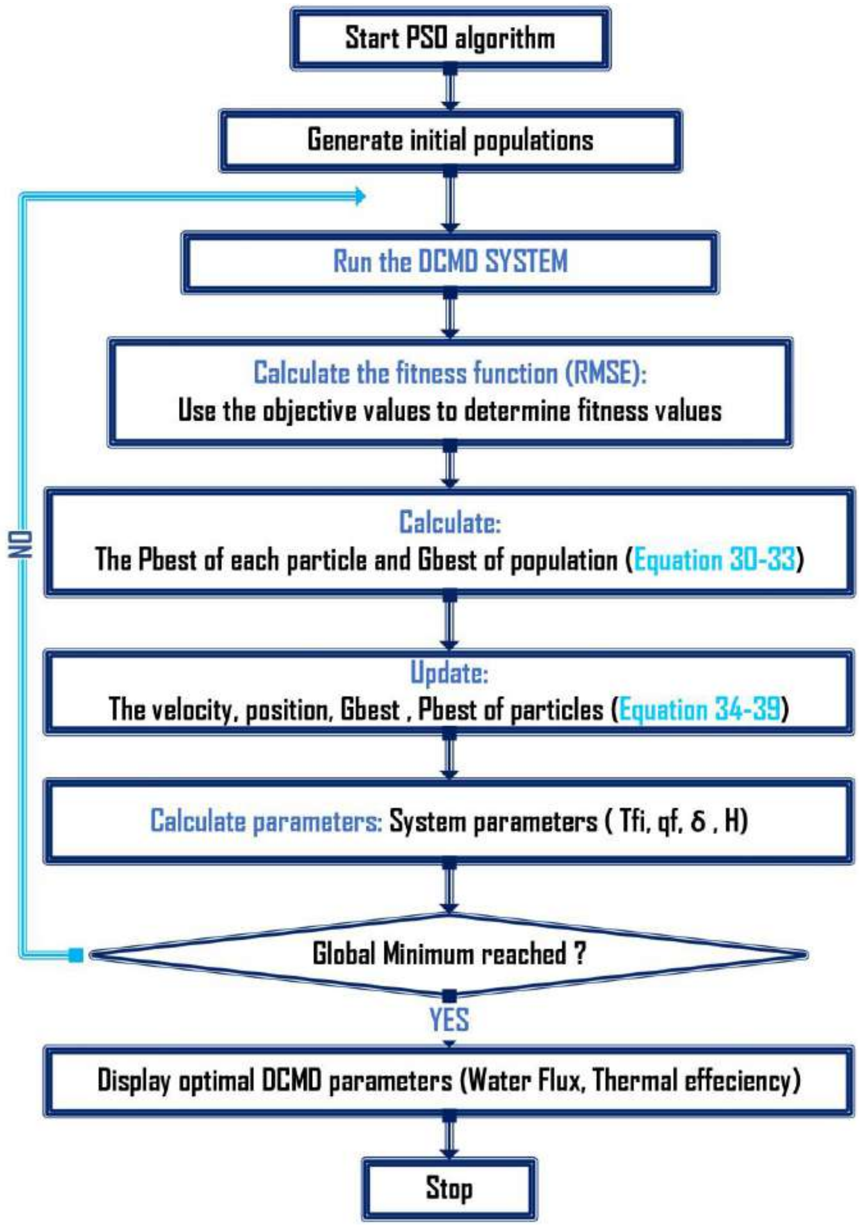


Figure II.5. flowchart of the proposed PSO algorithm.

- The *gbest* value represents the best solution found by the swarm up to the current iteration. It is updated whenever a particle finds a better solution than the current *gbest*.

1. Velocity Update:

The velocity of each particle *i* is updated based on its current velocity, the difference between its personal best position and its current position, and the difference between the global best position and its current position:

$$v_i(t+1) = w \times v_i(t) + c_1 \times r_1 \times (\text{pbest}_i - x_i(t)) + c_2 \times r_2 \times (\text{gbest} - x_i(t)) \quad \textbf{(34)}$$

- $v_i(t)$ is the velocity of particle I at time t.
- w is the inertia weight, which controls the momentum of the particle.
- c_1 and c_2 are cognitive and social coefficients, respectively.
- r_1 and r_2 are random numbers uniformly distributed in [0, 1].
- $x_i(t)$ is the position of particle I at time t.

2. Position Update:

The position of each particle I is updated based on its current position and its updated velocity:

$$x_i(t+1) = x_i(t) + v_i(t+1) \quad (35)$$

3. Personal Best (Pbest) Update:

For each particle i:

- Evaluate the fitness of the particle's current position: $f(x_i)$.
- If the current position has a better fitness than the personal best position, update the personal best:

For a **minimization** problem:

$$\text{pbest}_i = \begin{cases} x_i & \text{if } f(x_i) < f(\text{pbest}_i) \\ \text{pbest}_i & \text{otherwise} \end{cases} \quad (36)$$

For a **maximization** problem:

$$\text{pbest}_i = \begin{cases} x_i & \text{if } f(x_i) > f(\text{pbest}_i) \\ \text{pbest}_i & \text{otherwise} \end{cases} \quad (37)$$

4. Global Best (Gbest) Update:

After updating the personal best positions for all particles:

- The position with the best fitness among all the personal best positions becomes the global best position:

For a **minimization** problem:

$$\text{gbest} = argmin_i \; f(\text{pbest}_i) \quad (38)$$

For a **maximization** problem:

$$\text{gbest} = argmax_i \; f(\text{pbest}_i) \quad (39)$$

- The fitness function f is problem-specific.

- The values of w, c_1, and c_2 can be adjusted based on the specific problem and desired exploration/exploitation balance.
- The *pbest* and *gbest* values guide the particles towards better regions of the search space.

II.7. Presentation of the DCMD under Study

The DCMD module described has the following specifications:

- Membrane Length: 1 m
- Membrane Width: 0.5 m
- Feed Channel Height: 5 10^$^{-3}$ m
- Permeate Channel Height: 5 10^$^{-3}$ m
- Membrane Thickness: 120 µm
- Membrane Porosity: 75%
- Feed Inlet Temperature: 70°C (343.15 K)
- Feed Inlet Mass Flow Rate: 1 kg/s
- Feed Inlet NaCl Concentration: 35 g/kg
- Permeate Inlet Temperature: 20°C (293.15 K)
- Feed and Permeate Inlet Mass Flow Rate: 1 kg/s

DCMD is a membrane-based desalination operating on the principle of selective vapor permeation through a hydrophobic membrane. The module consists of a flat sheet membrane with specific dimensions. The feedwater, which is saline water in this case, enters the module through the feed inlet.

The feedwater enters the feed channel, which has a height of 5 10^$^{-3}$ m. The membrane acts as a barrier, allowing only water vapor molecules to pass through while retaining salts and other impurities. The length of the membrane used in this module is 1 m. The water flux indicates the rate at which water vapor permeates through the membrane surface area (expressed in kg/m^2.h).

The DCMD module also has a channel with a height of 5 10^$^{-3}$ m. The permeate inlet, which is the distilled water produced by the process, enters the module through this channel. The permeate inlet temperature is specified as 20°C (293 K) in this study. The performance of the DCMD module can be evaluated based on several parameters, including permeate flux and thermal efficiency.

Optimization strategies can be employed to improve the performance of the DCMD module. These strategies may include membrane modifications and system design improvements. Optimization aims to enhance water flux and thermal efficiency.

The given characteristics provide specific insights into the dimensions and operating conditions of the DCMD module, allowing for a better understanding of its configuration and potential performance.

II.8. Conclusion

In conclusion, this chapter has provided a comprehensive overview of Direct Contact Membrane Distillation (DCMD) modeling, covering various aspects of the membrane module, arrangement properties, heat and mass transfer, and polarization phenomena.

Firstly, the chapter discussed the importance of understanding the membrane module in DCMD systems, emphasizing factors such as module design, configuration, and material selection. These considerations are crucial in optimizing the overall performance and efficiency of the DCMD process.

Next, the chapter explored the arrangement properties in DCMD, including the arrangement of membranes, spacers, and flow channels. Proper arrangement is essential to ensure uniform flow distribution, minimize pressure drop, and maximize system heat and mass transfer efficiency.

The chapter then delved into the intricacies of heat and mass transfer in DCMD. It highlighted the significance of temperature gradients, latent heat transfer during evaporation, and the role of driving forces in the process. Understanding these transfer mechanisms is vital for accurately modeling and predicting the performance of DCMD systems.

Lastly, the chapter addressed the phenomenon of temperature polarization, a prevalent challenge in DCMD. Temperature polarization occurs due to the deviation of temperatures at the membrane surface from the bulk temperatures, affecting mass transfer across the membrane. The temperature polarization coefficient (TPC) was introduced as a metric to quantify and evaluate its impact. Mitigating temperature polarization through proper design and operation strategies is crucial for enhancing the efficiency and performance of DCMD systems.

In summary, this chapter has provided insights into the modeling aspects of DCMD, covering the membrane module, arrangement properties, heat and mass transfer, and the significance of addressing temperature polarization. These understandings are fundamental for developing accurate models, optimizing system design, and improving the overall effectiveness of DCMD processes.

Chapter III

Simulation Results and Discussions

III.1 Introduction

Membrane distillation (MD) is a promising thermal membrane technology with the potential for various applications, including seawater desalination. Its operation relies on a hydrophobic membrane to facilitate the transport of water vapor driven by a vapor pressure gradient. However, the efficiency and productivity of MD are impacted by challenges, particularly in water vapor flux. Different approaches have been explored to overcome these challenges and optimize MD performance.

One specific area of focus is the design of industrial-scale modules for seawater desalination using direct contact membrane distillation (DCMD). Achieving optimal pure water productivity requires careful module design, and module simulation has emerged as a valuable tool. The analyses and implementations were carried out using the (MATLAB R2021a) software on a laptop equipped with an Intel Core (TM) i7-7820HQ CPU, 2.90 GHz Processor, and 32 GB of RAM.

Additionally, there is a notable focus on investigating the total cross-membrane flux in membrane distillation to enhance overall process efficiency. The attention has been directed towards studying co-current PVDF flat sheet membranes for direct contact applications, aiming to improve the total cross-membrane flux and address this specific challenge in MD.

Given the ongoing research efforts, this study aims to provide valuable insights and practical guidance for the proper design module in DCMD for seawater desalination. By examining critical design criteria, this chapter seeks to enhance the understanding of module performance and contribute to advancing membrane distillation technologies. Finally, these endeavors will facilitate the development of efficient and sustainable seawater desalination and other relevant applications.

III.2 Contribution 01: Effect of operating parameters on the total cross-membrane flux

This section aims to enhance the total cross-membrane flux for membrane distillation using a co-current PVDF flat sheet direct contact approach. This study analyzed different operational factors that affect the performance of the system. These factors include the temperature of the feed inlet, which ranges from 333.15 K to 358.15 K, as well as the flow rate of the feed side, which varies from 1 kg/s to 2.5 kg/s. Also considered were the temperature of the permeate inlet, ranging from 288.15 K to 313.15 K, and the concentration of NaCl in the feed inlet, which is between 0.035 kg/kg and 0.485 kg/kg.

It should study how different operating parameters affect total cross-membrane flux to achieve the best possible value. In this aim, a MATLAB simulation obtains results for different scenarios, adjusting input parameters and creating curves for analysis through the Trial-and-error approach.

The study found that using a PVDF flat sheet membrane can lead to a significantly higher total cross-membrane flux when the feed input temperature increases. At a feed inlet temperature of 358.15 K, a permeate inlet temperature of 293.15 K, and a flow rate of 2.5 kg/s, the output achieved was 73.2075 kg/ (m^2.h). The feed inlet NaCl concentration used was 0.035 kg/kg. The temperature at which the feed enters significantly affects the total flow through the membrane. Meanwhile, the rate of flow, the temperature of the permeate inlet, and the concentration of NaCl in the feed inlet have a relatively minor effect.

III.2.1 The feed inlet temperature effect

MD stands for an evaporative thermal separation process. The driving force affected by temperature is the difference in vapor partial pressure between the feed and permeate sides. Therefore, the feed inlet temperature is a crucial operational parameter to investigate first.

The thermal-driven separation nature of the MD process has a significant effect on the total cross-membrane flux. The study covered feed inlet temperatures ranging from 313.15 K to 358.15 K with an interval of 278.15 K. The highest temperature was still lower than the feed solution's boiling point. Other factors like the permeate inlet temperature, feed inlet NaCl concentration, and flow rate are kept constant. The temperature of the permeate inlet maintains at 293.15 K, the concentration of NaCl in the feed inlet maintains at 0.035 kg/kg, and the flow rate on both feed and permeate sides adjusts at 2 kg/s. Figure III. 1 displays the cross-membrane flux for various feed inlet temperatures.

When the temperature of the feed inlet increases from 333.15 K to 343.15 K, the total cross-membrane flux increases from 25.6223 kg/ (m^2.h) to 39.5313 kg/ (m^2.h). At lower feed inlet temperatures, the total cross-membrane flux showed slight variation, and There was barely a difference in the total cross-membrane flux. However, at temperatures exceeding 343.15 K, there was a notable difference in flux, with the total cross-membrane flux rising from 39.5313 kg/ (m^2.h) to 68.3627 kg/ (m^2.h).

It observed that the greatest flux generation happens when the temperature is close to boiling and the permeate inlet temperature is low. This finding aligns with previous research on the effect of feed inlet temperature and transmembrane temperature difference on total cross-membrane flux.

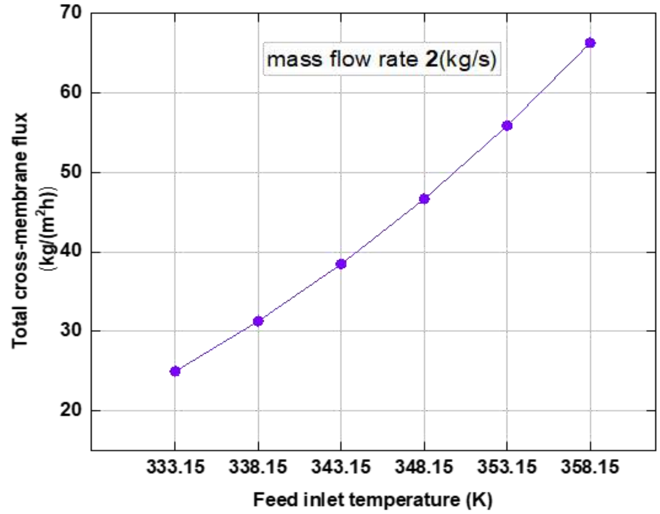


Figure III. 1: Total cross-membrane flux as a function of feed side temperature (Tp_{in} = 293.15 K).

Furthermore, the occurrence of temperature polarization diminishes with feed temperature increase. Consequently, the evaporation temperature becomes similar to the bulk temperature of the feed. This results in a greater flux. As shown by various research in the past [134].

III.2.2 The permeate inlet temperature effect.

The permeate inlet temperature also enhances total cross-membrane flux, while its effect is much smaller than the feed temperature effect. The total cross-membrane flux increased with a lower permeate temperature and a more significant vapor pressure differential. The permeate temperature ranges from 283.15 to 313.15 K in most DCMD experiments. In this particular investigation, the temperature of the permeate inlet varies between 288.15 and 313.15 K. As shown in Figure III. 1, the temperature of the feed inlet ranged from 328.15 K to 358.15 K, with a mean value of 278.15 K when there was a flow rate of 2 kg/s for both the feed and the permeate solutions.

The curves illustrate how the total cross-membrane flux increases as the permeate temperature decreases, with the highest quantities obtained at the most elevated temperatures; consequently, at 353.15 K and 358.15 K, the total cross-membrane flux increases to 61.2473 and 68.7062 kg / (m2.h), respectively, at the lowest permeate inlet temperature.

The highest temperatures allow for producing the most significant quantities. The decrease in the total cross-membrane flux at 288.15 to 313.15 K is due to the reduction of driving force as the temperature difference between the feed and permeate sides decreases. This significant decrease in total cross-membrane flux depends on increased permeate inlet temperature.

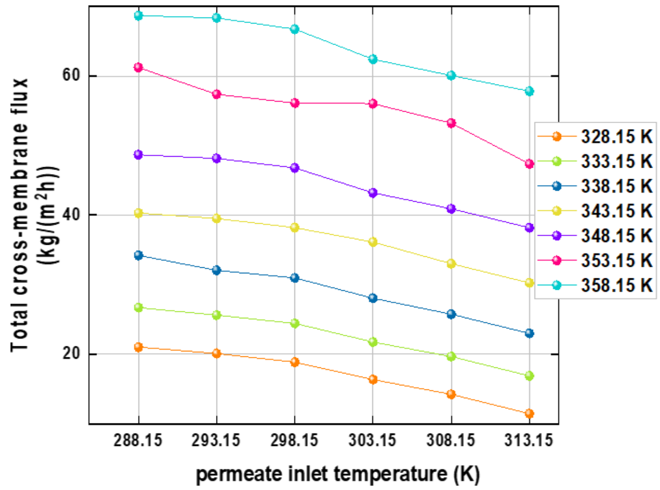


Figure III. 2: Effect of permeate inlet temperature on the total cross-membrane flux at different feed inlet temperatures

Even though the permeate inlet temperature increased, there was not a discernible improvement in the amount of the total cross-membrane flux. The influence of the temperature of the permeate input on the total cross-membrane flux is insignificant when the feed temperatures are held constant. According to Equation (1), at these temperatures, the total cross-membrane flux is solely influenced by the water vapor pressure at the permeate-membrane interface (Ppm) [135]. The Antoine equation varies less as the temperature decreases, as demonstrated by [136].

III.2.3 The feed and permeate flow rate effect.

Hydrodynamic conditions influence total cross-membrane flux. When the hydrodynamic conditions improve, the permeate flux increases. The efficiency of a DCMD system is directly related to the flow rate or the rate at which fluids are flowing through the system. Increasing the flow rates on both sides of the membrane is necessary to counteract the temperature and concentration polarization effects.

The four feed and permeate flow rates across all feed inlet temperature conditions varied from 1.0 kg/s to 2.5 kg/s, with a 0.5 kg/s difference between the lowest and highest values. The total cross-membrane flux increases as feed-side temperatures rise at a constant flow rate. As shown in Figure III. 3, increasing the flow rate significantly improves the total cross-membrane flux.

When feed inlet temperatures were low, the effect of increasing the feed flow rate was relatively negligible. It depends on the feed side cell, which may not be perfectly flat [137]. There is little change over the feed temperature range of (333.15K-343.15K) for flow rates of 1, 1.5, and 2 kg/s.

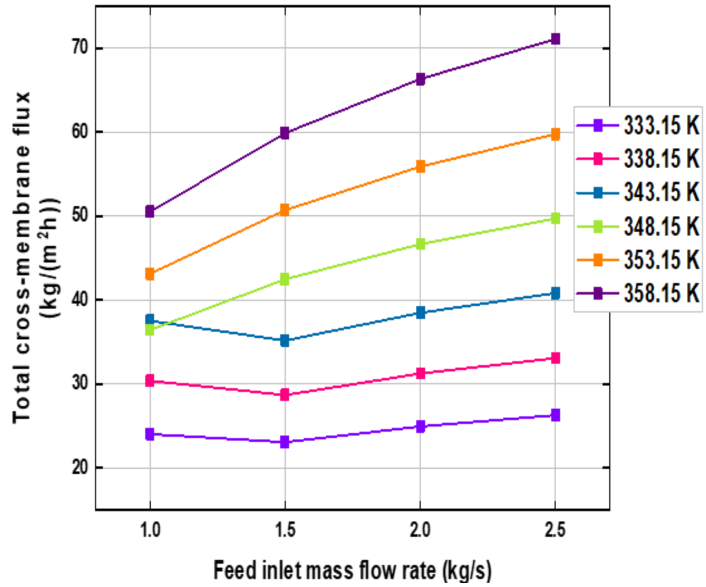


Figure III. 3 Total cross-membrane flux as a function of feed and permeate side flow rate at different feed inlet temperatures (Tpi_n = 293.15 K)

Further, while simulating a flow rate of 2.5 kg/s over a temperature range of (333.15-358.15 K), the highest levels of water vapor are acquired at temperatures of 348.15, 353.15, and 358.15 K, with corresponding total cross-membrane flux values of 50.4980, 61.1611, and 73.2075 kg/(m^2. h), respectively. The flux values improve with higher feed input temperatures and flow rates. As vapor molecules move from the feed side to the permeate side, they lower the membrane surface temperature to a lower temperature than the feed bulk temperature. This phenomenon is known as temperature polarization, and it causes a boundary layer to form close to the membrane surface. As the flow rate increases, the thermal boundary layer thins, weakening its effect [138].

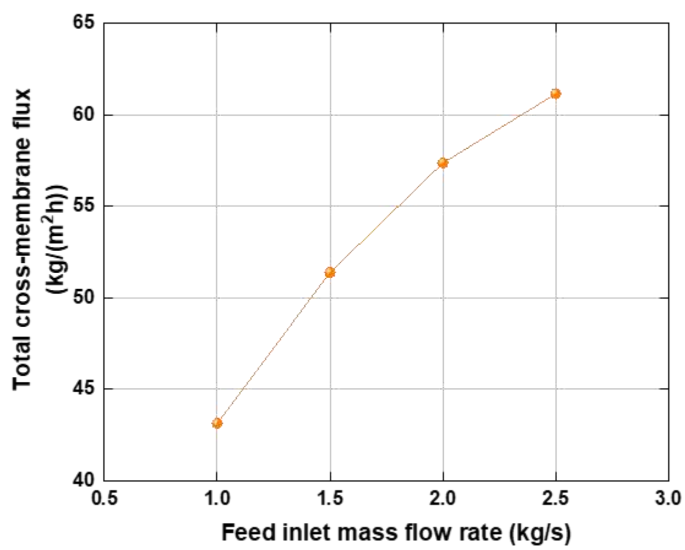


Figure III. 4: Overall effect of flow rate variation on the total cross-membrane flux

According to findings presented in Figure III.4, high flow rates increase the flux amount. This behavior pattern explains that the thermal boundary layer becomes thinner when the circulation rate is faster. As a result, heat transfer from the bulk to the membrane surface enhances increasing flux.

III.2.4 The feed inlet NaCl concentration effect

This investigation will analyze the total cross-membrane flux and the vapor pressure differential that drives the process to create the flux as a function of feed input NaCl concentration. The feed inlet NaCl concentrations ranged from 0.035 to 0.285 kg/kg, used to conduct the tests. Throughout the study, all other parameters maintain constants, including a flow rate of 2 kg/s, an input temperature of 358.15 K on the feed side, and an inlet temperature of 293.15 K on the permeate side.

Since the flux in membrane distillation is a function of feed temperature and concentration, the total cross-membrane flux and the pressure vapor difference are affected by the NaCl concentrations at the feed inlet. So, there is a dramatic reduction in the total cross-membrane flux product with increasing NaCl concentration in the feed inlet. The simultaneous drop in vapor pressure difference [136] may be the leading cause. Also, there is a continual change in concentration as the solvent moves from the feed side to the permeate side, which affects the vapor pressure and thermal conductivity on the feed side. This behavior demonstrated the link between low vapor pressure on the feed side and a reduced partial pressure gradient across the membrane (reduced driving force) [139].

Figure III. 5 shows that the total cross-membrane flux decreased when feed inlet concentration increased on the feed side. An increase in NaCl concentration from 0.035 to 0.335 kg/kg resulted in a 31.98 % drop in total cross-membrane flux, from 68.3627 to 46.5031 kg/ (m^2.h) and a 13.59 % drop in vapor pressure differential, from 11.33 to 9.79 kPa. Raising the vapor pressure differential affects the total cross-membrane flux less than raising the feed inlet NaCl concentration.

Furthermore, a continual change in concentration as the solvent moves from the feed side to the permeate side effects the vapor pressure and thermal conductivity on the feed side. This behavior demonstrated the link between low vapor pressure on the feed side and a reduced partial pressure gradient across the membrane (a reduced driving force) [139].

The decrease in flux is the result of three phenomena: first, temperature polarization [140], which is represented by layers formed on both sides of the membrane; second, concentration polarization increased due to the accumulated salt molecules on the membrane surface, which blocked the vapor from moving and resulted in resistance to mass transfer; and third, the membrane pore was

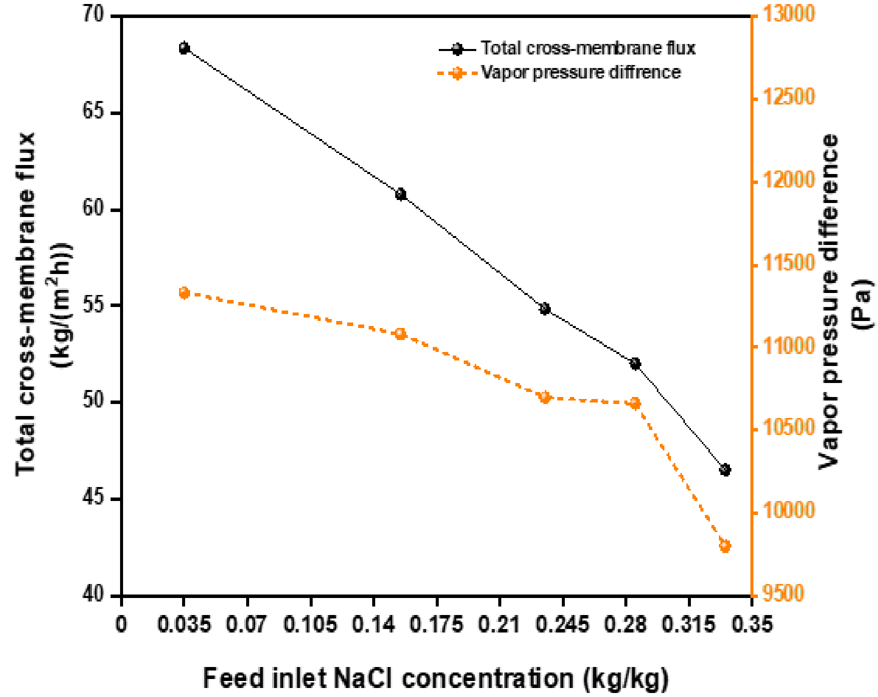


Figure III. 5: Effect of NaCl concentration on flux and vapor pressure difference (feed inlet temperature of 358.15 K, permeate inlet temperature of 293.15 K, and flow rate of 2 kg/s)

clogged, and the risk of scaling the membrane surface increased [140].

Second, the accumulation of salt molecules on the membrane surface forms the concentration polarization and impedes vapor movement, resulting in mass transfer resistance. This aids in the wetting of membrane pores [110].

Third, fouling decreases evaporation by partially wetting the membrane and allowing salt molecules to enter some membrane pores [141, 142]. The generation and quality of cross-membrane flux diminish due to these variables. Identical findings have been found by [110, 136, 139, 140, 141, 142, 143]. It is crucial to understand that if the temperature of the feed membrane surface is similar to the temperature of the feed bulk, the effect of temperature and concentration polarization in the MD process will be minimized [144].

Furthermore, the study analyzed how the NaCl concentration with temperatures varying from 343.15 to 358.15 K in 278.15 K increments at the feed inlet affects the total cross-membrane flux. The permeate inlet temperature remained at 293.15K, and the flow rate at the feed and permeate sides remained steady at two kg/s. In contrast, this feed NaCl concentrations varied between 0, 0.035, 0.085, and 0.185 kg/kg. Figure III. 6 shows the obtained results. The feed inlet NaCl concentrations increase from 0 to 0.285 kg/kg. At 358.15 K, the total cross-membrane flux decreased by 30.17 %, from 74.4823 to 52.0099 kg/ (m^2.h).

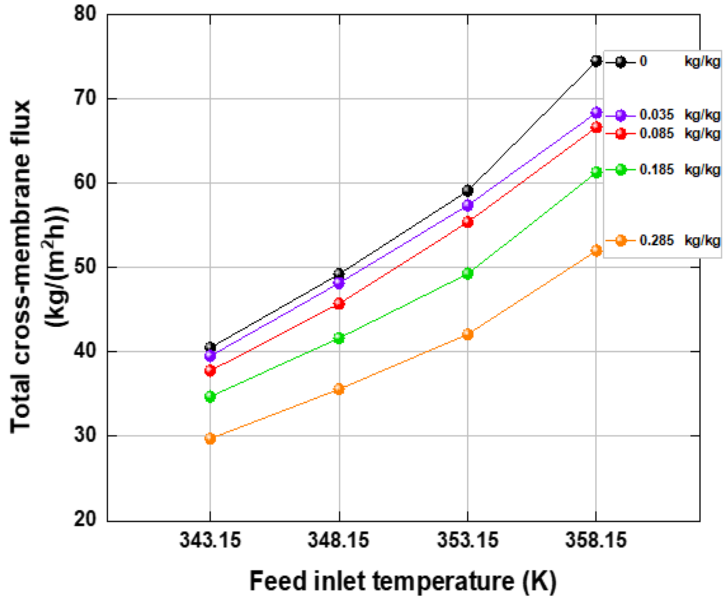


Figure III. 6: The effect of feed inlet NaCl concentration on total cross-membrane flux was predicted versus different feed inlet temperatures at a permeate inlet temperature of 293.15 K and a flow rate of 2 kg/s.

There is a direct correlation between the concentration of NaCl in the feed inlet and the steep drop-in water activity [145, 146]. This reduction occurs because a higher concentration of NaCl in the water makes the membranes less conductive[110]. Figure III. 7 illustrates the results.

Figure III. 8 depicts the occurrence of the reverse flux phenomenon. This phenomenon arises when the temperature difference fails to reach the threshold for producing a positive water flux.

Consequently, the pressure difference across the membrane decreases, owing to the concentrated salt that reduces the vapor pressure on the feed side. So, the driving force in the reverse direction increases due to the exponential relationship between water vapor pressure and temperature, resulting in the permeate vapor pressure rising faster than the feed side.

When the concentration of NaCl in the feed inlet increases, it impedes the evaporation process. Additionally, salt buildup on the membrane surface causes the pores to become wet, leading to faster membrane degradation when the water activity decreases [116].

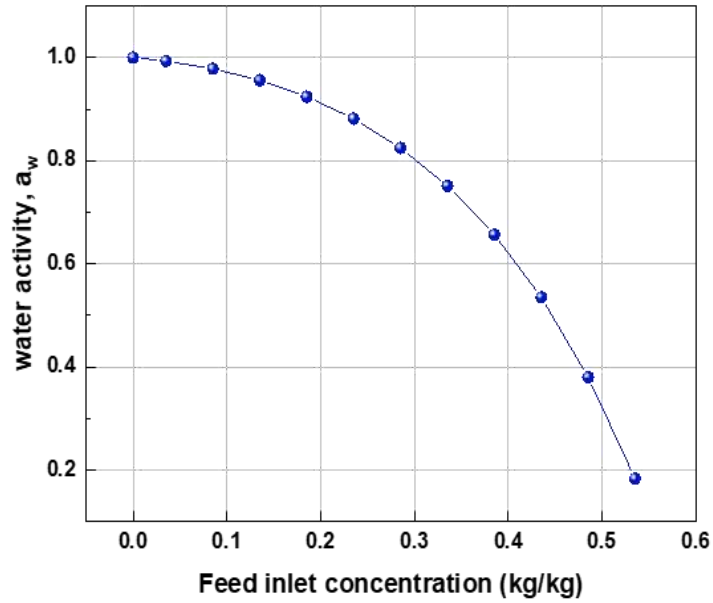


Figure III. 7: Water activity predicted different feed inlet NaCl concentrations at a feed inlet temperature of 358.15 K, permeate inlet temperature of 293.15 K, and flow rate of 2 kg/s.

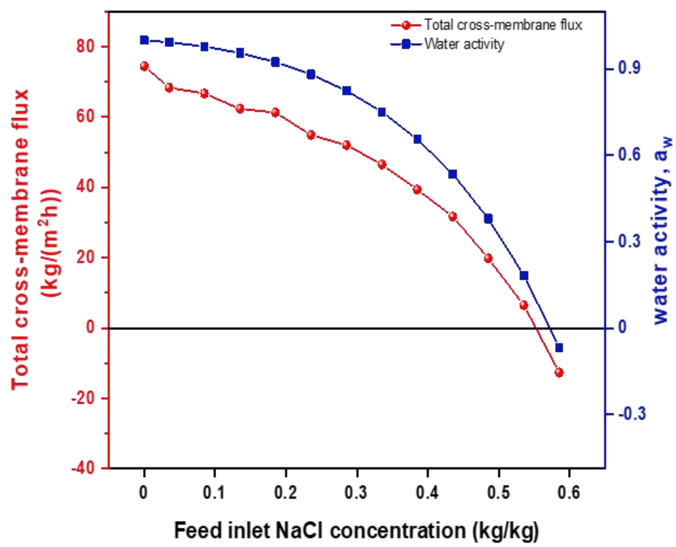


Figure III. 8: Effect of water activity on total cross-membrane flux vs. varied feed inlet NaCl concentrations at 358.15 K feed inlet, 293.15 K permeate inlet, and two kg/s flow rate.

The term membrane wetting describes the process of fluids penetrating the membrane. One of the crucial characteristics used to characterize the hydrophobicity of a membrane is the liquid entry pressure (LEP), which must be considered to prevent the membrane's hydrophobic pores from becoming wet. The LEP specifies the feed-side hydrostatic pressure critical value. This pressure is the lowest possible for membrane wetting [116]. The liquid entry pressure is established by the liquid-membrane contact angle, the pore's appropriate size, and shape to achieve a higher adequate LEP.

III.3. Comparison of operating conditions on MD performance: Feed temperature, flow rate, permeate temperature, and NaCl concentration

This comparison will investigate whether each operating parameter influences the permeate flux with another. Then, set who has the best effectiveness. Begin by comparing the feed inlet temperature with the permeate inlet temperature at a flow rate of 2 kg/s on both sides (see Figure III. 9).

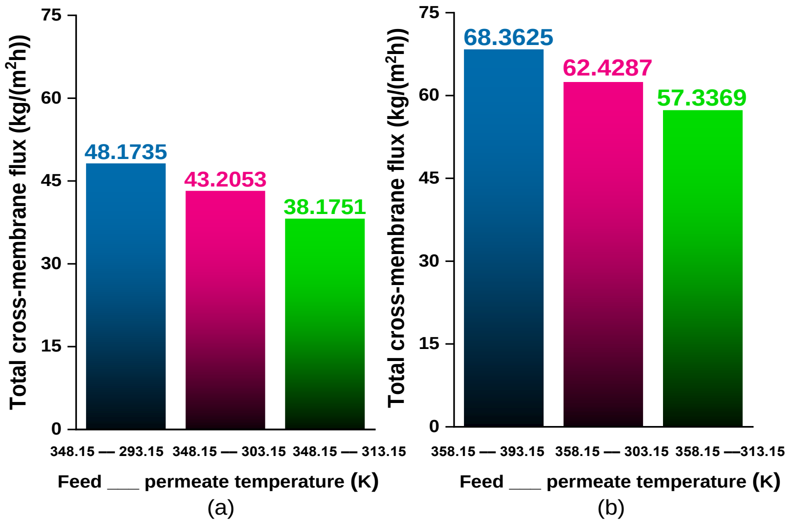


Figure III. 9: Overall fluxes at various temperature combinations ((a) Tfin = 348.15 K, (b) Tfin = 358.15 K) for a co-current PVDF flat sheet DCMD system with a feed and permeate flow rate of 2 kg/s

Based on these results, the total cross-membrane flux decreases as the temperature of the permeate increases, assuming the feed temperature remains constant. Figure III. 9 (a) shows a reduction of 20.75% in the total cross-membrane flux at a temperature of 348.15 K. On the other hand, Figure III. 9 (b) shows a reduction of 16.13% at a temperature of 358.15 K. In turn, it showed that the feed inlet with the highest temperature and the permeate inlet with the lowest temperature yielded the most significant amounts for the total cross-membrane flux.

Figure III. 10 provides an additional illustration, demonstrating that the effect of feeding temperature is more significant than that of permeation temperature when considering the same temperature difference (ΔT = 318.15 K). Specifically, in Figure III.10(a), the flux observed within the temperature range of (348.15–303.15 K) is compared to the flux observed at the temperature range of (358.15–313.15 K). The feed temperature effect is more significant, madding this notable disparity in water vapor pressure difference at elevated feed temperatures due to an exponential relation between pressure and temperature. Figure III.10 (b) shows a similar observation about another temperature difference (ΔT = 328.15 K).

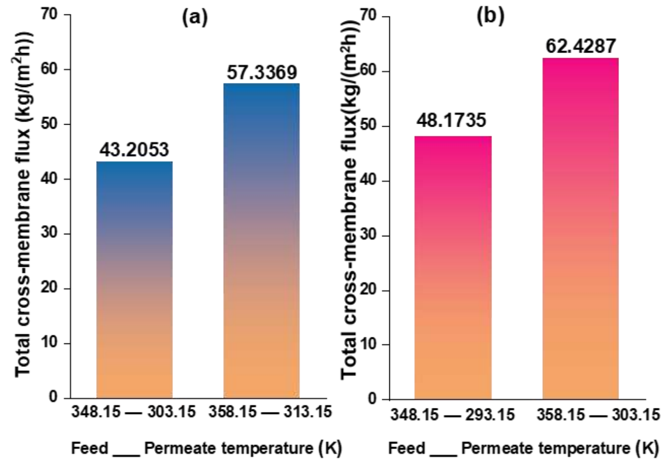


Figure III. 10: Overall fluxes at different temperature differences ((a) ΔT = 318.15 K, (b) ΔT = 328.15 K) for a co-current PVDF flat sheet DCMD system with a flow rate of 2 kg/s for the feed and permeate sides.

Figure III. 11 illustrates the effect of flow rate on the total cross-membrane flux under specific conditions, namely a feed inlet temperature of 358.15 K and permeate inlet temperature of 293.15 K.

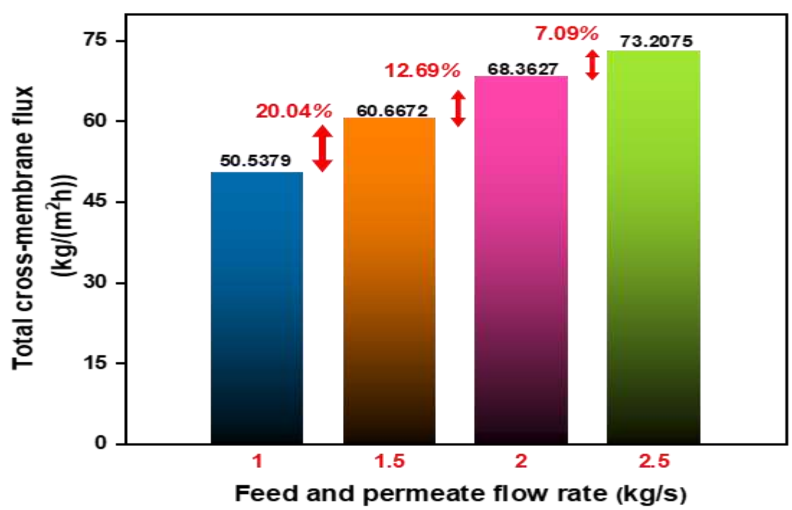


Figure III. 11: Effect of flow rates on total cross-membrane flux in a co-current PVDF flat sheet DCMD system with feed and permeate inlet temperatures of 358.15 K and 293.15 K, respectively.

The total cross-membrane flux observes an increase of 20.04% when the flow rate rises from 1 to 1.5 kg/s. Similarly, there is a 12.69% increase in flux between flow rates of 1.5 and 2 kg/s and a 7.09% increase between flow rates of 2 and 2.5 kg/s. Nevertheless, despite an increase in flow rate, the ratio of the change in total cross-membrane flux decreases from 12.69% to 7.09%. The effect of flow rate on the total cross-membrane flux to the feed temperature has a less critical effect.

Lastly, it is crucial to compare the effect of feed temperature and NaCl concentration, as shown in Figure III. 12. When comparing the two scenarios, the total cross-membrane flux can observe a significant increase of 64.08% when the feed temperature rises. The feed NaCl concentration is less effective than the feed temperature despite the increase in the total cross-membrane flux when the NaCl concentration decreases.

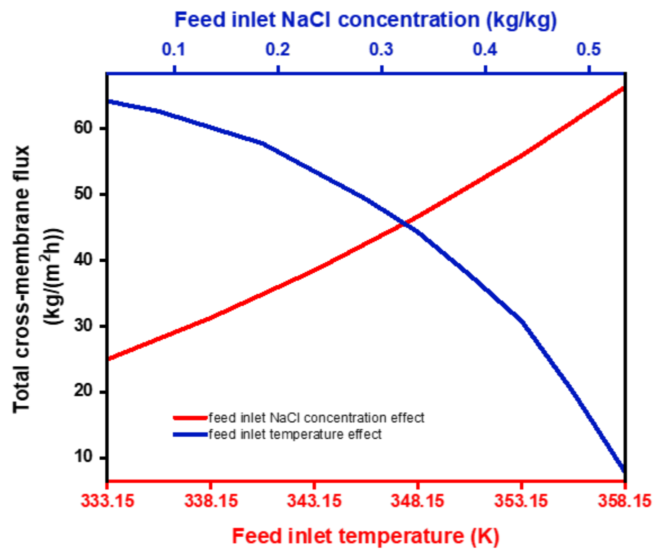
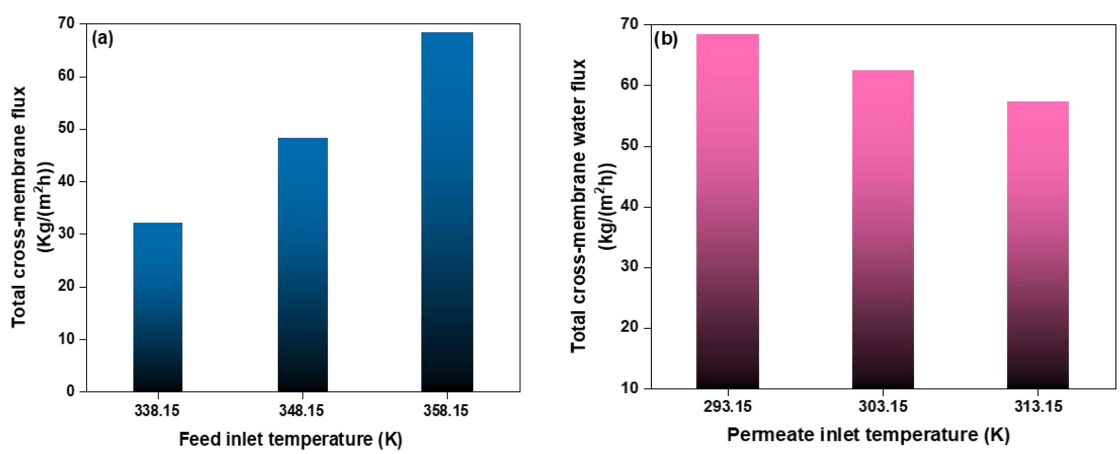


Figure III. 12: The feed inlet NaCl concentration effect vs. the feed inlet temperature on the total cross-membrane flux.

After analyzing and comparing the data, the results showed that the temperature at which the feed enters significantly affects the total cross-membrane flux, as depicted in Figure III. 13. The results attributed to the exponential rise in vapor pressure with increasing temperature, resulting in a more noticeable enhancement in total cross-membrane flux at higher temperatures.



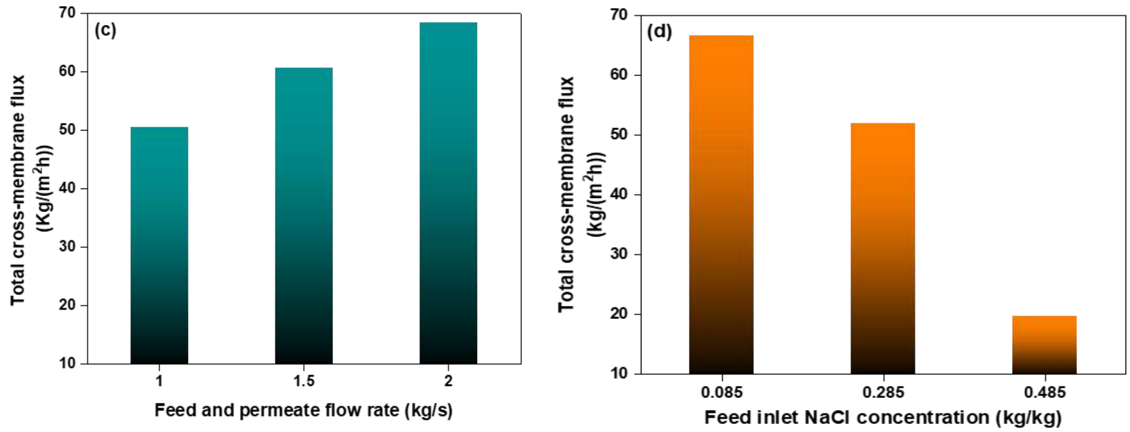


Figure III. 13: Comparison of main effects of operating parameters on the total cross-membrane flux: (a) feed inlet temperature, (b) permeate inlet temperature, (c) feed and permeate flow rate, and (d) feed inlet NaCl concentration.

III-4 Contribution 02: Optimization in DCMD performance

III.4.1. Results and discussions of the BO and PSO optimization on the DCMD module

The results and discussion of employing Bonobo optimization in a DCMD system are presented in this section. The Bonobo optimization algorithm was utilized to optimize the performance of the DCMD system by improving the permeate flux and the thermal efficiency.

The optimization process is attained using the Bonobo optimizer. The optimizer's parameters, fitness function, and cost function are included in Table III.1 below.

Table III.1 Input settings of the optimization algorithm and DCMD parameters

The Optimization method: BO / PSO optimizer				
Parameter		**Value**		
Iterations/population		**100 / 100**		
Used fitness function 'F': RMSE		**F_1 = sqrt (mean ((Error) .^2)); F_2 = sqrt (mean ((Error) .^2))**		
Used Cost function 'Cost'		**Cost 1 = RMSE(F1) * w_1 ; Cost 2 = RMSE(F2) * w_2**		
Number of parameters to optimize		**4**		
Optimization approach		**Single Objective | Multi-objective**		
Bounds of chosen DCMD parameters to optimize				
Parameters	**symbol**	**units**	**Lower bound**	**Upper bound**
Feed inlet temperature	**Tfi**	**K**	**333.15**	**353.15**
Feed flow rate	**q_f**	**kg/s**	**0.5**	**1.5**
Thickness	**δ**	**μm**	**60**	**120**
Height	**H**	**mm**	**1.5**	**2.5**

The optimization process aims to optimize the 04 selected DCMD parameters within their predetermined limits to enhance the overall DCMD performance, focusing on 02 cost functions: Permeate flux and Thermal efficiency. The whole optimization process of the DCMD system is attained as viewed in Figure III.14. The optimization organigramme shown in Figure II.4 illustrates the applied optimization cases using single and multi-objective approaches, besides highlighting the effects of each DCMD parameter on its overall performance. The discussion will be divided into:

III.4.1.1 Single-objective optimization using BO (parameter by parameter)

Figure III. 15 below displays the optimized parameters of the DCMD, along with the optimal computed values of the DCMD outputs in terms of Water flux, Thermal efficiency, and TPC.

Table III.2 Single-objective optimization using BO

Cases	Flux 1 (Kg.m^2.h)	Thermal efficiency 1	TPC 1	Flux 2 (Kg.m^2.h)	Thermal efficiency 2	TPC 2	Flux Basic	Thermal efficiency Basic	TPC Basic
T_{fi}	45.9427	0.63128	0.62608	42.7739	0.64271	0.56448	36.6548	0.6243	0.6424
q_f	41.4299	0.61564	0.6357	15.5729	0.48922	0.41267			
δ	39.2741	0.97921	0.78088	39.2741	0.97921	0.78088			
H	56.8765	0.62695	0.84854	56.8765	0.62695	0.84854			
	Single objective optimization using **Flux** as the cost function			Single objective optimization using **Thermal Efficiency** as the cost function			**Basic case**		

Optimization Criteria:

a. **Single Objective Optimization using Flux as the Cost Function**:

- **Flux 1**: This criterion represents the flux value obtained under single objective optimization with Flux as the cost function. It is evaluated for Cases 1, 2, 3, and 4. The corresponding values are 45.9427, 41.4299, 39.2741, and 56.8765 kg/m^2.h, respectively.
- **Thermal Efficiency 1**: This criterion indicates the thermal Efficiency achieved under single objective optimization using Flux as the cost function. Cases 1, 2, 3, and 4 values are 0.63128, 0.61564, 0.97921, and 0.62695, respectively.

- **TPC 1**: TPC 1 represents the total power consumption obtained under single objective optimization with Flux as the cost function. Cases 1, 2, 3, and 4 values are 0.62608, 0.6357, 0.78088, and 0.84854, respectively.

b. Single Objective Optimization using Thermal Efficiency as the Cost Function:

- **Flux 2**: This criterion represents the flux value achieved under single objective optimization with Thermal Efficiency as the cost function. It is evaluated for the four Cases. The corresponding values are 42.7739, 15.5729, 39.2741, and 56.8765, respectively.
- **Thermal Efficiency 2**: This criterion indicates the thermal Efficiency obtained under single objective optimization using Thermal Efficiency as the cost function. The values for 4 Cases are 0.64271, 0.48922, 0.97921, and 0.62695, respectively.
- **TPC 2**: TPC 2 represents the total power consumption obtained under single objective optimization with Thermal Efficiency as the cost function. The values for 4 Cases are 0.56448, 0.41267, 0.78088, and 0.84854, respectively.

c. Regular Operation Mode without Optimization (Basic):

- **Flux Basic**: This criterion represents the flux value obtained under regular operation mode without optimization. The value is 36.6548 $kg/m^2.h$.
- **Thermal Efficiency Basic**: This criterion indicates the thermal Efficiency achieved under regular operation mode without optimization. The value is 0.6243.
- **TPC Basic**: TPC Basic represents the total power consumption under regular operation mode without optimization. The value is 0.6424.

Table III.3 The BO Optimization Process and Optimal Parameters

Optimal parameters	case 1	case 2	case 3	case 4	case 5	case 6	case 7	case 8
T_{FI}	**352.7488**	basic	basic	basic	**352.748**	basic	basic	basic
q_f	basic	**1.0159**	basic	basic	basic	**0.029983**	basic	basic
δ	basic	basic	**0.03**	basic	basic	basic	**0.03**	basic
H	basic	basic	basic	**0.0015278**	basic	basic	basic	**0.0015278**
Optimization cases	Single objective optimization using **Flux** as the cost function				Single objective optimization using **Thermal Efficiency** as the cost function			

1. The optimization process used the Bonobo optimizer to tune the optimal parameters for the DCMD process. The optimal values of the parameters are provided for specific cases:

- Cases 1, 2, 3, and 4 represent **single** objective optimization using **Flux** as the cost function. The optimal parameters are as follows:
- Optimal Feed Inlet Temperature (K) (T_{FI}): The values are 352.7488, basic, basic, and basic for Cases 1, 2, 3, and 4, respectively.
- Optimal Feed Inlet Mass Flow Rate (kg/s) (q_f): The values are basic, 1.0159, basic, and basic for Cases 1, 2, 3, and 4, respectively.
- Optimal Membrane Thickness (mm) (δ): The values are basic, basic, 0.03, and basic for Cases 1, 2, 3, and 4, respectively.
- Optimal Feed Channel Height (mm) (H): The values are basic, basic, basic, and 0.0015278 for Cases 1, 2, 3, and 4, respectively.
- Cases 5, 6, 7, and 8 represent **single** objective optimization using **Thermal Efficiency** as the cost function. The optimal parameters are as follows:
- Optimal Feed Inlet Temperature (K) (T_{FI}): The values are 352.748, basic, basic, and basic for Cases 5, 6, 7, and 8, respectively.
- Optimal Feed Inlet Mass Flow Rate (kg/s) (q_f): The values are basic, 0.029983, basic, and basic for Cases 5, 6, 7, and 8, respectively.
- Optimal Membrane Thickness (mm) (δ): The values are basic, basic, basic, and 0.03 for Cases 5, 6, 7, and 8, respectively.
- Optimal Feed Channel Height (mm) (H): The values are basic, basic, basic, and 0.0015278 for Cases 5, 6, 7, and 8, respectively.

2. Based on the analyses of the provided data, we can draw the following main conclusions:

Optimization Criteria:

- Flux-based optimization: When Flux is used as the cost function for optimization, the following results are observed:
- Cases 1, 2, 3, and 4 achieve higher flux values than the basic operation mode. The flux values for these cases are 45.9427, 41.4299, 39.2741, and 56.8765 kg/m^2.h, respectively.

- The thermal efficiencies for these cases are 0.63128, 0.61564, 0.97921, and 0.62695, respectively.
- These cases' (TPC) values are 0.62608, 0.6357, 0.78088, and 0.84854, respectively.

➢ Thermal Efficiency-based optimization: When Thermal Efficiency is used as the cost function for optimization, the following results are observed:

- Cases 5, 6, 7, and 8 achieve higher thermal efficiencies than the basic operation mode. The thermal efficiencies for these cases are 0.64271, 0.48922, 0.97921, and 0.62695, respectively.
- The flux values for these cases are 42.7739, 15.5729, 39.2741, and 56.8765 kg/m^2.h, respectively.
- These cases' (TPC) values are 0.56448, 0.41267, 0.78088, and 0.84854, respectively.

3. Bonobo Optimizer and Optimal Parameters:

The Bonobo optimizer was used to tune the optimal parameters for the DCMD process. The basic values of the 4 DCMD's parameters are (Basic T_{FI} = 80+273.15 (K), Basic q_f = 1 (kg/s), Basic δ = 0.00012 (m), and Basic H = 0.005 (m)), while optimal parameter values for different cases are as follows:

➢ Cases 1, 2, 3, and 4 (Flux optimization):

- Optimal Feed Inlet Temperature (T_{FI}): 352.7488 (K).
- Optimal Feed Inlet Mass Flow Rate (q_f): the basic value 1 (kg/s).
- Optimal Membrane Thickness (δ): the basic value 0.00012 (m).
- Optimal Feed Channel Height (H): the basic value is 0.005 (m).

➢ Cases 5, 6, 7, and 8 (Thermal Efficiency optimization):

- Optimal Feed Inlet Temperature (T_{FI}): 352.748 (K).
- Optimal Feed Inlet Mass Flow Rate (q_f): the basic value is 1 (kg/s).
- Optimal Membrane Thickness (δ): The basic value is 0.00012 (m).
- Optimal Feed Channel Height (H): the basic value is 0.005 (m).

In summary, the provided data includes comparative analyses of the optimization criteria for the DCMD process using the Bonobo optimizer. It involves two different cost functions (Flux and

Thermal Efficiency) for single objective optimization. The optimization process resulted in different values for Flux, thermal Efficiency, and temperature polarization coefficient (TPC) based on the chosen cost function. Additionally, Table III.3 presents the optimal parameters for different cases, indicating the values of feed-inlet temperature, feed-inlet mass flow rate, membrane thickness, and feed channel height under optimization for both Flux and thermal efficiency objectives.

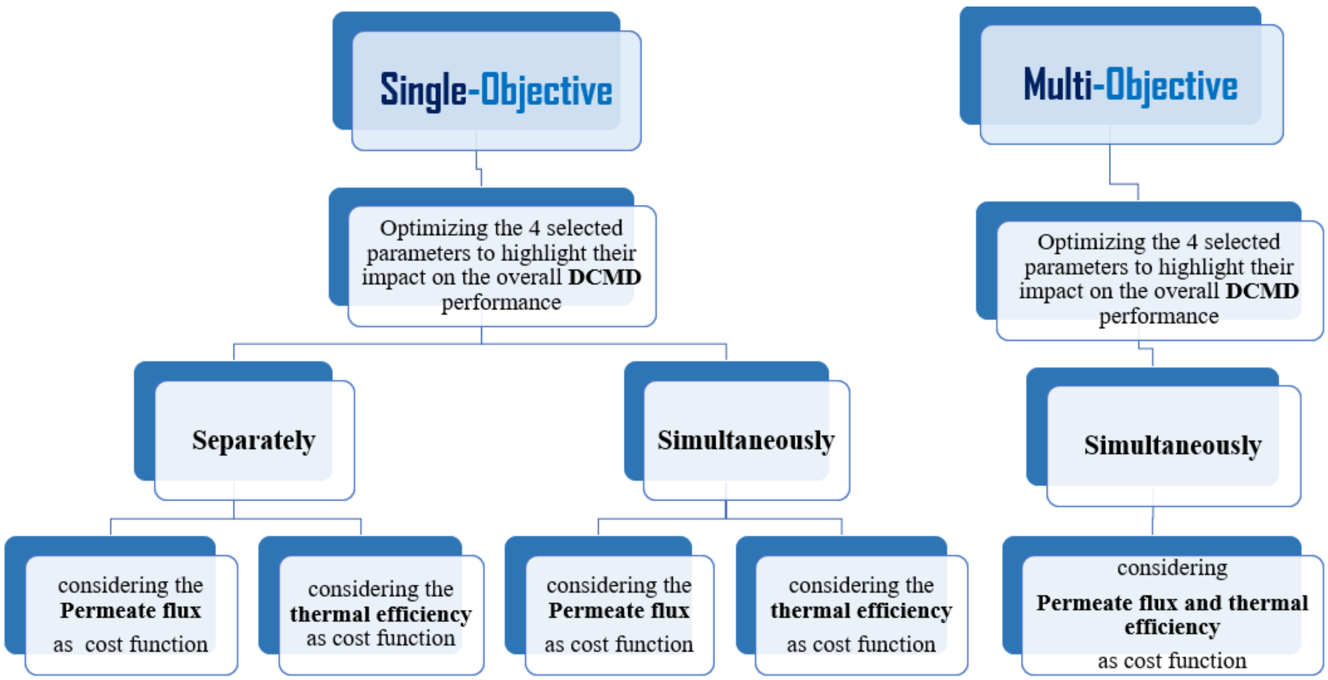


Figure III. 14: The optimization process of the DCMD process under study

In figure III.15, the eight optimization scenarios revealed varying performance based on the evaluated outputs when tuning the four selected parameters. The main conclusions are as follows:

1- Water Flux parameter:

- The maximum water flux (J_w) was achieved with the height (H) variable, using the flux as a cost function.

- The minimum water flux (J_w) was achieved with the feed flow rate (q_f) variable, using the thermal efficiency as a cost function.

2- Thermal efficiency parameter:

- The maximum thermal efficiency (Th_eff) was achieved with the thickness (δ) variable, using the flux as a cost function.

- The minimum thermal efficiency (Th_eff) was achieved with the feed flow rate (q_f) variable using the thermal efficiency cost function.

3- TPC parameter:

- The maximum temperature polarization coefficient (TPC) was achieved with the height (H) variable, using the Flux as a cost function.
- The minimum temperature polarization coefficient (TPC) was achieved with the feed flow rate (q_f) variable, using the thermal efficiency as a cost function.

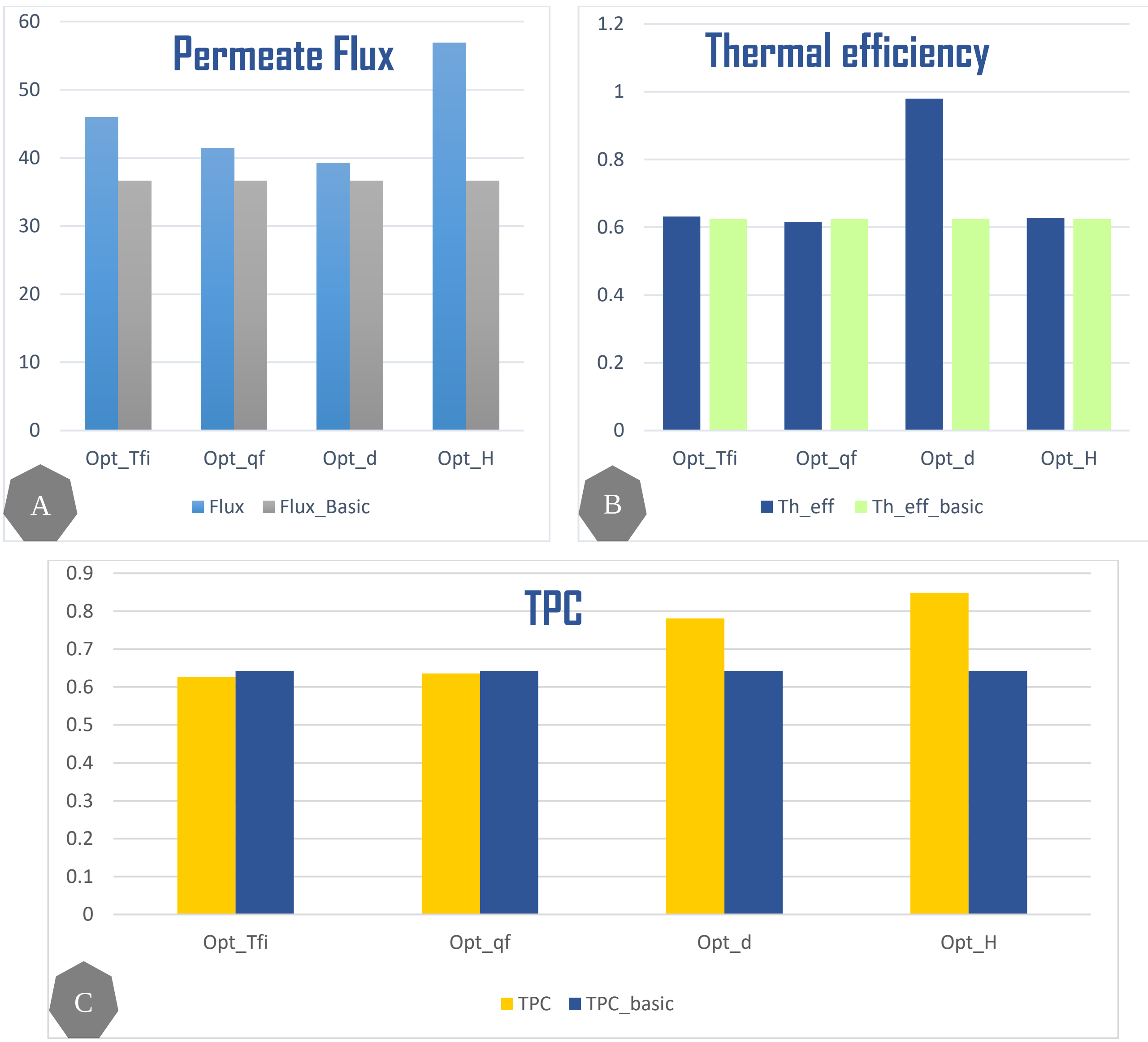


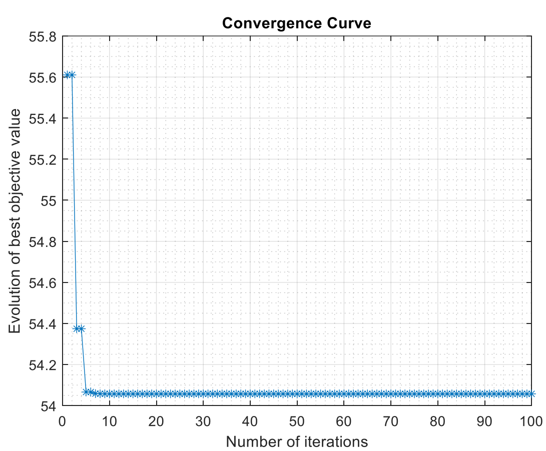
Figure III. 15: Obtained optimized parameters of the DCMD with its outputs.

Based on these observations, it can be concluded that the height (H) variable is associated with achieving higher water flux and TPC values, while the feed flow rate (q_f) variable tends to result in lower water flux and thermal efficiency values.

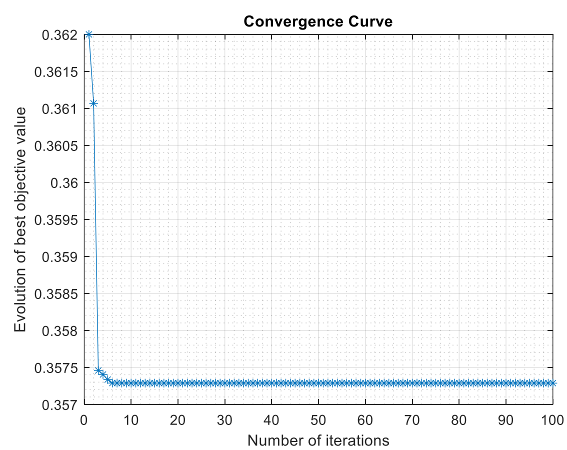
The thickness (δ) variable is linked to higher thermal efficiency values. These findings provide insights into the impact of the selected parameters on the performance of the DCMD system. Figure III. 16 shows the convergence curves versus the best objective values of the optimized parameters during the eight optimization scenarios. In cases (1,3,5,7), the objective or the cost function is the flux, whereas in cases (2,4,6,8) is thermal efficiency.

As seen, the optimal obtained values of the 04 DCMD parameters were attained using the Bonobo optimizer, representing the end values of each given curve above. These curves vary in convergence speed and global minima of selected parameter errors.

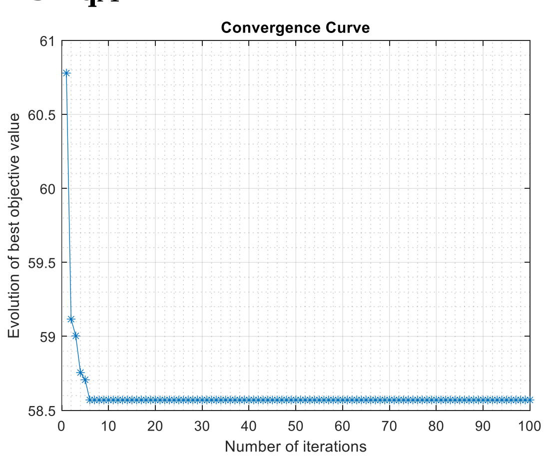
1- $T_{Fi\,1}$



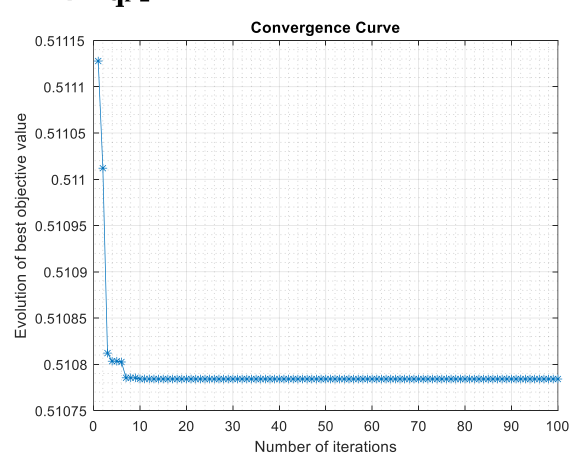
2- T_{Fi2}



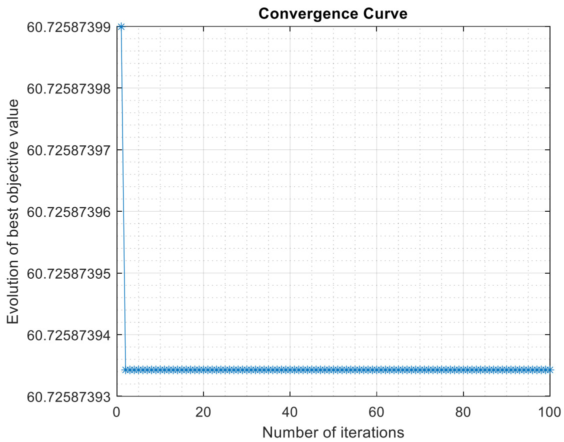
3- $q_{f\,1}$



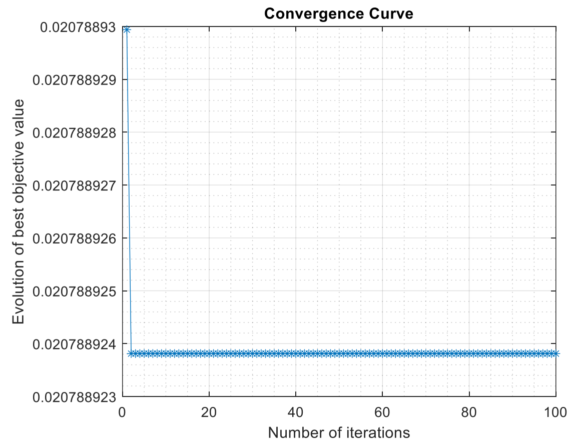
4- $q_{f\,2}$



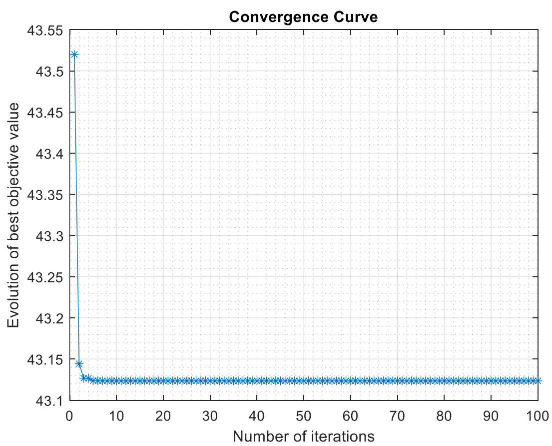
5- δ_1



6- δ_2



7- H_1



8- H_2

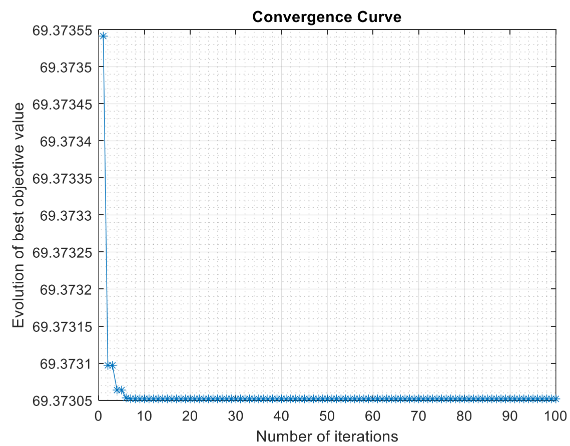


Figure III. 16:Convergence curves versus best objective values of the optimized parameters.

The Bonobo optimizer's fast convergence speed and ability to minimize parameter errors are valuable advantages in optimization tasks. These features contribute to efficient optimization processes and help in achieving highly accurate parameter settings, resulting in improved system performance and desired outcomes.

The next step involves the simultaneous optimization of all four DCMD parameters using a single objective and multi-objective optimization approach besides the BO and PSO optimizers. This step aims to enhance the already obtained values of the DCMD outputs (Flux, Thermal efficiency, and TPC) to enhance the overall performance of the DCMD system.

III.4.1.2 Single vs. multi-objective optimization using BO and PSO (all parameters)

PSO Optimizer:

- The highest Flux achieved by the PSO optimizer is 87.8313 kg/m^{2}h.
- The highest thermal Efficiency achieved by the PSO optimizer is 0.68463.
- The highest combined objective value (Flux + Thermal Efficiency) the PSO optimizer achieves is 0.82843.

BONOBO Optimizer:

- The highest Flux achieved by the BO optimizer is 87.8313 kg/m^2.h, the same as the PSO optimizer.
- The highest thermal Efficiency achieved by the BO optimizer is 0.68463, the same as the PSO optimizer.
- The highest TPC value (Flux + Thermal Efficiency) achieved by the BO optimizer is 0.82843, the same as the PSO optimizer.

a) Comparison of T_{Fi}, q_f, δ, and H:

- T_{FI} remains constant at 354.15 K for both PSO and BO optimizers.
- Q_f also remains constant at 0.9345157 kg/s for both optimizers.
- δ remains constant at 0.000100386 m for both optimizers.
- H remains constant at 0.0015 m for both optimizers.

Conclusion: The DCMD performance has not been highly affected by the T_{FI}, q_f, δ, and H values, indicating that the optimizers are not manipulating these parameters.

b) Comparison of Flux:

- The highest Flux achieved by both optimizers is 87.8313 kg/m^2.h.
- The lowest Flux achieved by both optimizers is 85.4195 kg/m^2.h..

Conclusion: The range of flux values achieved by both optimizers is relatively small, suggesting that the optimization process has a limited impact on the Flux.

c) **Comparison of Thermal Efficiency (Th_eff):**

- The highest thermal Efficiency achieved by both optimizers is 0.68463.
- The lowest thermal Efficiency achieved by the PSO optimizer is 0.65433.
- The lowest thermal Efficiency achieved by the BONOBO optimizer is 0.65518.

Conclusion: The thermal efficiency values achieved by both optimizers are similar, with a slight variation in the lowest values. However, the difference between the highest and lowest thermal efficiency values is relatively small, indicating a relatively stable system performance.

d) **Comparison of Temperature Polarization Coefficient (TPC):**

- The highest TPC value achieved by both optimizers is 0.82843.
- The lowest TPC value achieved by the PSO optimizer is 0.8158.
- The lowest TPC value achieved by the BO optimizer is 0.81596.

Conclusion: Both optimizers' temperature polarization coefficient values are similar, with a slight variation in the lowest values. However, the difference between the highest and lowest TPC values is relatively small, indicating a relatively stable system performance.

Overall, the analysis suggests that the PSO and BO optimizers perform comparably in achieving similar flux, thermal efficiency, and TPC values. The system appears to be relatively stable, and there is no significant difference between the two optimization processes. However, further analysis and comparison with other optimization methods or additional data may provide a more comprehensive understanding of the system's behavior and the effectiveness of the optimizers.

In the end, the analyses discussed above of the obtained results from the DCMD system revealed the rate of improvement of the studied DCMD system, as can be observed in the water flux, thermal efficiency, and, thus, the temperature polarization coefficient. Table III.4 below resumes and summarizes the main obtained results and supports the discussions above to highlight the impact of the optimization and their contributions to enhance the system operation at various conditions.

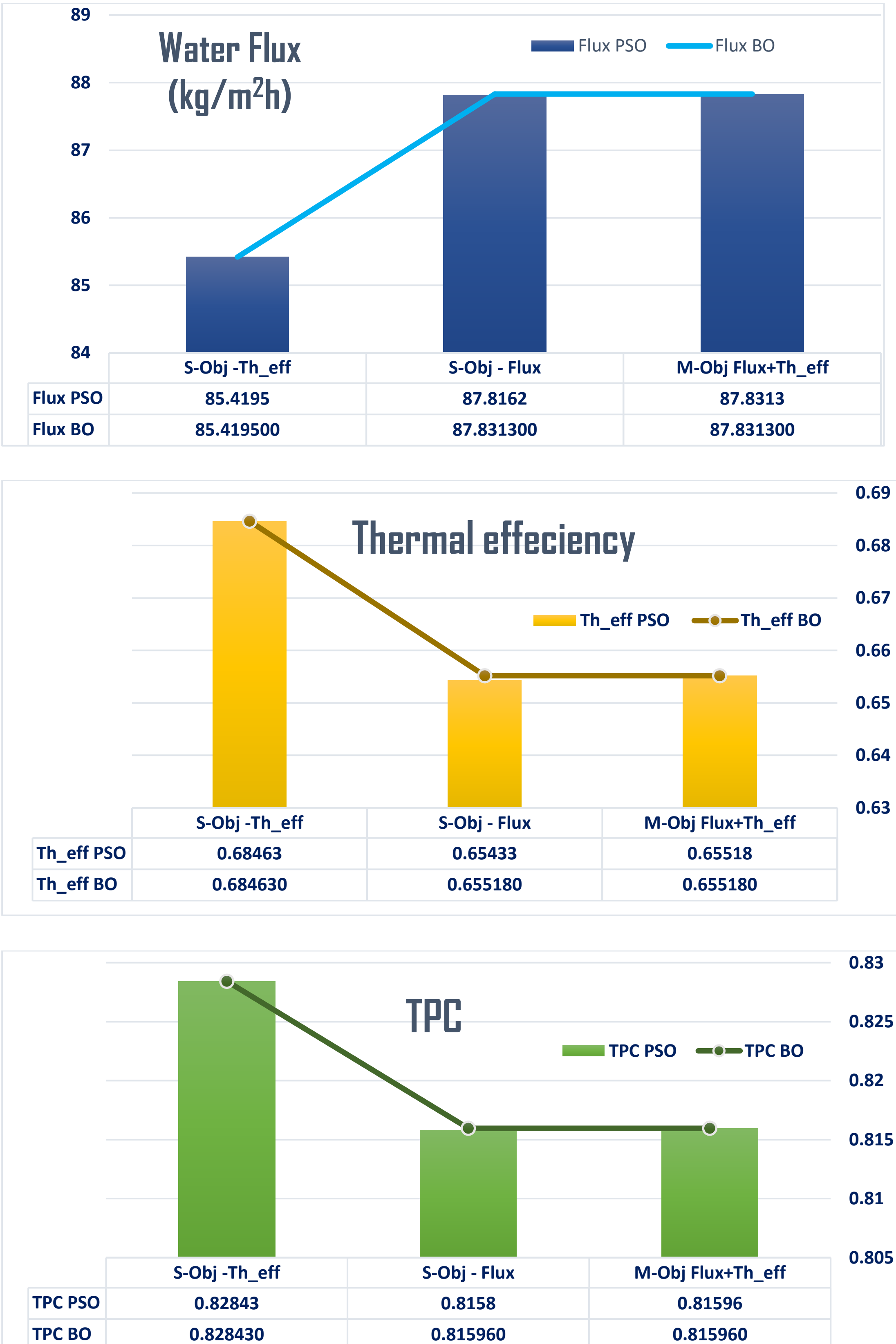


Figure III.17: Single-objective vs. multi-objective optimization using PSO and BO

Table III.4 Final values of optimized DCMD parameters and outputs (all parameters)

	Thermal efficiency	**Flux**	**Flux & Thermal eff**
BO	**S-Obj -Th_eff**	**S-Obj - Flux**	**M-Obj Flux+Th_eff**
T_{FI} (K)	**354.15**	**354.15**	**354.15**
qf (kg/s)	**0.9345157**	**0.9345157**	**0.9345157**
δ (m)	**0.000100386**	**0.000100386**	**0.000100386**
H (m)	**0.0015**	**0.0015**	**0.0015**
Flux (kg/m²h)	**85.419500**	**87.831300**	**87.831300**
Th_eff	**0.684630**	**0.655180**	**0.655180**
TPC	**0.828430**	**0.815960**	**0.815960**
PSO	**S-Obj -Th_eff**	**S-Obj - Flux**	**M-Obj Flux+Th_eff**
T_{FI} (K)	**353.15**	**354.15**	**355.15**
qf (kg/s)	**0.9296576**	**0.9355795**	**0.934516**
δ (m)	**0.00012**	**0.0001**	**0.000100385**
H (m)	**0.0015**	**0.0015**	**0.0015**
Flux (kg/m²h)	**85.4195**	**87.8162**	**87.8313**
Th_eff	**0.68463**	**0.65433**	**0.65518**
TPC	**0.82843**	**0.8158**	**0.81596**

As an outcome, it can said that:

- In the realm of optimizing Direct Contact Membrane Distillation (DCMD), both the Bonobo Optimizer (BO) and Particle Swarm Optimization (PSO) have demonstrated commendable efficacy, yielding analogous optimized flux and thermal efficiency values. However, a nuanced examination reveals subtle disparities in their operational mechanisms and outcomes, which become pivotal in specific application contexts.

- BO is a favorable choice in scenarios where a balanced optimization is sought. It meticulously enhances the selected objective while concurrently maintaining other variables at levels that do not detrimentally impact the overall system performance. This characteristic of BO is particularly vital in multifaceted systems where the alteration of one parameter could inadvertently cascade into undesired alterations in interconnected variables. The ability of BO to navigate through the optimization landscape while ensuring a harmonious balance among all variables underscores its applicability in scenarios demanding a holistic optimization approach.

- Conversely, PSO relentlessly pursues the desired objective, often sidelining the equilibrium of other parameters in the process. This unidirectional focus can sometimes necessitate the sacrifice of other variables, which might be acceptable in scenarios where the attainment of the primary objective is of paramount importance, overshadowing all secondary considerations. With its inherent capability to navigate swiftly toward the optimal solution, PSO can be particularly beneficial in applications where a rapid achievement of the objective is crucial, even if it comes at the cost of other parameters.

- Therefore, the dichotomy between BO and PSO hinges on the specific demands of the application at hand. BO might be aptly suited for applications demanding a meticulous and balanced optimization of all variables, ensuring a stable and harmonious operational regime. On the other hand, PSO might be the optimizer of choice for scenarios where the swift and unequivocal attainment of the primary objective takes precedence over all other considerations.

III.5 Conclusion

In conclusion, this chapter has examined the effect of various operating parameters, including feed inlet temperature, permeate inlet temperature, flow rate, and NaCl concentration, on the total cross-membrane flux in DCMD systems. The analysis of these parameters has provided valuable insights into their influence on the process's overall performance.

The investigation revealed that the feed inlet temperature and permeate inlet temperature significantly impact the total cross-membrane flux. Higher feed inlet temperatures generally result in increased flux due to enhanced vapor pressure difference, while lower permeate inlet temperatures promote condensation and higher driving forces. Additionally, the flow rate affected the flux, with higher flow rates typically leading to higher flux values. Furthermore, the NaCl concentration in the feed solution was observed to have an inverse relationship with the flux, as higher concentrations tend to increase the solution viscosity and hinder mass transfer.

Moreover, the chapter presented an optimization study utilizing the Bonobo Optimizer (BO) and the Particle Swarm Optimization (PSO) method to enhance the total cross-membrane flux. By comparison, the two methods, BO and PSO, effectively found optimal operating conditions by iteratively adjusting the parameters to maximize the flux and the thermal efficiency, highlighting the potential for enhancing the performance of DCMD systems.

In summary, this chapter has explored the impact of operating parameters on the total cross-membrane flux in DCMD systems, including feed inlet temperature, permeate inlet temperature, flow rate, and NaCl concentration. The findings emphasize the importance of carefully selecting and optimizing these parameters to maximize the efficiency and performance of the process. Additionally, the successful application of the BO and PSO method for optimization purposes demonstrates its potential as a valuable tool for enhancing the performance of DCMD.

General Conclusion

GENERAL CONCLUSION

In conclusion, this thesis has provided a comprehensive and in-depth examination of desalination methods, explicitly focusing on membrane desalination (MD) as a thermal desalination technique. The study has explored various technologies employed in producing safe drinking water, such as membrane properties, module design, optimization strategies, and operating parameters impact.

The research conducted in this thesis has highlighted the importance of understanding and distinguishing between different desalination procedures. By establishing a solid foundation of knowledge, readers are equipped with a comprehensive understanding of the complexities and nuances associated with each method. In particular, membrane technology, specifically membrane distillation (MD), has emerged as a competitive and promising alternative to conventional separation methods in desalination. Furthermore, the thesis has emphasized the significance of operating parameters in influencing the total cross-membrane flux in MD systems.

Through in-depth investigations, valuable insights have been gained into the effects of feed inlet temperature, permeate inlet temperature, flow rate, and NaCl concentration on the flux. The findings have contributed to optimizing the performance of DCMD systems and maximizing the productivity of high-quality pure water.

An optimization study utilizing the Bonobo Optimization (BO) and particle swarm optimization (PSO) methods enhanced the total cross-membrane flux and thermal efficiency. This approach has demonstrated its effectiveness in finding optimal operating conditions by iteratively adjusting the parameters, leading to significant improvements in flux values. By simulating and analyzing module behavior, various designs can be explored into considerations and criteria, ultimately contributing to developing efficient and sustainable solutions for seawater desalination.

In summary, this thesis offers valuable insights into membrane distillation systems for seawater desalination. The research contributes to understanding membrane behavior, module performance, and operating parameters' influence on high-quality water production. By exploring optimization strategies, it paves the way for advancements in membrane technology and sustainable desalination processes. With ongoing efforts, membrane distillation holds great potential for meeting global demand for safe drinking water.

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