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MEMBRANE DISTILLATION FOR WATER GENERATION

by

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Abstract

This thesis concentrates on optimizing the efficiency of freshwater production via a membrane distillation system. The Membrane Distillation system offers purified water by a thermal separation process, which permits the water vapor to go through the membrane, and aids in separating the salt and other impure materials. The main goal of this study is to get the optimum value of the membrane properties, such as porosity, pore size, contact angle, and membrane thickness, such that it can influence and make positive changes on permeate flux (J_p), mass transfer coefficient (K_m), and Liquid Entry Pressure (LEP).

This study uses mathematical equations to develop the prediction models to explain the relationship between membrane properties and outputs. Mathematical equations are taken from the principles of thermodynamics, and the equations are validated by using the data from the experiment results of peer-reviewed articles to ensure the accuracy of the model. When the equations were validated, it was used to run the code and build the prediction model via MATLAB, which helps to understand the impacts of membrane properties on the permeate flux, mass transfer coefficient, and Liquid Entry Pressure (LEP). Next, the desirability function had been applied to identify the most optimized membrane design. This approach aids in identifying the optimal balance to maximize permeate flux, mass transfer coefficient while Liquid Entry Pressure is maintained in a safe limit of 300 kPa to protect the membrane from wetting. Furthermore, this study tried to identify the best combination of membrane properties to get the enhanced performance of the system by improving permeate flux, mass transfer coefficient, and Liquid Entry Pressure.

The findings of the study reveal that the membrane, which has higher porosity and higher contact angles, improves the transportation of vapor and aids in preventing leakage. Moreover, a smaller membrane thickness can improve the permeate flux, but it loses the

strength of the membrane. In short, this study introduces optimization models for designing the membrane distillation system to get sustainable freshwater production.

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Dear Dr Jonathan Dong,

I, S M Abul Fatha Rifat, hereby submit my thesis entitled “Membrane Distillation for Water Generation,” as part of my requirements for completion of the Master of Professional Engineering in Mechanical.

I declare that this thesis is entirely my own work with the exception of the acknowledgements and references mentioned.

Yours sincerely,



S M ABUL FATHA RIFAT

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Declaration of published work

I also acknowledge that parts of the paper-style literature review presented at the end of the first semester of this project have been used in the following chapters of this thesis, and the report has been properly referenced:

- Literature Review

I also acknowledge that parts of the progress report presented at the end of the first semester of this project have been used in the following chapters of this thesis, and the report has been properly referenced:

- Methodology and Implementation of Results

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1.0 INTRODUCTION

This study focuses on the prediction model to track the functionality of the Membrane Distillation system via MATLAB software. This project emphasizes membrane properties, such as membrane thickness, porosity, pore size & contact angle, to improve the permeate flux, liquid entry pressure, and mass transfer efficiency. This study approaches on computational framework of previous research works toward the efficiency of the desalination system by identifying the best combination of membrane properties in the membrane distillation system. The study addresses the shortage of experimental resources and the constraint on time. That's why the study is based on a computational framework, which works on building up the prediction model to enhance the performance of the membrane distillation system by identifying the best combinations of the membrane properties.

Nowadays, freshwater is becoming scarce according to human needs and is established as a global problem, also having an impact on the environment and society. Khilchevskyi et al. [1] emphasize that the total volume of the Earth's water is massive, but the problem is the availability of fresh water, which is around 2.5% of the total water, and an even smaller portion of it is accessible for the use of humans. The problem of getting freshwater is rising due to the geographical factors, such as the Middle East and Africa, in those places, huge areas are covered by deserts, where lots of people live, who are deprived of getting fresh water, also temporal factors, socio-economic factors, which includes the increasing tendency of the population, the expansion of the agriculture and prone to attract in luxury lifestyle and so on [1]. Researchers are predicting that if no alternate solution comes up and people use freshwater in this way, 40% of the world population will face water scarcity issues by 2025, especially in South Asia and China, North Africa, and so on, as shown in Figure 1.1 [1].

Moreover, Figure 1.1 provides the visual representations of the water scarcity issues and the availability of freshwater in different demographic locations of the world. According to Lopez-Gunn and Llamas [2], the issues with Water Scarcity are rising not only for the geographic locations of nature, but also for the mismanagement of people. For instance, Governments are not collaborating with others, instead creating a dam, which is harmful for everyone, and people are using it with a defective setup, which wastes lots of water, and people are using rivers and lakes excessively without allowing the water sources to recover. Though theory proves that freshwater sources are still enough to meet the demand of the populations, the mismanagement of the system, the wrong approach to the utilization of the water sources, and discrepancies in water distribution according to demographic location make the water scarcity issue intensify in the developed and developing countries of the world [3].

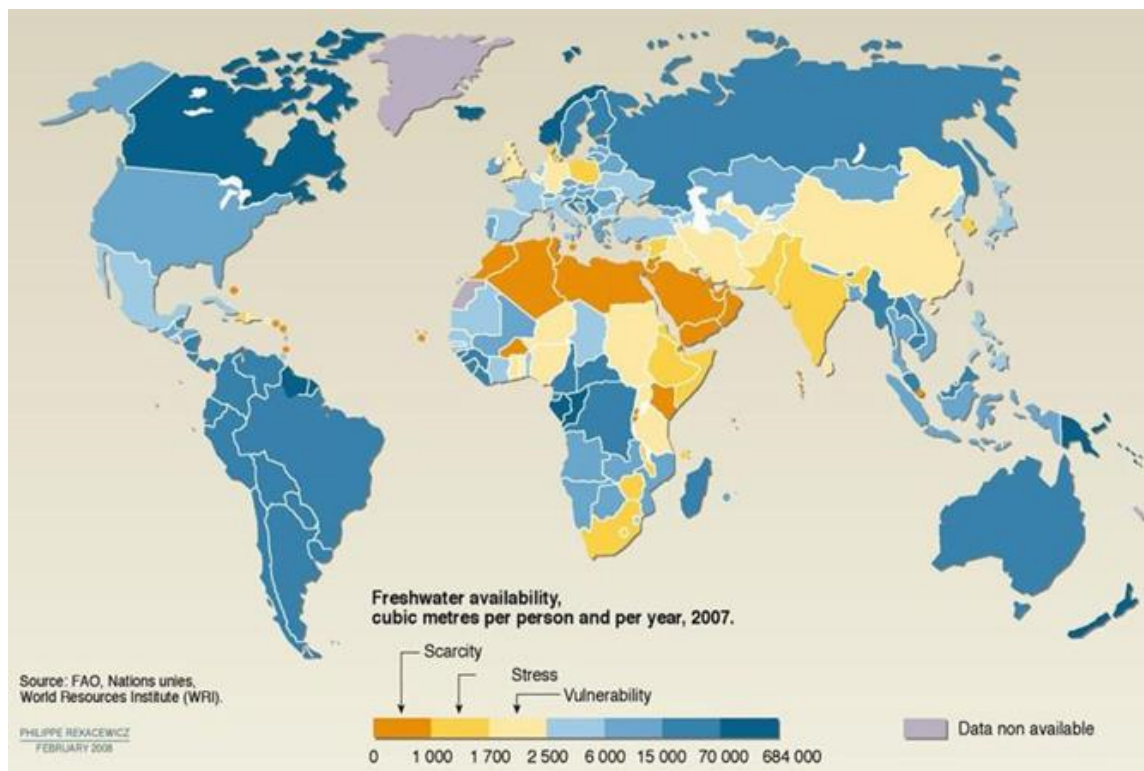


Figure 1.1: The Sources of Freshwater around the World [1]

This study has some drawbacks. The study is based on the computational framework, planning to build prediction models to get an insightful idea about the combination of membrane properties. This study lacks an experimental approach to validate the prediction model due to a lack of resources and time constraints. Moreover, this study takes the numerical data from the peer-reviewed articles and validates the results by comparing them with one journal article. It could be better if more datasets engage in the validation of the results, which can strengthen the validation of the research work. Furthermore, the optimized model assumes the steady-state operational environments, which means that it doesn't depend on the effects of time-dependent factors, such as polarization, temperature, and fouling, which influence the performance over time. Moreover, the optimized model works on uniform properties of the membrane, but the membranes could have minor variations in pore diameter. Moreover, the surface is assumed to be uniform, but it can be rough over time, which can affect the performance of the system. In addition, experimental data is taken from only one journal article, where more datasets can strengthen the comparison of the research work.

The primary aim of the research is to enhance the performance of the membrane distillation by identifying the best combinations of membrane properties, such as membrane thickness, pore size, porosity, and contact angle. The computational modelling is planned to be developed by MATLAB software, which aids in identifying the optimum value of membrane properties by using some equations. The study focuses on building optimization models to present the enhanced performance of output parameters, such as permeate flux, mass transfer coefficient, and liquid entry pressure. Later, the results of the optimized membrane design are compared with the peer-reviewed article to validate the research work.

This study is organized to represent the investigation and findings of the research work in a structured way. First, it starts with an introduction, where it discusses the background,

research goal, and the limitations of the project. Next, it discusses the literature review, which summarizes previous research works on the design of the membrane and the performance metrics, such as membrane thickness, pore size, porosity, and contact angle. Next, the study presents the methodology, presenting the operation procedures and all-important equations for use on MATLAB software. Next, the study analyzes the outcomes of the optimized model by presenting plots, graphs, and bar charts. Later, it discusses the relevance to be engineering standards, identification of the limitations, and scope for future research.

2.0 LITERATURE REVIEW

The dearth of water becomes a global crisis, which requires a potential solution. Desalination is the process that removes minerals, salts, impurities, and other harmful materials from brackish water & seawater to generate fresh water and provides a potential approach to meet the demand for freshwater [4]. Shemer et al. [5] state that the desalination technique is crucial for those geographical locations where the sources of fresh water are limited. The desalination technique has some operational stages that include intaking impure water and going through pre-treatment, desalination by membrane, and post-treatment to produce fresh water, which are shown in Figure 2.1. While the Desalination technique becomes a potential solution to meet the demand for freshwater, researchers need to examine the advancements of the technology to reduce the cost, energy consumption, the negative impacts on the environment, and enhance performance by producing freshwater [6].

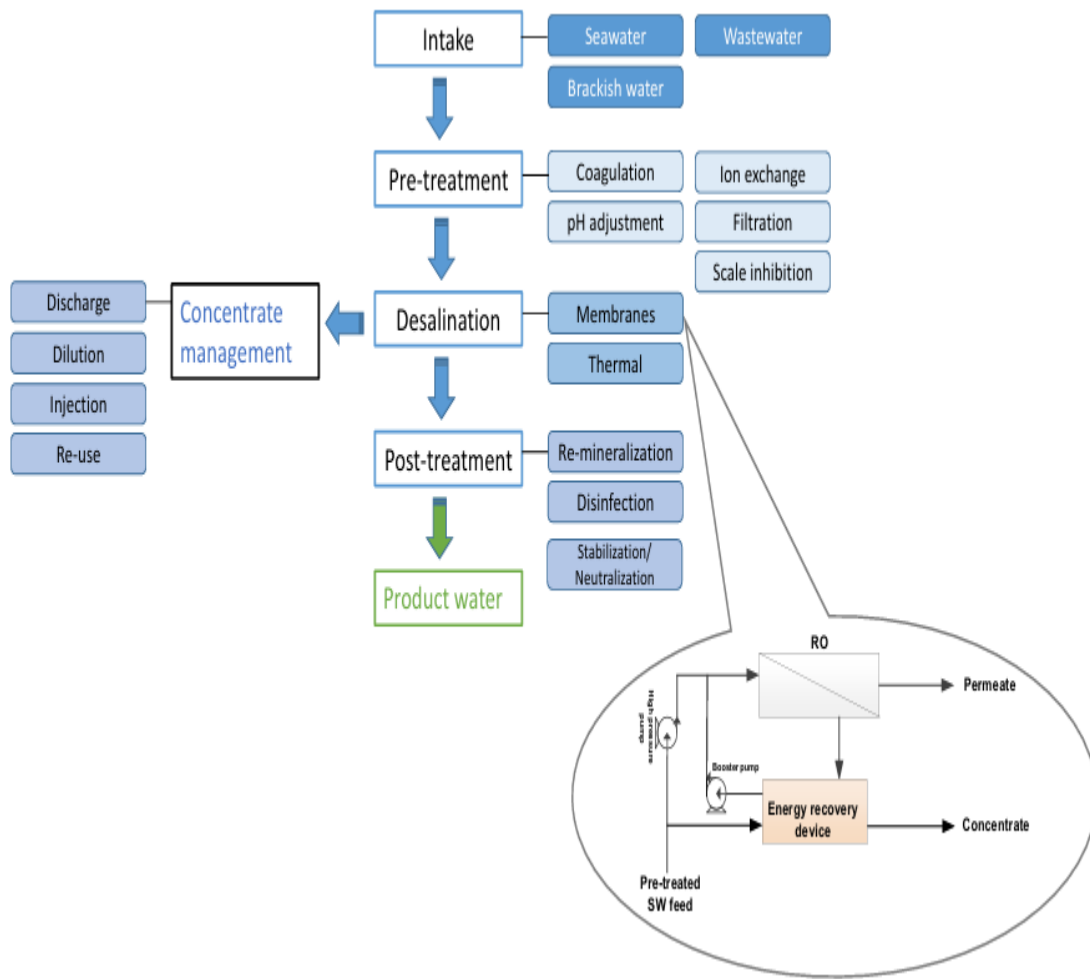


Figure 2.1: Stages for the Desalination Process [5]

2.1 MEMBRANE DISTILLATION

Desalination is offering a solution to fulfil the rising demand for freshwater production, where further research is needed to reduce costs, lower energy consumption, and reduce detrimental effects on nature. At this point, membrane distillation can be a potential solution for the desalination process to produce water because the Membrane has obtained intensified attention for its capability to produce more fresh water by lowering the project cost, saving the consumption of energy, and considering all impacts on nature [7].

Radadiya et al. [8] use hydrophobic membranes to remove impure particles by separating vapor from brackish water, effectively obtaining the purified water under medium thermal

conditions. Researchers utilize micro-nanotube technology to reduce fouling on the membrane and enhance its long-term operational stability. Figure 2.2 illustrates the schematic diagram of a Micro-nanotube technology with a Membrane Distillation system. Similarly, Gupta et al. [9] tried to enhance performance by increasing permeate flux, removing more bacteria, and saving power throughout the operation. The authors used a microwave-induced membrane distillation system that integrates the radiation of the microwave and the membrane with a nano-carbon coating. This system shows better performance than the traditional membrane distillation system, and biocidal performance is increased up to 99.6%. Moreover, the permeate flux is improved by 39%, and the system saves energy by 20% to 25%. However, this study lacks long-term operational performance, simulations to observe the performance in extreme conditions, and requires more experiments to verify the application worldwide.

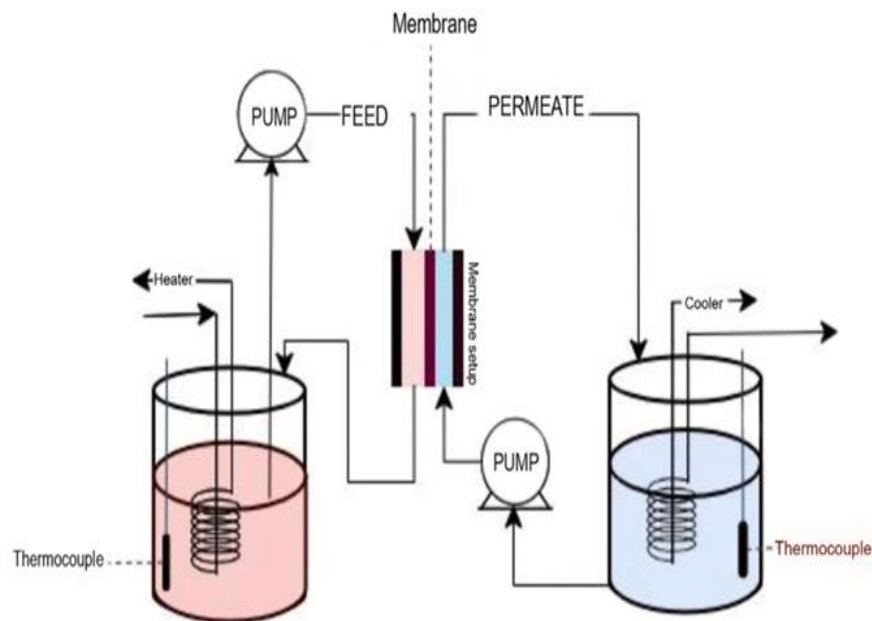


Figure 2.2: Schematic Diagram for Membrane Distillation [8]

To address the issue with Gupta et al., Lee et al. [10] focused on the Simulation Framework and suggested a hybrid system that combines a Phosphoric Acid Fuel Cell and a direct

Contact Membrane Distillation to produce purified water from the sea as well as generate electricity, also working with the waste heat from the system to save energy. The system shows better performance than the traditional PFAC and gets enhanced power density, superior effectiveness in energy saving. Lee et al. [10] illustrate different fouling systems in Figure 2.3, where BSA stands for Bovine Serum Albumin, SA for Sodium Alginate, and AHA for Alginate Humic Acid, which are protein-based foulants, biofouling components, and organic foulants, respectively. These fouling systems react variously with the surfaces of the membrane, resulting in surface deposition, sometimes blocking the pores, as well as forming a gel layer on the surface of the membrane, which can drop the performance of the system significantly. Researchers advise some anti-fouling techniques, which include pretreatment of the feedwater such that it can remove organics, protein, bio-fouling components, and other particles that can create fouling on the membrane. Moreover, Researchers also suggested applying superhydrophobic or omniphobic coatings on the membrane surface to resist foulants in the system. Furthermore, Lee et al. not only discuss about varieties of fouling as shown in Figure 2.3 but also advise some techniques to reduce fouling on the Membrane Distillation System.

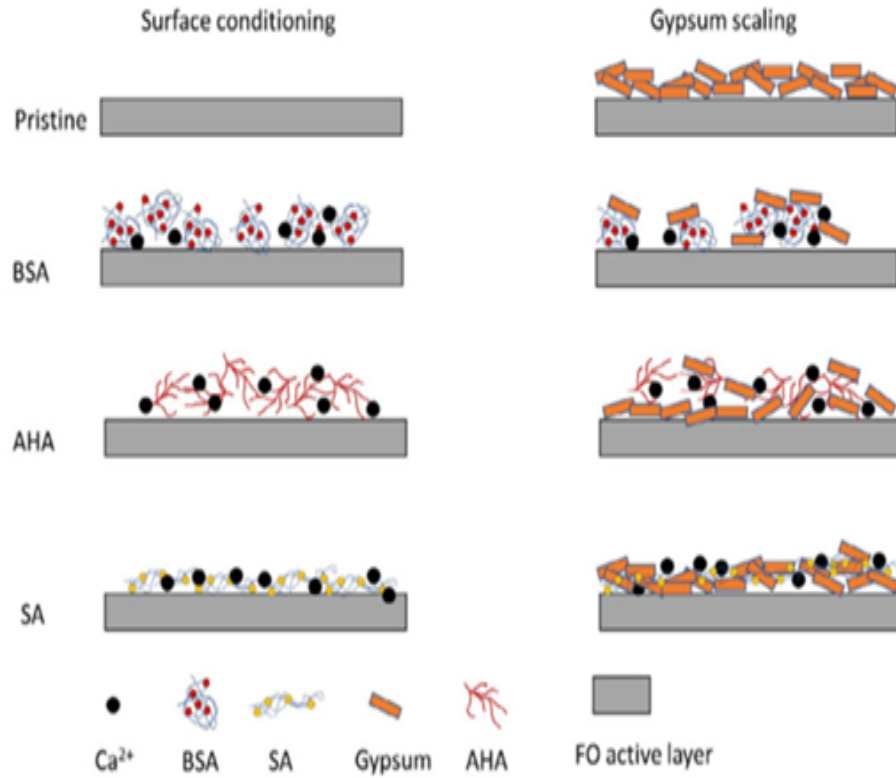


Figure 2.3: Different types of Fouling Mechanisms [10]

2.2 MECHANISM OF THE MEMBRANE DISTILLATION FOR WATER PRODUCTION

Water Generation in the Membrane Distillation system is solely run by the pressure difference of vapor, which is controlled by the temperature gradient around the membrane. Typically, the high temperature of the system is maintained at the feed side, which creates vapor and provides pressure to the vapor such that it goes through the pores of the membrane and gradually condenses the vapor on the permeate side and generates fresh water [11]. Zuo et al. [12] use a hydrophobic membrane where the pore sizes are 0.3 micrometres, just allowing the vapor to enter the membrane and resisting the water from going through the membrane, as shown in Figure 2.4.

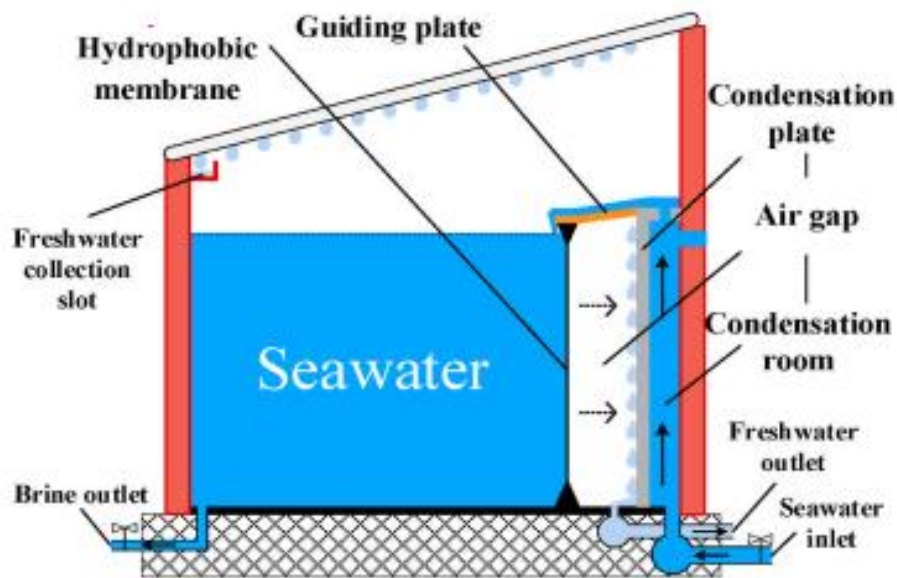


Figure 2.4: Mechanism of the system for Water Production [12]

Moreover, Liu et al. [13] support this study by explaining that the Membrane Distillation system includes three steps for freshwater production. First, evaporate the liquid molecules at the connection of the hot feed membrane. Second, the distribution of the vapor around the membrane pushes to go through into the pores, which is driven by the pressure of the vapor. Third, condensation of vapor is occurring on the cooler permeate side. Besides, this project focuses on keeping the membrane hydrophobicity and reducing the heat loss around the surface of the membrane.

Moreover, Ding and Han [14] state that the vapor flows through the pores of the membrane and gradually condenses on the cooler side of the membrane; that's how the membrane organizes the process of separation. Researchers focus on maintaining the high temperatures of the membrane, which is supplied by solar energy, and this setup is suitable for rural places. It's important to keep high temperatures for a long time with solar energy sources, which ensures a higher amount of freshwater production by effective separation of brackish water from salt, impure particles, and so on.

2.3 INFLUENCING FACTORS FOR WATER PRODUCTION

The performance of the membrane distillation system depends on several influencing factors, which are explained below:

2.3.1 TEMPERATURE GRADIENT

A temperature gradient is one of the influential factors that generate the vapor pressure around the hydrophobic membrane. Since the portion of the feed is kept at a higher temperature than the permeate portion, and that temperature difference creates a vast amount of vapor pressure and provides enough pressure to evaporate water at the connecting section of the feed-membrane, such that it can go through the pores of the membrane. Furthermore, maintaining a higher temperature is beneficial for the operation because it increases the vapor pressure and maximizes the transportation of liquid vapor to improve the production of permeate flux [15]. Moreover, Cath et al. [16] show in their experiment that a rise of temperature around 3 degrees to 5 degrees Celsius improves the production of the permeate flux significantly.

On the other hand, when the temperature gradient reduces because of losing heat in the membrane or membrane fouling and wetting, the production of permeate flux drops significantly. Zhang et al. [17] also state that a little bit reduction of the temperature difference can make the system worse, resulting in a reduction in water production.

Elmarghany et al. [18] illustrate the relationship of the permeate flux with the influence of feed temperature in Figure 2.5. It shows that the increasing nature of feed temperature makes the permeate flux production higher, as well as the salt rejection rate is also higher.

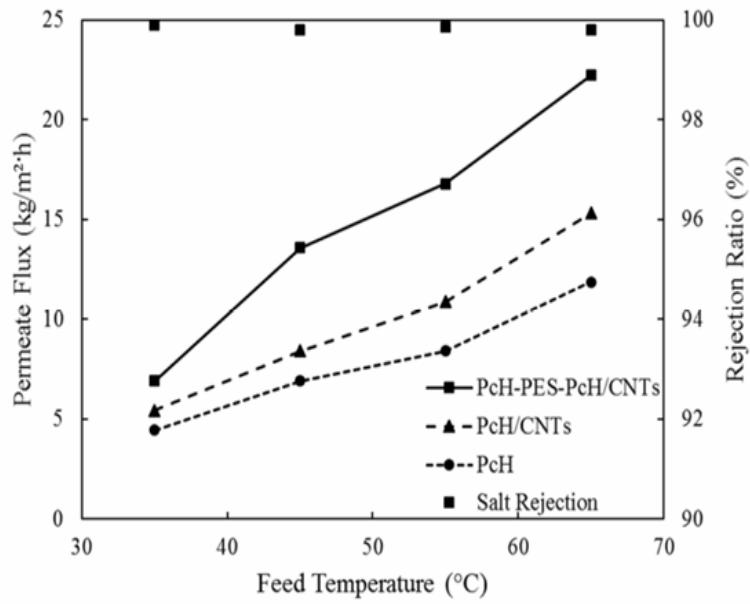


Figure 2.5: The Relationship Between Permeate Flux and Feed Temperature

Membrane properties such as porosity, pore size, the thickness of the membrane, and the contact angle also influence the production of fresh water.

2.3.2 POROSITY

Porosity is the pathway through which vapor passes inside the membrane from the feed side to the permeate portion to enhance the freshwater production. Porosity is the pathway through which vapor passes inside the membrane from the feed side to the permeate portion to enhance the freshwater production. Ramlow et al. [19] investigate high porosity membranes, for instance, PTFE & PP, for the experiment. Researchers state that a higher porosity membrane is an advantage to get a larger amount of permeate flux, as a higher porosity membrane allows vapor to go through the system and makes it capable of increasing the mass transfer, but the drawback is that there is chance of facing some issues like membrane wetting, membrane fouling and structure failure. Baroud [20] illustrates the visual representation of the membrane porosity by showing the SEM images of the different types of PVDF membranes, exhibiting the roughness of the structure, which are shown in Figure 2.6. Figure 2.6(a) and Figure 2.6(b) illustrate the feed side and permeate side of the PVDF-

G membrane, respectively, which has visibly lower porosity, allowing less transportation of the vapor inside the membrane but having lower chances of issues like membrane wetting and structural failures, but failing to produce a larger amount of permeate flux due to having smoother surfaces.

The more downward movement in figure 2.6, like moving from figure 2.6(c) & figure 2.6(d) to figure 2.6(k) & figure 2.6(i), the surface becomes rougher, exhibits higher porosity, and enhances the fresh water. Figure 2.6(k) and Figure 2.6(i) show the feed side and permeate side of the PVDF-S150 membrane, which displays higher porosity and generates more permeate flux due to having a rougher surface, but still has a high chance of issues like membrane wetting & structure failures.

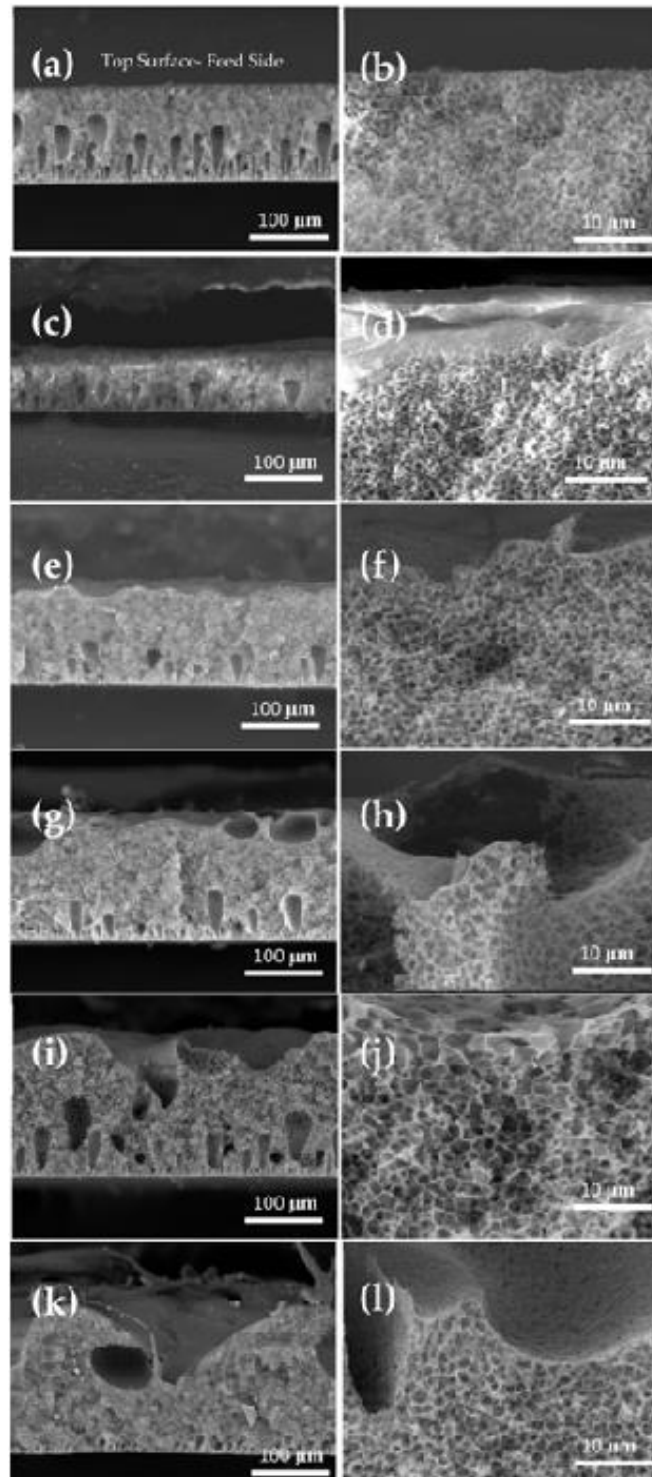


Figure 2.6: SEM Image of Different Types of Polyvinylidene Fluoride Membrane for visual understanding of the influence of the Porosity on the System [20]

2.3.3 PORE SIZE

Pore size is another significant factor that affects a lot to the performance of the Membrane Distillation System. According to McGaughey et al. [21], Pore size facilitates the vapor transport inside the membrane and improves water generation. Though pore sizes minimize

the Liquid Entry Pressure and increase the chance of pore wetting as well as the tendency to mix the contamination with the fresh water. This project also focuses on the tuning of pore size is crucial to resist contamination on fresh water as well as lower the chance of pore wetting, such that it can perform well and provide better output. Hong et al. [22] illustrate visually the relationship between the permeate flux and the pore sizes in Figure 2.7, which explains about two curves, one is the ideal vapor transportation from the simulation, another curve is obtained from the lab experiments, and both curve matches the relationship between the pore sizes and permeate flux, which validates the simulation model. Moreover, it supports McGaughey et al.'s statement about the pore sizes influencing the output. Moreover, it shows the advantage of having larger pore sizes for getting more permeate flux, but increasing the chances of pore wetting. Furthermore, it depicts a reduced amount of permeate flux for smaller pore sizes but reduces the chances of pore wetting.

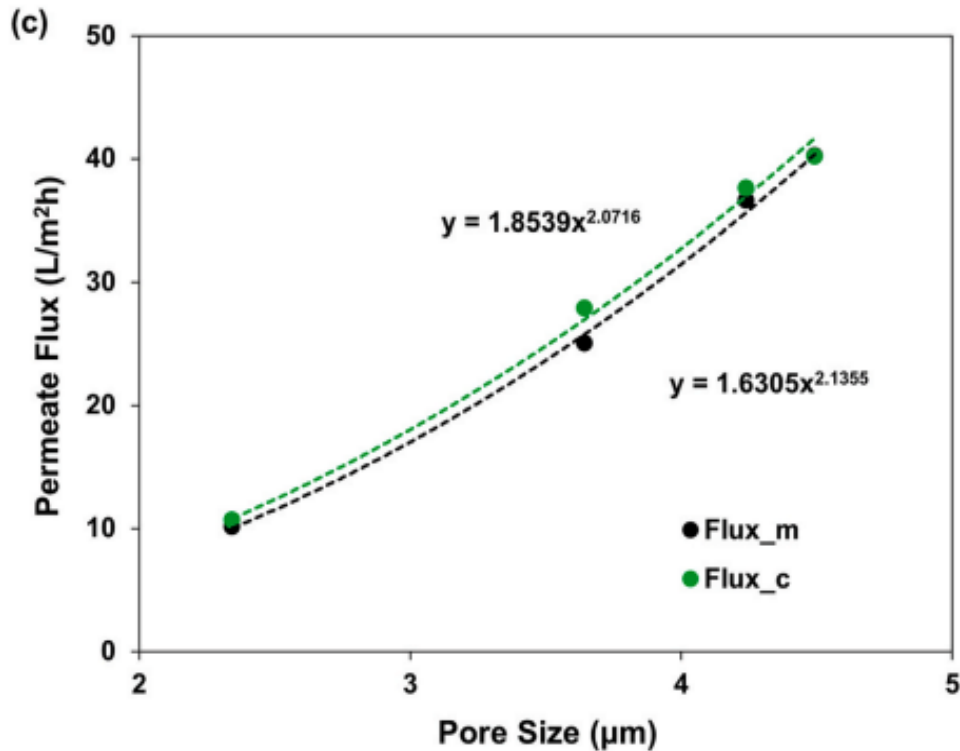


Figure 2.7: The Relationship Between Permeate Flux and Pore Size [22]

2.3.4 MEMBRANE THICKNESS

Membrane Thickness directly impacts the performance of the membrane distillation system, as well as affects the energy efficiency of the system. Deshmukh and Elimelech [23] work on the theoretical prediction model and find that the thinner membrane can pass the liquid vapor easily due to having a lower resistance to the mass transfer. Researchers also state that a thinner membrane can enhance the energy efficiency of the system initially, but gradually it can be worse if heat conduction becomes prominent, resulting in uncontrolled excessive heat to the system and loss of performance on the membrane distillation system. Furthermore, an extremely thin membrane can pass the vapor-liquid so smoothly, but may face some issues like structural failure or excessive heat during the operation of the system. This study proves that the optimal thickness of the membranes is essential to get the maximum output by ensuring the stability of the operation.

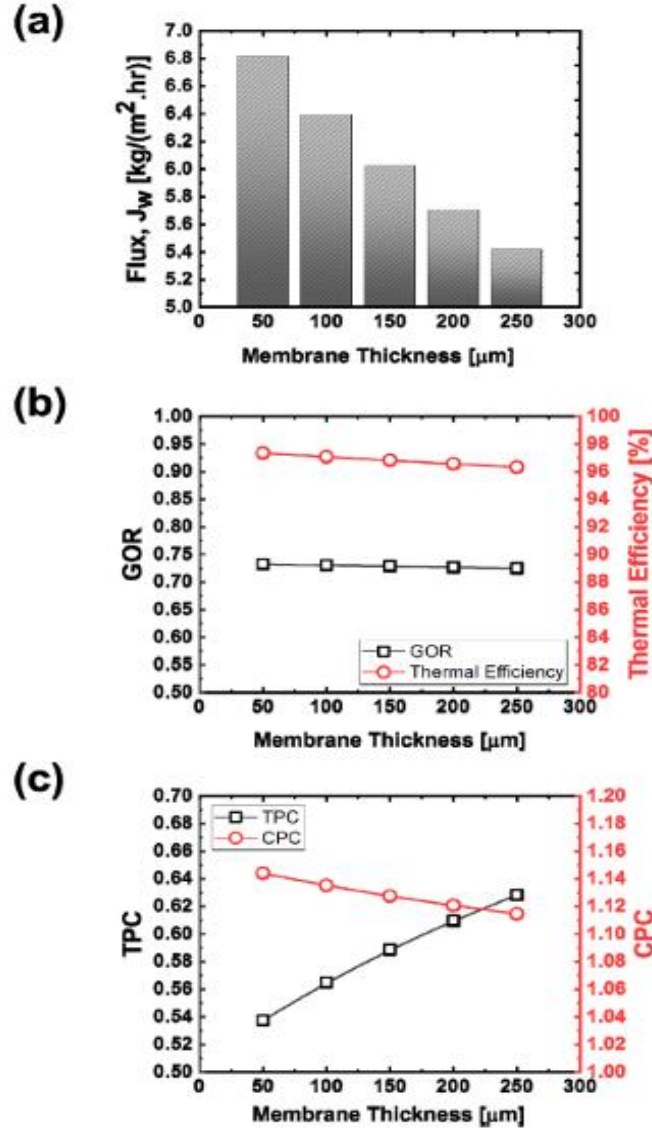


Figure 2.8: The Relationship of the Membrane Thickness with GOR, TPC, and Flux [24]

Noamani et al. [24] depict the relationship of the membrane thickness with the output of the system, for instance, Permeate Flux, Gained Output Ratio (GOR), and Thermal Performance Coefficient (TPC) in Figure 2.8. When the thickness of the membrane increases, the overall performance drops, which is visible in Figure 2.8 because the thick membrane becomes a resistance for the mass transfer inside the system, which minimizes vapor transportation inside the system as well as losing heat from the system, which directly affects the performance of the system. While thinner membranes show superior vapor transportation capability, but face challenges like structure integrity or creating excessive heat on the surface, which reduces the efficiency of the system. So, the optimal thickness of the

membrane is important not only for getting a better amount of permeate flux but also for improving the energy efficiency of the system.

2.3.5 CONTACT ANGLE

The contact angle plays a significant role in the performance of the system. Dumée et al. [25] state that higher contact angles enhance hydrophobicity, which means better transportation of the liquid vapor inside the system as well as reducing the chances of pore wetting.

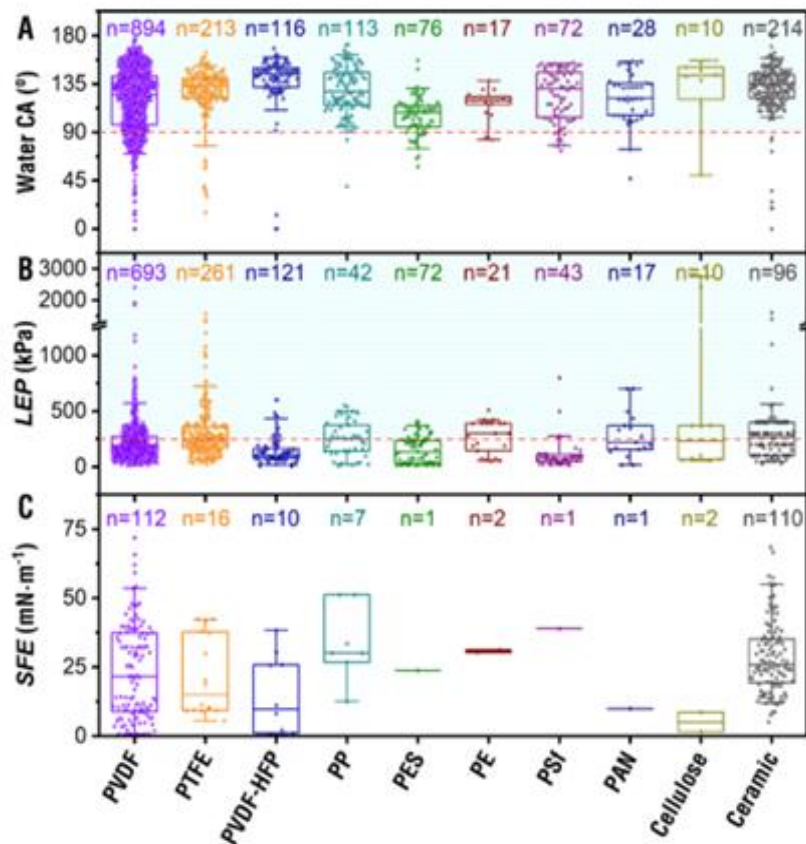


Figure 2.9: The Impact of Contact Angle on System's Performance

This study ensures that higher contact angles produce a vast amount of permeate flux and minimize the wetting of the pore membrane by maintaining a stable operation, which is crucial for continual mass transfer and other operations for achieving better performance. On the other hand, lower contact angles lower the hydrophobicity, which means reducing the production of fresh water, also increasing the chance of other challenges like pore

wetting, which can significantly impact the system. So, a higher contact angle is not only crucial for getting more permeate flux by reducing the pore wetting, but also maintaining a stable operation in the system.

Chang et al. [26] illustrate the analysis of the chance of Membrane wetting by presenting the relation between the Water Contact Angle (WCA), Liquid Entry Pressure (LEP) & Surface Free Energy (SFE) around different types of membranes used in the system, as shown in Figure 2.9, that categorizes into three types, which are unmodified, hydrophobic and superhydrophobic. Superhydrophobic membranes show higher contact angles, lower values of SFE, and higher LEP, which ensures a lower chance of pore wetting and confirms the stable operation with better output. On the other hand, unmodified membranes depict the lower contact angles, higher value of SFE, and lower values of LEP, which increase the chance of pore wetting, resulting in unstable operation with loss of efficiency.

2.4 OPTIMIZATION TECHNIQUES OF MD (MEMBRANE DISTILLATION) SYSTEMS

The introduction of the hybrid systems in Membrane Distillation is a great approach for energy utilization as well as improving the freshwater production. This hybrid system focuses on overcoming the limitations of the Membrane Distillation system by enhancing the durability of the operation as well as the energy efficiency of the system.

Tian et al. [27] provide a comparative review of two different technologies of the membrane system; one is about solar interfacial distillation (SID) and photothermal membrane distillation (PMD), emphasizing their structures & mechanisms, efficiency of the system & performance to generate water and electricity. SID shows better performance in water generation and energy utilization, while PMD shows better performance in vapor separation from the membrane. Both systems analyze salt rejection and water purification. The research

papers need to work on simulations to observe the performance in different conditions, as well as needs to analyze durability and sustainability.

To develop the importance of hybridization for advancement, Lin et al. [28] suggested another hybrid system that integrates the Pressure Retarded Osmosis with the Membrane Distillation to produce water and electricity from low heat. The system utilizes concentrated and dilute streams for salt rejection and water generation, as well as the utilization of the energy, which provides enhanced performance as well as superior conversion of heat into work. However, the system is based on theory, lacking experimental validation, but analyzes identify flow rates, enhanced conversion of heat into work & energy recovery.

Similarly, building on the need for reliable membrane performance in such hybrid systems, Chen et al. [29] worked with a decentralized cogeneration system that combines the concentrated photovoltaic/thermal (CPV/T) collectors and vacuum multi-effect membrane distillation (V-MEMD) to generate continuous water and electricity. This system is successful in utilizing solar energy properly and produces electricity of 562 kWh annually, and produces 5.25 m³ of water per square meter of the solar collector area. However, this study is based on simulations and needs experimental validation to observe the performance of the system. Similarly, Li et al. [30] also worked with only theoretical modelling and suggested a hybrid system that combines a Phosphoric Acid Fuel Cell and a direct Contact Membrane Distillation to produce purified water from the sea as well as generate electricity, also working with the waste heat from the system to save energy. The system shows better performance than the traditional PFAC and gets enhanced power density, superior effectiveness in energy saving. However, the study relies on theoretical models, requires more economic analysis and experiments to implement the system on a large scale.

In response to the gap of real-world implementation, Wang & Chung [31] work to solve ongoing challenges with the Vacuum Membrane Distillation (VMD), where the wetting

resistance and permeation flux don't show stable performance. The researcher used a multi-bore hollow fibre membrane, changed its shape, and turned it into a lotus root shape to provide more strength. The result appears that antiwetting performance increased by more than 65%, and salt rejection was higher than the standard VMD. The study requires research on the durability, analysis of the long-term performance, and economic considerations. These projects mainly highlight the need for a hybrid Membrane Distillation system to achieve enhanced performance, as well as the utilization of energy in the system.

2.5 MODELLING WITH EXPERIMENTAL IMPLEMENTATION IN MEMBRANE DISTILLATION SYSTEM

The Computational Framework is crucial for understanding the model's performance under challenging conditions. Zhao et al. [32] tried to figure out the solutions for low-efficiency Photovoltaic Modules (PVM) with Direct Contact Membrane Distillation (DCMD), utilizing the waste heat for electricity generation and water production. This proposed system showed 4.44 times better performance than the standard PVM, measured by MATLAB modelling. However, this research lacks actual experiments, indicating the need for a validation experiment, but it provides alternative solutions in the PVM system.

To address the issue with the validation of the experiment, Kumar and Martin [33] proposed a pilot-scale system that combines solar domestic hot water (SDHW) and air-gap membrane distillation (AGMD) to generate hot water and drinkable water to meet the demand in the UAE, under actual climate conditions. The study of Kumar and Martin not only provides the validation of the experiment, but also generates the analysis of the computational framework, where Zhao et al.'s study is completely MATLAB-based and lacks experimentation under realistic weather conditions. The system can generate 2.2 L of drinking water per hour and successfully satisfies the domestic demand for hot water. Though the system provides a detailed analysis and performs well in the real-world experiment, but still has issues like

membrane wetting, the fluctuations of thermal efficiency, as well as requires the evaluation of the long-term operational performance. So, experimental validation is important while working with a model; otherwise, it's impossible to understand the feasibility of real-world implementation unless resources for experiments are not limited.

In short, this study investigates the membrane distillation system as an impactful technology to minimize the issue of water scarcity, focusing on improving the performance of the system by producing more permeate flux and the utilization of energy. It highlights the development of the membrane properties, such as porosity, pore size, membrane thickness, and contact angle, which are the influencing factors to improve the performance of the system, as well as resisting the membrane pore wetting. Moreover, this thesis also investigates the importance of modelling to understand the performance of the system under various challenging conditions and also emphasizes the validation of the experiment according to the modelling. Furthermore, this study introduces the hybrid system to the membrane distillation system, which works on enhancing energy efficiency with improved permeate flux. Overall, this report emphasizes the need for the introduction of advanced materials or technology for the membrane distillation system, a hybrid system for enhanced energy efficiency, and the importance of experimental validation of the modelling to understand the durability and sustainability for long-term operational performance.

3.0 METHODOLOGY

The Membrane Distillation system is one of the most popular and effective desalination technologies, which can produce a vast amount of fresh water by consuming lower power energy. This thesis analyses the membrane properties, such as membrane thickness, pore size, porosity & contact angle, and evaluates the membrane properties, which have a great influence on the performance of the system. The study analyses the performance of the system through MATLAB modelling and evaluates the influence of membrane properties on generating fresh water with minimal energy consumption. The study is planned to design a model that includes the equations of heat and mass transfer to calculate the permeate flux, Liquid Entry Pressure (LEP), and mass transfer coefficient. Furthermore, the thesis aims to find out the optimal values of membrane properties, for instance, minimizing the membrane thickness, as increasing the membrane thickness reduces in production of freshwater, as well as figure out the optimal value for the pore size, porosity, as maximizing the value has a positive impact on permeate flux but negative consequences on Liquid Entry Pressure, which leads to membrane wetting. The MATLAB model provides a robust analysis to achieve better performance of the system through the evaluation of the membrane properties and focuses on parameters for enhancing the performance of desalination.

3.1 PROGRESS

Lots of ideas have been generated from the Literature review, focusing on freshwater production and energy saving to operate the Membrane Distillation System. The study of the researchers helps to identify some gaps and findings in that area, which are given below:

- Influence of the Membrane Properties, such as pore size, porosity, contact angle, and membrane thickness, on the performance of the system.
- The crisis of fresh water and the introduction of technology for desalination to solve the ongoing issue.

- Different varieties of Membrane Distillation System.
- Importance of temperature difference and pressure gradient to produce fresh water.
- Brief ideas to utilize the heat loss from the system to save energy.
- Importance of prediction and optimized model with experiments to monitor the performance under different challenging situations.
- Gaining knowledge about the surface treatment of the membrane for enhanced wetting resistance and durability.

3.2 COMPONENTS OF THE MEMBRANE DISTILLATION SYSTEM

The basic working principle of the membrane system is shown in Figure 3.1, which represents a small-scale laboratory experiment under a controlled setup, where all the necessary components are shown, which is beneficial for understanding the operation of the membrane distillation system.

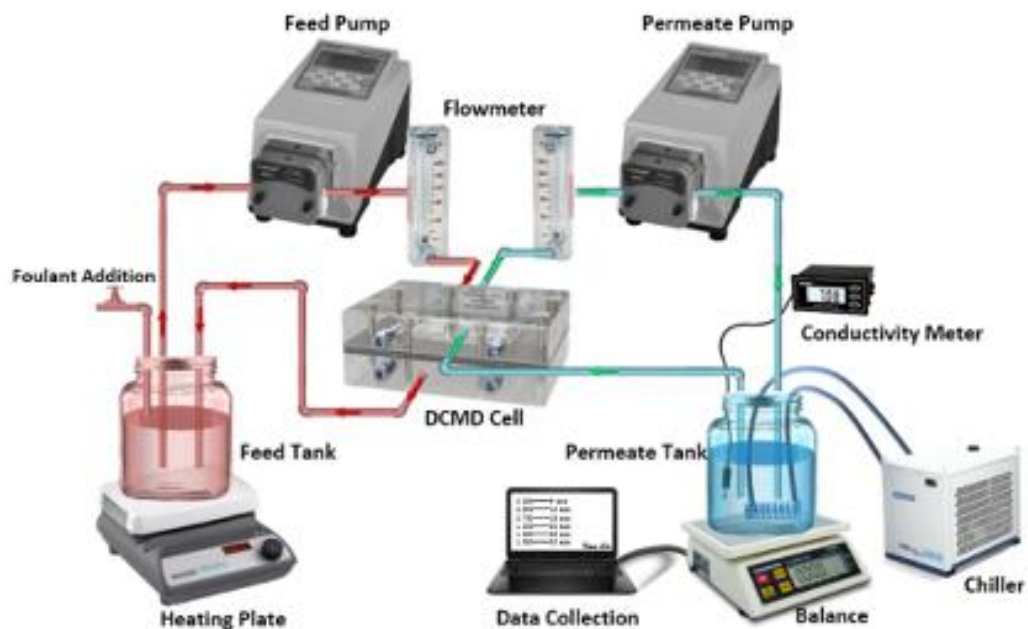


Figure 3.1: Schematic Diagram of the Membrane Distillation System for basic understanding [35]

Figure 3.1 illustrates two different sections: one is for the saline water, which is contained inside the feed tank, and another is for the permeate flux, which is contained in the Permeate

Tank. Furthermore, the feed water tank is connected to a heating plate, which helps to maintain a temperature of 66 °C, and the permeate tank is connected to a chiller, which also helps to maintain a temperature of 44 °C. A conductivity meter is connected to determine the purification of the water and calculate the rejection rate of salt and other impurities. Here, the feed pump helps to circulate hot water along the hydrophobic membrane, and the permeate pump aids in circulating the cold water around the membrane surface to maintain the temperature difference, which generates vapor pressure and repeatedly pushes the water vapor inside the membrane surface. The water vapor goes through the pores of the membrane, condenses into liquid, and is stored as freshwater.

3.3 MATLAB MODELLING

The thesis is designed to develop a prediction model using MATLAB Software for a Direct Contact Membrane Distillation (DCMD) system. The main objective is to monitor the performance of the membrane system by modifying the membrane properties, such as porosity, pore size, contact angle, and membrane thickness.

The prediction model is designed via MATLAB by using a block diagram to evaluate the thermal behaviour and the production of freshwater by saving the energy of the Direct Contact Membrane Distillation System. The predication model includes some equations to calculate the permeate flux, the liquid entry pressure (LEP), and the mass transfer coefficient under various challenging conditions.

The optimization model is a work in progress at this moment. At this stage, the equations are selected for the calculation and are used to build the block diagrams to evaluate the performance of the system under various operating conditions. The study focuses on the membrane properties to enhance the permeate flux by saving energy.

3.4 EQUATIONS

Some equations are used in MATLAB to calculate the permeate flux, Mass Transfer coefficient & Liquid Pressure Entry (LEP), which are given below [35].

Permeate Flux:

$$J_p = C_w \left(\frac{H_{fg}}{(R_{const} \times (T_m + 273) \times P_m)} \right) (T_{hi} - T_{ci})$$

Where,

J_p = Permeate Flux, C_w = Mass Transfer Coefficient, H_{fg} = Latent Heat Vaporization, R_{const} = Specific Gas Content, T_m = Mean Temperature, P_m = Mean Pressure, T_{hi} = Inlet Heat Temperature, T_{ci} = Inlet Cold Temperature

Liquid Entry Pressure:

$$LEP = \left[\frac{-2 \times y_i}{r_{memb}} \right] \times \cos \theta$$

Where,

y_i = sea water surface tension, θ = Contact angle between water and membrane surface,

r_{memb} = largest pore size

Mass Transfer Coefficient:

$$K_m = \left[\frac{J_p \times H_{fg}}{T_{hi} - T_{ci}} \right] \times 1$$

3.5 DISCUSSION ABOUT PARAMETERS

Some Parameters are considered fixed, and the values are given below:

The area of the Membrane = $0.22 \times 10.13 \text{ m}^2$, Thermal Conductivity = $0.000189 \text{ kW/m} \cdot ^\circ\text{C}$, Feed water Tank Temperature = $66 ^\circ\text{C}$, Permeate tank temperature = $44 ^\circ\text{C}$, the salinity of feed = 35020 ppm, the efficiency of pump = 0.76

Some parameters change to enhance the permeate flux and durability of the system, which are given below:

Porosity, Pore Size, Membrane thickness, and contact angle vary from 0.48 to 0.91, $0.21 \text{ }\mu\text{m}$ to $0.98 \text{ }\mu\text{m}$, $70.31 \text{ }\mu\text{m}$ to $190.18 \text{ }\mu\text{m}$, 85° to 145° , respectively.

In short, the progress report highlights the planning, early stages of the calculation, setting up the goals, and developing the strategy to work on the MATLAB software. Moreover, the idea has been generated from the Literature Review, which provides an insightful idea about membrane properties, for instance, membrane thickness, porosity, pore size & contact angle, which remarkably impact the performance of the system. Next, the planning with MATLAB software, the equations, and the parameters have been defined, but the optimized model is now in the development stage. So, the next stage of the study will focus on the numerical modelling to calculate the enhanced permeate flux, liquid pressure entry, and mass transfer coefficient by changing the parameters of the membrane properties.

3.6 EQUATIONS FOR OPTIMIZATION

The performance metrics of the MD system mostly rely on the structure and properties of the membrane, which can present four variables, and all equations are obtained from [35] [36].

$$x = [\varepsilon, d, \delta, \theta]^T$$

Here,

ε = membrane porosity (no dimension)

d = pore diameter (μm)

δ = membrane thickness (μm)

θ = contact angle ($^\circ$)

The properties of the membrane impact how effectively the vapor goes through the membrane and efficiently separates the impurities without membrane wetting. Each variable has been limited by some practical bounds [36], which are shown below:

$$\varepsilon \in [\varepsilon_{min}, \varepsilon_{max}], d \in [d_{min}, d_{max}], \delta \in [\delta_{min}, \delta_{max}] \quad \& \quad \theta \in [\theta_{min}, \theta_{max}]$$

We know,

$$H_{fg} = \text{latent heat of vaporization } (J \cdot kg^{-1})$$

$$R_{const} = \text{specific gas constant for water vapor } (J \cdot kg^{-1} \cdot K^{-1})$$

$$T_{hi}, T_{ci} = \text{hot/cold bulk temperatures } (^\circ C)$$

$$\text{Mean Temperature, } T_m = \frac{T_{hi} + T_{ci}}{2}$$

$$\Delta T = T_{hi} - T_{ci}$$

$$P_m = \text{mean pore pressure } (Pa)$$

$$\gamma = \text{surface tension } (N \cdot m^{-1})$$

$$\tau = \text{tortuosity}$$

Permeate Flux:

Permeate Flux illustrates how much vapor is going through the surface of the membrane, and turns the vapor into fresh water in the permeate tank. It relies on the temperature difference around the surface of the membrane and the mass transfer coefficient of the substances.

$$J_p(\varepsilon, d, \delta) = C_w(\varepsilon, d, \delta) \left(\frac{H_{fg}}{(R_{const} \times (T_m + 273) \times P_m)} \right) (T_{hi} - T_{ci}) [kg \cdot m^{-2} \cdot s^{-1}]$$

$$C_w(\varepsilon, d, \delta) \propto \frac{\varepsilon d}{\tau \delta} \quad [35] [36]$$

Here,

J_p = Permeate Flux, C_w = Mass Transfer Coefficient, H_{fg} = Latent Heat Vaporization, R_{const} = Specific Gas Content, T_m = Mean Temperature, P_m = Mean Pressure, T_{hi} = Inlet Heat Temperature, T_{ci} = Inlet Cold Temperature

Liquid Entry Pressure:

Liquid Entry Pressure measures the pressure difference before the water enters the hydrophobic membrane. The equation below is obtained from the Laplace equation:

$$LEP(d, \theta) = \left[\frac{-2 \times y_i}{r_{memb}} \right] \times \cos \theta$$

Here,

y_i = sea water surface tension, θ = Contact angle between water and membrane surface,

r_{memb} = largest pore size

A larger contact angle and smaller pore diameter increase LEP, improving resistance to pore wetting. The combination of a higher contact angle and a smaller diameter of the pore increases the liquid entry pressure and enhances the performance of resistance for membrane wetting.

Mass Transfer Coefficient:

The mass transfer coefficient works on the movement of the vapor transfer inside the membrane.

$$K_m(J_p) = \left[\frac{J_p \times H_{fg}}{T_{hi} - T_{ci}} \right] \times 1$$

It is related to the permeate flux because it deals with the required energy for vapor transfer, and a higher value of the mass transfer coefficient indicates more efficient mass transportation and effective heat transfer.

Desirability Functions:

This study focuses on identifying the ideal design for a membrane distillation system by converting three performance metrics, such as Permeate Flux, Mass Transfer Coefficient, and Liquid Entry Pressure, into a desirability function, which responds 0 for unacceptable performance, and responds 1 for the ideal value.

For each response $y_i \in \{J_p, K_m, LEP\}$ define lower acceptable bound L_i , target T_i ($T_i > L_i$), and shape exponent $r_i > 0$:

$$d_i(y_i) = \begin{cases} 0, & y_i \leq L_i \\ \left(\frac{y_i - L_i}{T_i - L_i} \right)^{r_i}, & L_i < y_i < T_i \\ 1, & y_i \geq T_i \end{cases}$$

- d_1 for J_p , d_2 for K_m , d_3 for LEP
- $r_i > 1$ emphasizes values near the target; $r_i < 1$ rewards modest gains
- $LEP \geq 300 \text{ kPa}$

$$\theta_0 = 1$$

$$-2.25 \theta_1 + \theta_2 = -1$$

$$\theta_1 - 2.25 \theta_2 + \theta_3 = 0$$

$$\theta_2 - 2.25 \theta_3 + \theta_4 = 0$$

$$2\theta_3 - 2.25 \theta_4 = 0 \quad \text{for } i = M \text{ [Tip]}$$

Desirability to maximize:

The combined performance is measured using a weighted geometric mean:

The combination of the optimized performance metric is measured by using the geometric mean.

Here, w_i are the weights of the substances.

Assign importance weights $w_i > 0$ (e.g., equal $w_1 = w_2 = w_3$). The overall desirability is the weighted geometric mean:

$$D(x) = (d_1(x)^{w_1} d_2(x)^{w_2} d_3(x)^{w_3})^{\frac{1}{w_1+w_2+w_3}} \in [0,1]$$

The final goal is to find the membrane configuration that maximizes

The main aim is to identify the behavior of the membrane properties, which maximizes the value of $D(x)$

Now, the objective is to get the maximum values for $\max D(x)$ because it will help to identify the best combinations of the membrane properties.

$$x \in X$$

$$s.t. \varepsilon_{min} \leq \varepsilon \leq \varepsilon_{max}, d_{min} \leq d \leq d_{max}, \delta_{min} \leq \delta \leq \delta_{max}, \theta_{min} \leq \theta \leq \theta_{max} \\ , (optional \text{ Safety}) LEP(d, \theta) \geq L_{req} \text{ (e.g., 300 kPa)}$$

Outputs: the optimal $x = [\varepsilon, d, \delta, \theta]$ and the corresponding J_p, K_m, LEP [35]

3.7 RESEARCH DESIGN

This study deals with explaining the design of the membrane, data collection, optimization, and validation of the model by building an optimized model. The study works on prediction models to identify the performance of the Membrane Distillation System for producing fresh water. A lab experiment is avoided in this study due to a lack of resources. Instead of doing lab experiments, this study completely focused on building up the MATLAB-based

prediction model by taking data, theoretical concepts, and equations from peer-reviewed articles. The way so far has been approached is acceptable because it permits the performance of the membrane distillation system via checking the parameters, such as the properties of the membrane, without requiring time-consuming lab experiments. Though lab experiments are crucial to identify the effectiveness of the proposed model, the lack of resources and time constraints for lab experiments moves the research work to a MATLAB-based optimization model approach. Moreover, it still saves waste of minerals and materials and ensures a safe environment by showing the accuracy of the result.

This study uses lots of parameters, such as the temperature of the feed and the properties of the membrane, which were taken from the peer-reviewed articles and data sheets of the membrane manufacturers. When the values were taken from the datasheet, all units were converted into SI units. Later on, these parameters were used in MATLAB. Next, the Data were sorted and organized into arrays to create variations on one parameter while keeping other parameters fixed, which helps identify the behavior of the properties. Moreover, it is helpful to understand the impact of individual properties on the system.

Model Structure depends on three equations.

1. Permeate Flux: It measures the amount of fresh water produced from the vapor, which goes through the surface of the membrane by creating a pressure difference and a temperature difference across the membrane.
2. Mass Transfer Coefficient: It measures the amount of vapor passing through the pores of the membrane, and the parameter is directly related to producing the permeate flux.
3. Liquid Entry Pressure: This parameter tries to protect the membrane from liquid penetration, which may cause membrane wetting. This parameter is directly connected to the performance of the distillation system due to membrane wetting.

These equations are connected in the MATLAB software such that any small change to one property can affect the system, and record the behavior of changes on the output, which provides an idea about the effective values in the system.

MATLAB software has been used to build the optimization model by sweeping the parameters. All parameters of membrane properties, such as porosity, pore size, membrane thickness, and contact angle, have different effects on the output of the system. The results were analyzed and plotted for visual representation to know about the trends in the performance. The plots and graphs were recorded and verified from the journal articles. Next, multi-objective optimization is applied by using the desirability function. The main objective was to identify the most optimized combination of the membrane properties, which provides the maximum permeate flux and mass transfer coefficient by keeping the Liquid Entry Pressure on the safety threshold, which is around 300 kPa. Next, the results were verified and compared with the journal article to validate the prediction model. The value from the prediction model closely aligns with the data in peer-reviewed articles, which ensures the reliability of the model. Next, sensitivity analysis was applied to change some input parameters by 10%. This study presents the minimum deviation occurring in performance trends, representing the stable and reliable model.

Several assumptions and boundary conditions were applied to modify the Prediction Model:

- It's important to ensure a Steady-state operational environment of the Membrane Distillation system.
- It's crucial to maintain inlet feed and balanced permeate temperatures.
- The system can lose a negligible amount of heat to the environment.
- The membrane should be protected from fouling and wetting of the membrane.

3.8 UPGRADED METHODOLOGY FROM ENGR6009

In ENGR6009, some basic equations were developed from peer-reviewed articles.

Moreover, it discussed several fixed and variable parameters. Furthermore, it discussed some basic operations of MATLAB. But in ENGR 6010, lots of methodological improvements have been made:

- Lots of new equations and functions have been introduced for optimization from peer-reviewed articles.
- Equations have been modified and prepared to use them for building the prediction model via MATLAB software.
- The desirability function has been developed to understand the performance of the permeate flux, mass transfer coefficient, and Liquid Entry Pressure.
- An optimization function has been introduced to use the desirability approach.
- Parameter sweeping techniques have been developed on MATLAB to observe the individual performance of the membrane properties.
- Lots of plots have been presented to show the performance of the Membrane properties, such as pore size, porosity, membrane thickness, and contact angle. Data visualization has been enhanced by providing complete ideas. It also compares the value with the literature data.
- It validates the model by comparing it with peer-reviewed articles.

Besides, it works on the future work and limitations of the study. It provides a strong idea about theoretical membrane design by protecting the membrane from fouling and wetting, which can degrade the membrane in the long term, but it does not discuss the polarization of temperature and scaling. So, there is a scope to figure out those in the future because it could improve the performance of the membrane. Besides, CFD (Computational Fluid Dynamics) could be applied to combine the MATLAB model to observe the distributions of temperature

and flow visually. Next, lab experiments could be applied according to the design of the membrane to validate the model.

4.0 IMPLEMENTATION OF RESULTS

The Membrane Distillation system is an iconic technique that aids in producing a substantial amount of purified water by saving energy. This study examines properties of the membrane, such as membrane thickness, pore size, porosity & contact angle, and assesses the membrane properties and their impacts on the system performance. The thesis examines the performance of the system by building up the prediction model via the MATLAB software and evaluates the impact of membrane properties on producing fresh water with minimum supply of energy. The thesis is designed to create a prediction model, including the equations to calculate the heat and mass transfer coefficient, the permeate flux, and Liquid Entry Pressure (LEP).

The thesis is working on finding out the optimum values of the properties of the membrane. Initially, this study tries to find out the behavioural characteristics of the membrane properties in the system. Findings are given below:

- Membrane thickness minimization is important to increase the production rate of fresh water because increasing the membrane thickness drops the production rate of fresh water.
- Determination of the optimal value for the pore size, porosity is crucial to get the enhanced freshwater production, as maximization of pore size and porosity has positive consequences on permeate flux but has negative impacts on Liquid Entry Pressure, which may result in membrane wetting.

The MATLAB prediction model provides an insightful idea to get better performance of the system through the evaluation of the membrane properties, such as porosity, pore size, membrane thickness, and contact angle, and concentrates on the parameters for enhancing the performance of desalination.

4.1 SUMMARIZATION OF THE MEMBRANE DISTILLATION SYSTEM

The Membrane Distillation System is shown in Figure 3.1, which represents a small-scale laboratory experimental setup under a controlled environment, where all components are visible, aiding in understanding the membrane distillation system.

A membrane distillation system may have two sections: one is for the saline water, contained in the feed tank, and another is for the permeate flux, contained in the Permeate Tank. Here, the heating plate connects to the feed water tank, maintaining a temperature of 66 °C. Furthermore, the permeate tank is connected to a chiller, maintaining a temperature of 44 °C. A conductivity meter calculates the rejection rate of salt and other impurities. Here, the feed pump helps to circulate hot water along the membrane, and the permeate pump circulates the cold water around the membrane to create the temperature difference, aiding in repeatedly pushing the water vapor through the membrane, gradually going through the pores of the membrane, and condensing into freshwater.

4.2 THE REVIEW OF EQUATIONS AND PARAMETERS

This study is planned to develop a prediction model by using some equations, which aids in building an optimized model via MATLAB Software for the Membrane Distillation system. Some equations are used in MATLAB to calculate the permeate flux, Mass Transfer coefficient & Liquid Pressure Entry (LEP), which are given below [35].

Permeate Flux:

$$J_p = C_w \left(\frac{H_{fg}}{(R_{const} \times (T_m + 273) \times P_m)} \right) (T_{hi} - T_{ci})$$

Here,

J_p = Permeate Flux, T_{hi} = Inlet Heat Temperature, T_{ci} = Inlet Cold Temperature, C_w = Mass Transfer Coefficient, T_m = Mean Temperature, P_m = Mean Pressure, H_{fg} = Latent Heat Vaporization, R_{const} = Specific Gas Content

Liquid Entry Pressure:

$$LEP = \left[\frac{-2 \times y_i}{r_{memb}} \right] \times \cos \theta$$

Here,

r_{memb} = largest pore size, y_i = sea water surface tension, θ = Contact angle between water and the membrane surface

Mass Transfer Coefficient:

$$K_m = \left[\frac{J_p \times H_{fg}}{T_{hi} - T_{ci}} \right] \times 1$$

Fixed parameters are given below:

The area of the Membrane = $0.22 \times 10.13 \text{ m}^2$, Thermal Conductivity = $0.000189 \text{ kW/m} \cdot ^\circ\text{C}$, Feed water Tank Temperature = 66°C , Permeate tank temperature = 44°C , the salinity of feed = 35020 ppm, the efficiency of pump = 0.76

The parameters of membrane properties are adjusted in MATLAB software to understand their impact on the system, which will aid in improving the permeate flux. Variable parameters are shown below:

Porosity, Pore Size, Membrane thickness, and contact angle vary from 0.48 to 0.91, $0.21 \mu\text{m}$ to $0.98 \mu\text{m}$, $70.31 \mu\text{m}$ to $190.18 \mu\text{m}$, 85° to 145° , respectively.

4.3 MATLAB WORKFLOW

MATLAB Software is designed to perform complex calculations, but before doing so, it needs to establish a solid foundation of knowledge. Based on that knowledge, it is important to work on some equations according to the target output. After getting the equations, it is crucial to have proper knowledge about the parameters from the equations. Moreover, it

needs to be mentioned about the boundary conditions or any other assumptions for the controlled setup.

All necessary steps are taken to work on the MATLAB Software. For instance, insightful knowledge of membrane distillation was learnt from the peer-reviewed articles. Next, it was documented in the literature review section, which helped to identify the goals of the research. Next, the foremost task is to find out the equations that align with the target of the research. Then, it's necessary to have profound knowledge of the parameters of the equation, as well as needs to consider boundary conditions and assumptions.

Some assumptions for this thesis are given below:

- Steady-state operation environment is considered for the membrane distillation system
- The temperatures for the inlet are constant for two separate sides of the membrane surface.
- Heat loss is considered negligible to the environment.
- Pore size is uniform

Once the equation is set and already documented about the fixed and variable parameters, it is the perfect time to start the MATLAB coding to get the prediction model.

The MATLAB code for presenting the prediction model is given below:

<pre> %% MD Validation using governing equations clear; clc; close all; %% ----- Constants ----- Hfg = 2.406e6; % J/kg (latent heat of vaporization) Rconst = 461.5; % J/kg.K (specific gas constant for water vapor) Thi = 66; % °C, feed hot side Tci = 44; % °C, cold side Tm = (Thi + Tci)/2; % mean temperature dT = Thi - Tci; % temperature difference Pm = 1.013e5; % Pa (mean pore pressure, ~1 atm) gamma = 0.067; % N/m (surface tension of water) tau = 2; % tortuosity (assumed) %% ----- Parameter sweeps ----- th_um = [70.31 80 90 110 130 160 190.18]; % thickness μm epsil = [0.50 0.60 0.70 0.80 0.90]; % porosity (-) d_um = [0.22 0.30 0.40 0.50 0.60 0.70 0.80]; % pore diameter μm theta = [90 100 110 120 130 140 150]; % contact angle deg % Baseline eps0 = 0.80; d0 = 0.22; th0 = 70.31; theta0 = 120; %% ----- Mass transfer coefficient function ----- % Overall mass transfer coefficient $Cw \propto (\epsilon * d) / (\tau * \delta)$ Cw_fun = @(eps, d_um_loc, th_um_loc) ... (eps .* d_um_loc*1e-6) ./ (tau .* th_um_loc*1e-6); % Baseline scaling to match $J_p = 66.79 \text{ kg/m}^2\cdot\text{h}$ Cw_base = Cw_fun(eps0, d0, th0); scaleFact = 66.79/3600 / (Cw_base * (Hfg/(Rconst*(Tm+273)*Pm)) * dT); % Final calibrated Cw function Cw_fun_cal = @(eps, d_um_loc, th_um_loc) ... scaleFact * ((eps .* d_um_loc*1e-6) ./ (tau .* th_um_loc*1e-6)); %% ----- Governing equations ----- % Permeate flux Jp_fun = @(eps, d_um_loc, th_um_loc) ... Cw_fun_cal(eps, d_um_loc, th_um_loc) .* ... (Hfg ./ (Rconst*(Tm+273).*Pm)) .* dT; % kg/m2.s % Convert to kg/m2.h Jp_fun_h = @(eps, d_um_loc, th_um_loc) 3600 * Jp_fun(eps, d_um_loc, th_um_loc); % Mass transfer coefficient Km_fun = @(Jp_h) ((Jp_h/3600) * Hfg) / dT / 1000; % kJ/m2.s.°C % LEP LEP_fun = @(d_um_loc, theta_deg) ... (2*gamma*abs(cosd(theta_deg))) ./ (d_um_loc*1e-6) / 1000; % kPa %% ----- Model predictions ----- % Thickness sweep Jp_th_mod = Jp_fun_h(eps0, d0, th_um); Km_th_mod = Km_fun(Jp_th_mod); LEP_th_mod = LEP_fun(d0, theta0) * ones(size(th_um)); % Porosity sweep Jp_eps_mod = Jp_fun_h(epsil, d0, th0); Km_eps_mod = Km_fun(Jp_eps_mod); LEP_eps_mod = LEP_fun(d0, theta0) * ones(size(epsil)); % Contact angle sweep Jp_tht_mod = Jp_fun_h(eps0, d0, th0) * ones(size(theta)); Km_tht_mod = Km_fun(Jp_tht_mod); LEP_tht_mod = LEP_fun(d0, theta); %% ----- Plotting ----- plotDv(th_um, Jp_th_mod, 'Thickness (\num)', 'Permeate flux (kg m⁻² h⁻¹)', 'Permeate flux vs Thickness (\num)'); plotDv(epsil, Jp_eps_mod, 'Porosity (-)', 'Permeate flux (kg m⁻² h⁻¹)', 'Permeate flux vs Porosity (-)'); plotDv(d_um, Jp_d_mod, 'Pore diameter (\num)', 'Permeate flux (kg m⁻² h⁻¹)', 'Permeate flux vs Pore diameter (\num)'); plotDv(theta, Jp_tht_mod, 'Contact angle (deg)', 'Permeate flux (kg m⁻² h⁻¹)', 'Permeate flux vs Contact angle (deg)'); plotDv(th_um, Km_th_mod, 'Thickness (\num)', 'Mass transfer coefficient (kJ m⁻² s⁻¹ °C⁻¹)', 'Mass transfer coefficient vs Thickness (\num)'); plotDv(epsil, Km_eps_mod, 'Porosity (-)', 'Mass transfer coefficient (kJ m⁻² s⁻¹ °C⁻¹)', 'Mass transfer coefficient vs Porosity (-)'); plotDv(d_um, Km_d_mod, 'Pore diameter (\num)', 'Mass transfer coefficient (kJ m⁻² s⁻¹ °C⁻¹)', 'Mass transfer coefficient vs Pore diameter (\num)'); plotDv(theta, Km_tht_mod, 'Contact angle (deg)', 'Mass transfer coefficient (kJ m⁻² s⁻¹ °C⁻¹)', 'Mass transfer coefficient vs Contact angle (deg)'); plotDv(th_um, LEP_th_mod, 'Thickness (\num)', 'LEP (kPa)', 'LEP vs Thickness (\num)'); plotDv(epsil, LEP_eps_mod, 'Porosity (-)', 'LEP (kPa)', 'LEP vs Porosity (-)'); plotDv(d_um, LEP_d_mod, 'Pore diameter (\num)', 'LEP (kPa)', 'LEP vs Pore diameter (\num)'); plotDv(theta, LEP_tht_mod, 'Contact angle (deg)', 'LEP (kPa)', 'LEP vs Contact angle (deg)'); %% ----- Helper function ----- function plotDv(x, x1, y1, ttl) figure('Color','w'); plot(x, y, 'bo-', 'LineWidth',1.6, 'MarkerFaceColor','b'); grid on; xlabel(x1, 'Interpreter','tex'); ylabel(y1, 'Interpreter','tex'); title(ttl, 'Interpreter','tex'); end </pre>	
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Figure 4.1: MATLAB Code Generation

Figure 4.1 presents MATLAB code for building the prediction model. The MATLAB code was organized from the equations of permeate flux, mass transfer coefficient, and liquid entry pressure. Moreover, it explains the performance of the system, like how well the

system can separate the impure materials from the saline water and produce fresh water efficiently.

Initially, the code starts by introducing all fixed and variable parameters, for instance, the latent heat of vaporization, specific gas constant for water vapor, and the temperature difference between hot feed and cold feed, mean temperature, mean pressure of pore, tortuosity, and so on, as fixed parameters. Variable parameters are the membrane thickness, porosity, pore size & contact angle. In MATLAB code, ranges were set for the variable parameters, and these values are taken from the peer-reviewed articles. Next, the MATLAB code works on the equations of the permeate flux, mass transfer coefficient, and Liquid Entry Pressure to understand the impacts of the variable parameters on the performance of the system. Furthermore, MATLAB uses the parameter sweeping technique, which changes one parameter by making fix to other parameters to observe the influence of the variable parameters, such as pore size, porosity, membrane thickness, and contact angle, on the performance metrics, which are permeate flux, mass transfer coefficient, and Liquid Entry Pressure.

The function plot0v is introduced in the MATLAB code, which is used to plot the graphs to exhibit the relationship between the variable parameters and the output of the system. For instance, some plots show how the increasing pattern of membrane thickness decreases the production rate of permeate flux, and how a higher contact angle enhances the Liquid Entry Pressure. MATLAB code generates lots of plots, which are beneficial for understanding the importance of the membrane design.

4.4 INFLUENCE OF THE MEMBRANE PROPERTIES ON OUTPUT

This section discusses the influence of membrane properties, such as membrane thickness, pore size, porosity, and contact angle, on permeate flux, mass transfer coefficient, and Liquid Pressure Entry. This section explains the relationship between the membrane properties and

performance metrics by illustrating the plot, which aids in understanding with clear ideas. First, starting with presenting the relationship between Permeate Flux and Membrane Thickness, which is given below:

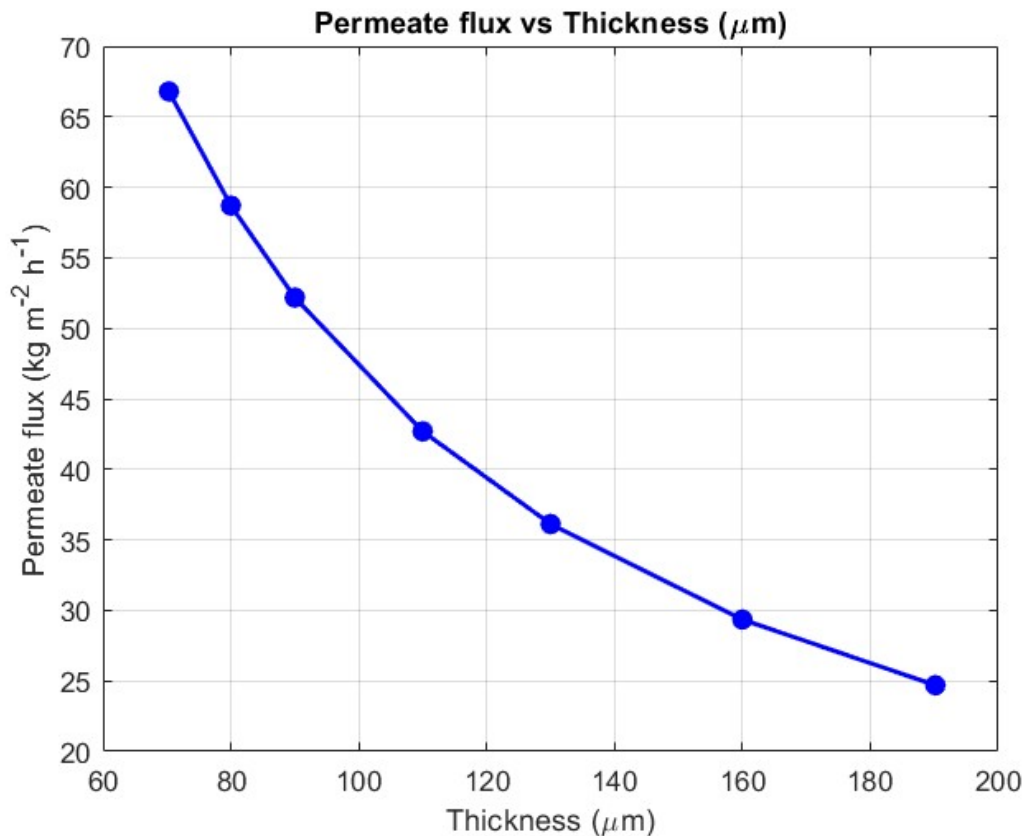


Figure 4.2: The relationship between Membrane thickness and Permeate Flux

Figure 4.2 represents the relationship between the membrane thickness and permeate flux. Moreover, it depicts how the permeate flux responds to the change in the membrane thickness in the direct contact membrane distillation system. It is visible in Figure 4.2 that the increasing pattern of membrane thickness reduces the production of permeate flux. This is occurring because a thicker membrane makes a longer path and creates more resistance for water vapor to pass through the membrane and requires more pressure to transfer the water vapor to the permeate tank, which has a negative effect on energy efficiency. That's why water vapor moves more slowly and goes through more resistance inside the membrane

and produces less amount of fresh water [37]. In Contrast, a thin membrane is easier for water vapor to go through the membrane, which leads to the production of a huge amount of permeate flux. Though a thinner membrane may affect the mechanical strength of the membrane, it may lead to the membrane wetting, which reduces the durability of the membrane. Lastly, a thinner membrane enhances the performance of producing permeate flux but may affect the mechanical strength of the membrane. That's why it is crucial to find out the optimal value of membrane thickness, which may aid in producing the permeate flux by maintaining stability in the Membrane Desalination system [38].

Next, this section discusses the influence of the porosity on the permeate flux production. This section describes the relationship between the porosity and permeate flux by depicting a graph that makes it easier to understand with clear views. Now, it's time to present the relationship between Permeate Flux and Porosity, which is shown below:

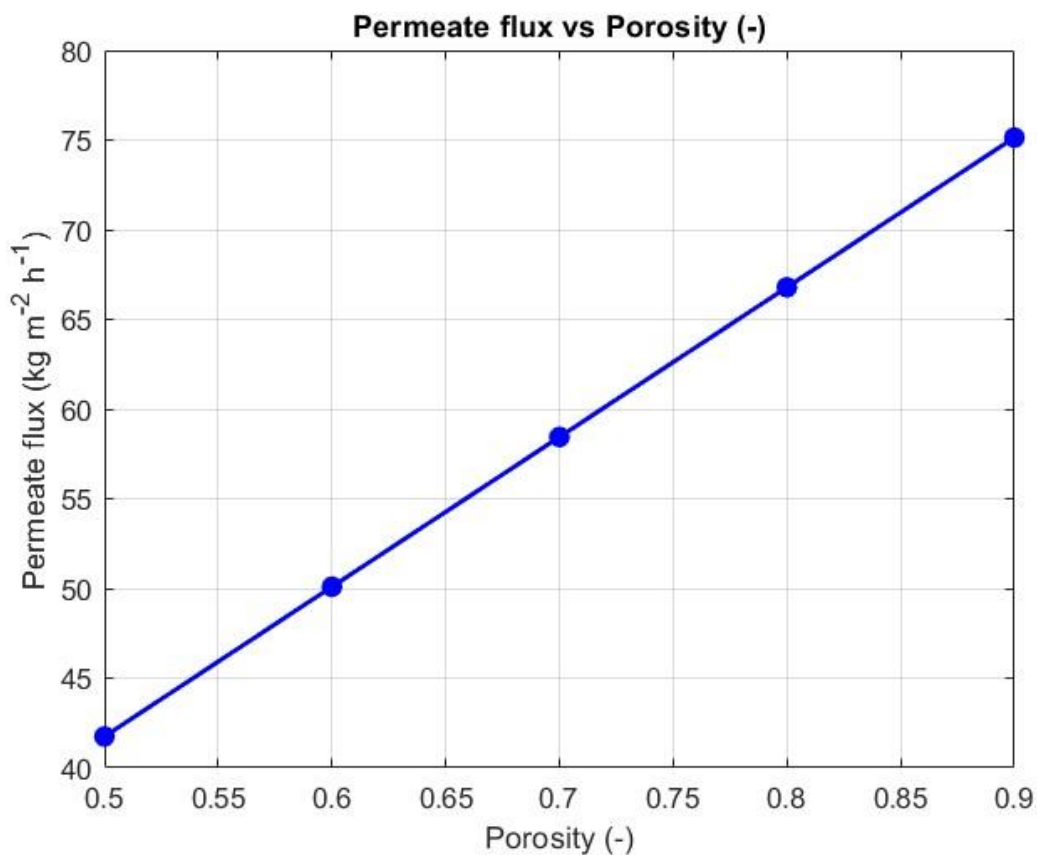


Figure 4.3: The relationship between Porosity and Permeate Flux

Figure 4.3 illustrates the relationship between the porosity and permeate flux. Furthermore, it explains the response of the permeate flux under the influence of porosity in the membrane distillation system. It is clearly shown in Figure 4.3 that the higher amount of porosity increases the production of fresh water because the membrane with a higher amount of porosity permits more water vapor to go through the surface of the membrane, which leads to producing more water. On the other hand, the lower amount of porosity makes it difficult for water vapor to travel through the surface of the membrane due to the blockage on the way for water vapor, leading to a drop in the production of purified water. On the other hand, a higher amount of porosity makes it easier for travel through the membrane because it opens more ways for water vapor to go through the surface of the membrane, also easier to produce more fresh water due to having fewer restrictions. A lower amount of porosity restricts the way for the vapor to travel through the membrane surface due to having a smaller number of open pores, which results in a drop in the production of fresh water [39]. On the other hand, higher porosity creates more scope for mass transfer through the open pores, which lowers the resistance to mass transfer and enhances vapor transportation across the membrane surface, resulting in the production of more fresh water. Although higher porosity makes it easier to produce more fresh water, it weakens the membrane and increases the likelihood of membrane wetting, which has a detrimental impact on the system's performance. Therefore, it's important to identify the optimum level of porosity for maximum production of purified water by maintaining the durability and stability of the membrane distillation system [40]. Next, this part discusses the influence of the pore diameter on the permeate flux production, which is presented below:

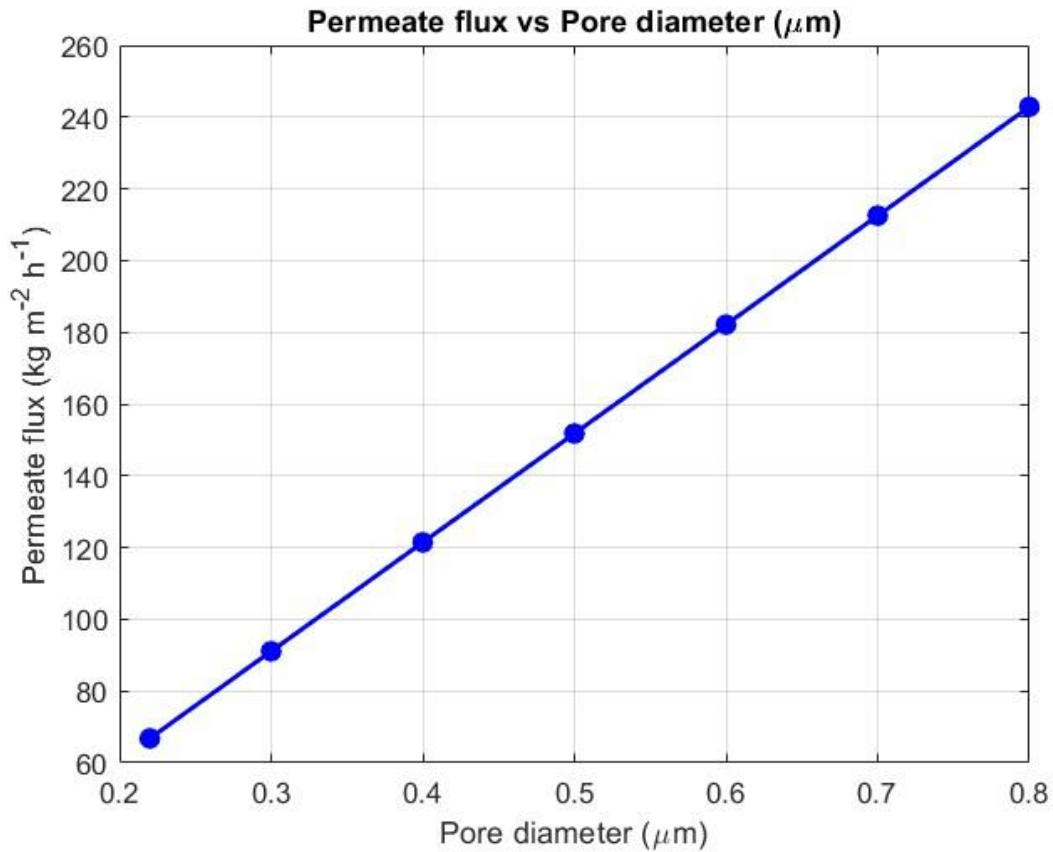


Figure 4.4: Pore Diameter vs Permeate flux

Figure 4.4 depicts the relationship between the pore diameter and permeate flux. Moreover, it explains how well the pore diameter responds to the production of the purified water in the membrane distillation system. It is visible in Figure 4.4 that a larger pore diameter increases the production of fresh water because the membrane with a larger pore diameter allows more water vapor to go through the surface of the membrane, enhancing the permeate flux. In contrast, the lower pore diameter makes it difficult for water vapor to go through the surface of the membrane due to restricting the water vapor from traveling, leading to a drop in the production of purified water. On the other hand, a larger pore diameter has the advantage for travel through the membrane because it opens more ways for water vapor to go through the surface of the membrane, also easier to produce more fresh water due to having fewer restrictions. A lower pore diameter restricts the way for the vapor to travel through the membrane surface due to having a smaller number of open pores, which results

in a drop in the production of fresh water [41]. On the other hand, a higher pore diameter creates more scope for mass transfer through the open pores, which lowers the resistance to mass transfer and enhances vapor transportation across the membrane surface, resulting in the production of more fresh water. Although a higher pore diameter makes it easier to produce more fresh water, it weakens the membrane and increases the likelihood of membrane wetting. Therefore, it's crucial to determine the optimum value of pore diameter for enhancing the permeate flux while maintaining the durability and stability of the membrane distillation system [42]. Now, this section discusses the influence of the contact angle on the permeate flux production, which is presented below:

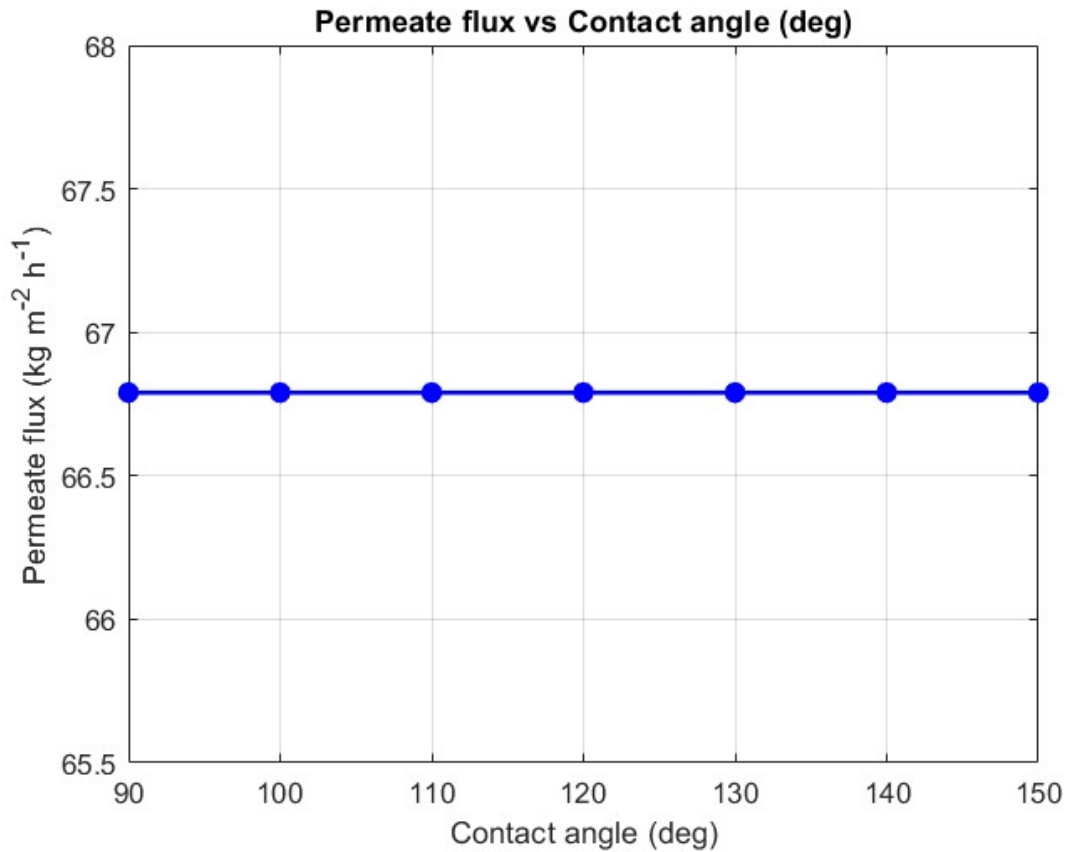


Figure 4.5: The relationship between Contact Angle and Permeate Flux

Figure 4.5 depicts the relationship between the contact angle and permeate flux in the membrane distillation system. Furthermore, it illustrates the influence of the contact angle on permeate flux in the membrane distillation system. It is shown in Figure 4.5 that the permeate flux remains constant when the contact angle changes from 90 degrees to 150 degrees. It establishes that the contact angle does not have any impact on fresh water production. Moreover, the contact angle can't change anything in the system when the water vapor moves and goes through the surface of the membrane. However, the contact angle doesn't make any difference during the production of fresh water; it directly affects the wetting tendency of the membrane. A higher contact angle makes the membrane surface more hydrophobic, which aids in protecting the pores from water penetration. Furthermore, it helps to improve the wetting resistance of the membrane. Although the contact angle does

not have any direct impact on the freshwater production, it protects the membrane from wetting and makes the membrane more durable. Therefore, higher contact enhances the performance of the membrane distillation system by protecting the membrane from wetting, which makes the membrane more durable, but doesn't have any influence on the freshwater production [43].

This section discusses the influence of membrane properties, such as membrane thickness, pore size, porosity, and contact angle, on permeate flux. Next, this section is planned to identify the relationship between the membrane properties and mass transfer coefficient by illustrating the plot, which aids in understanding with insightful ideas. Now, starting with presenting the relationship between the Mass Transfer coefficient and Membrane Thickness, which is given below:

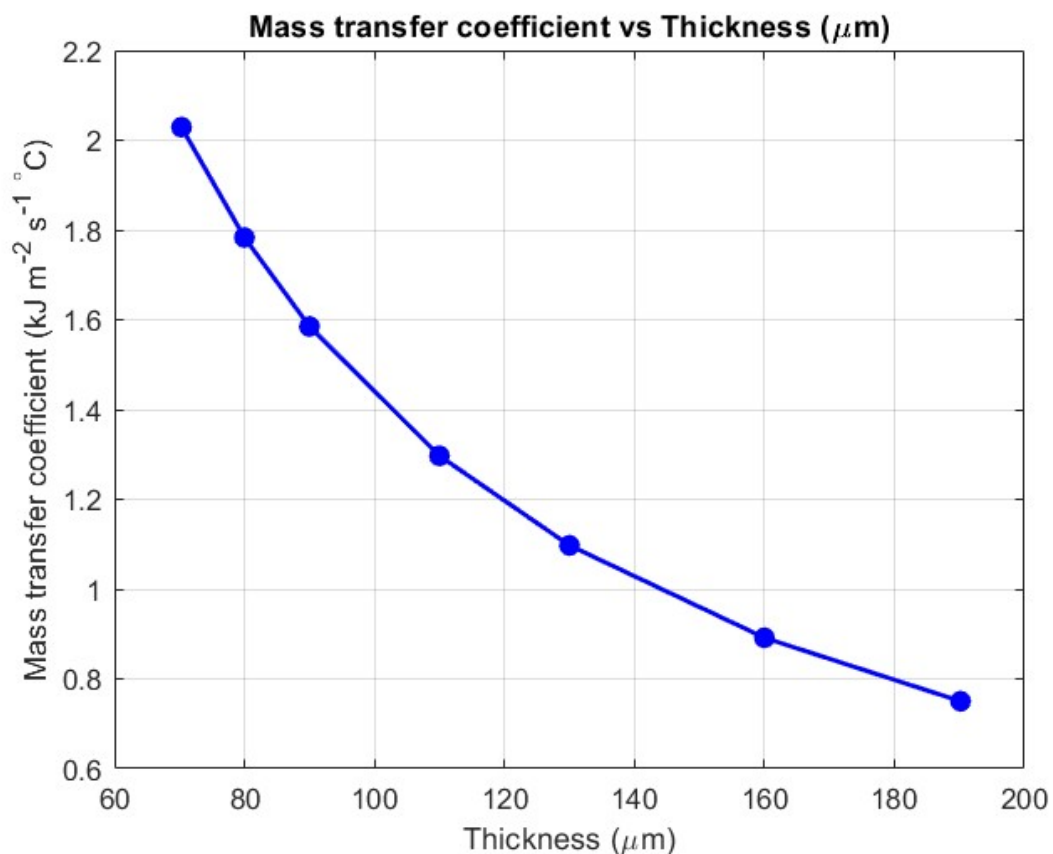


Figure 4.6: Membrane thickness vs Mass Transfer Coefficient

Figure 4.6 represents the relationship between the membrane thickness and mass transfer coefficient. Furthermore, it illustrates how the mass transfer coefficient responds to the change in the membrane thickness in the direct contact membrane distillation system. It is visible in Figure 4.6 that the increasing pattern of membrane thickness reduces the transfer of molecules of water vapor, which drops in the mass transfer coefficient. This is occurring because a thicker membrane makes a longer path and creates more resistance for water vapor to pass through the membrane, and requires more pressure to transfer the water vapor to the permeate tank, which has a negative effect on energy efficiency. That's why water vapor moves more slowly and goes through more resistance inside the membrane, transferring a smaller amount of vapor molecules, resulting in less amount of permeate flux [44]. In Contrast, a thin membrane is easier for water vapor to go through the membrane, creating a scope to pass through a huge amount of vapor molecules, which leads to the production of a huge amount of fresh water. Though a thinner membrane may affect the mechanical strength of the membrane, it may lead to the membrane wetting, which reduces the durability of the membrane. Lastly, a thinner membrane enhances the performance of the mass transfer coefficient but may affect the mechanical strength of the membrane. That's why it is crucial to find out the optimal value of membrane thickness, which may aid in enhancing the performance of the mass transfer coefficient by maintaining stability in the Membrane Desalination system [45].

Next, this section discusses the influence of porosity on the mass transfer coefficient. This section describes the relationship between the porosity and mass transfer coefficient by depicting a graph that makes it easier to understand with clear views. Now, it's time to present the relationship between mass transfer coefficient and Porosity, which is shown below:

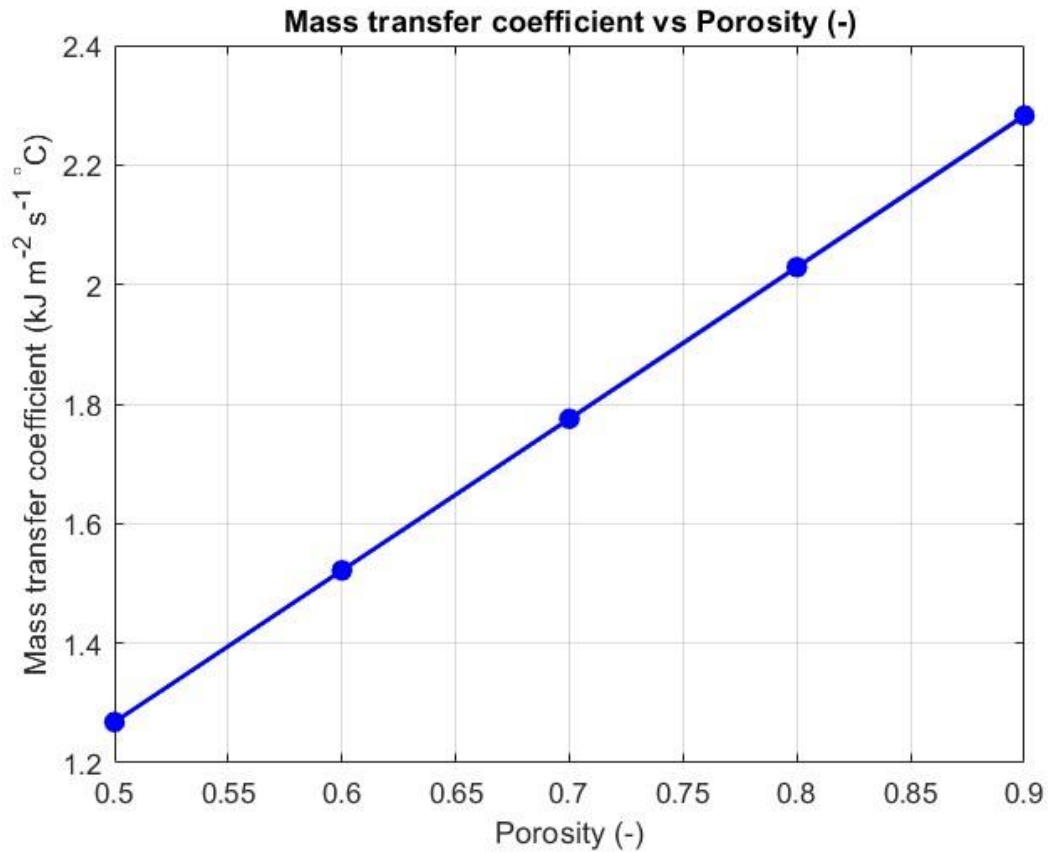


Figure 4.7: Mass Transfer Coefficient vs Porosity

Figure 4.7 illustrates the relationship between the porosity and the mass transfer coefficient. Furthermore, it explains the response of the mass transfer coefficient under the influence of porosity in the membrane distillation system. It is clearly shown in Figure 4.7 that the higher amount of porosity increases the production of fresh water because the membrane with a higher amount of porosity permits more vapor molecules to pass through the surface of the membrane, leading to an enhancement of the performance of the mass transfer coefficient. On the other hand, the lower amount of porosity makes it difficult for water vapor molecules to travel through the surface of the membrane due to the blockage on the way for water vapor, leading to a drop in the mass transfer coefficient. On the other hand, a higher amount of porosity makes it easier for water vapor molecules to travel through the surface of the membrane, also easier to produce more fresh water due to having fewer restrictions. A lower amount of porosity restricts the way for the molecules of water vapor to travel through the

membrane surface due to having a smaller number of open pores, which results in a drop in the production of fresh water [46]. On the other hand, higher porosity creates more scope for mass transfer through the open pores, which lowers the resistance to mass transfer and enhances vapor transportation across the membrane surface, resulting in a higher mass transfer coefficient. Although higher porosity makes it easier to produce more fresh water, it weakens the membrane and increases the likelihood of membrane wetting, which has a detrimental impact on the system's performance. Therefore, it's important to identify the optimum level of porosity for an enhanced mass transfer coefficient by maintaining the durability and stability of the membrane distillation system [47]. Next, this part discusses the influence of the pore diameter on the mass transfer coefficient, which is presented below:

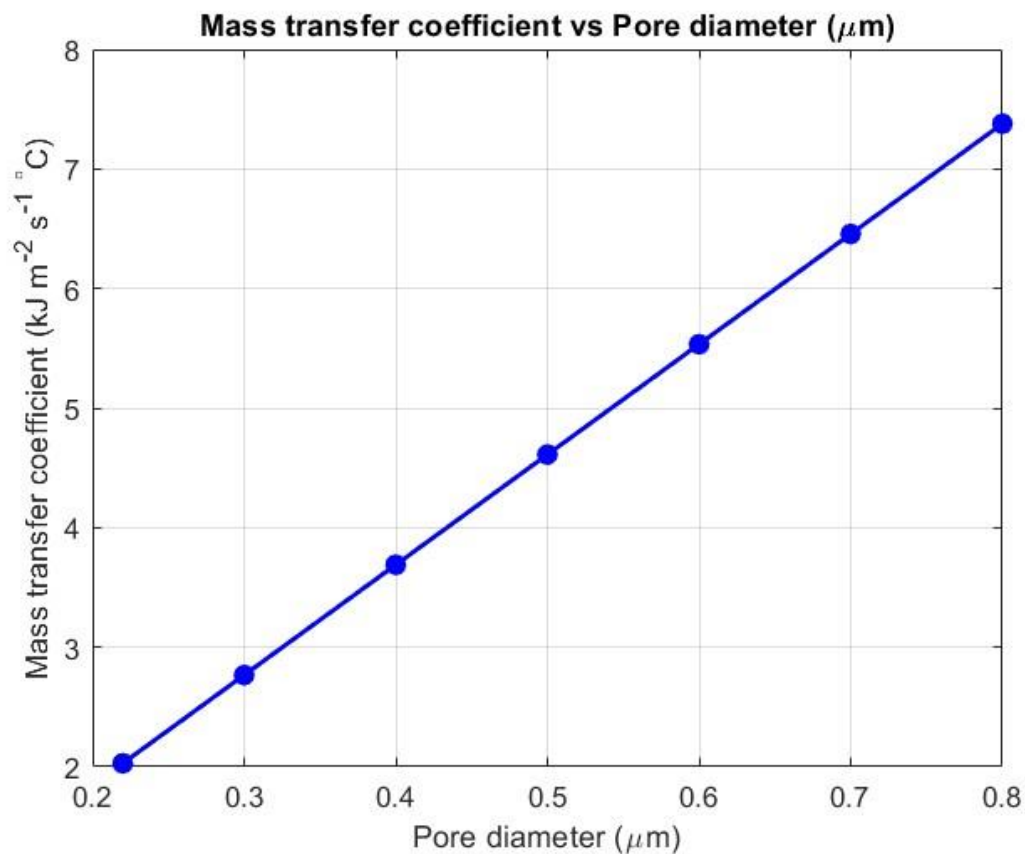


Figure 4.8: Mass Transfer Coefficient vs Pore Diameter

Figure 4.8 depicts the relationship between the pore diameter and mass transfer coefficient. Moreover, it explains how well the pore diameter responds to the mass transfer coefficient

in the membrane distillation system. It is visible in Figure 4.8 that a larger pore diameter increases the scope for more vapor molecules to travel because the membrane with a larger pore diameter allows more water vapor molecules to go through the surface of the membrane, increasing the value of the mass transfer coefficient. In contrast, the lower pore diameter makes it difficult for water vapor to go through the surface of the membrane due to restricting the water vapor from traveling, leading to a drop in the mass transfer coefficient. On the other hand, a larger pore diameter has the advantage for travel through the membrane because it opens more ways for water vapor to go through the surface of the membrane, also easier to transfer more water vapor molecules due to having fewer restrictions. A lower pore diameter restricts the way for the vapor to travel through the membrane surface due to having a smaller number of open pores, which results in a drop in the mass transfer coefficient [48]. On the other hand, a higher pore diameter creates more scope for mass transfer through the open pores, which lowers the resistance to mass transfer and enhances vapor transportation across the membrane surface, increasing the mass transfer coefficient. Although a higher pore diameter makes it easier to transfer more molecules of water vapor, it weakens the membrane and increases the likelihood of membrane wetting. Therefore, it's crucial to determine the optimum value of pore diameter for enhancing the mass transfer coefficient while maintaining the durability and stability of the membrane distillation system [49]. Now, this section discusses the influence of the contact angle on the mass transfer coefficient, which is presented below:

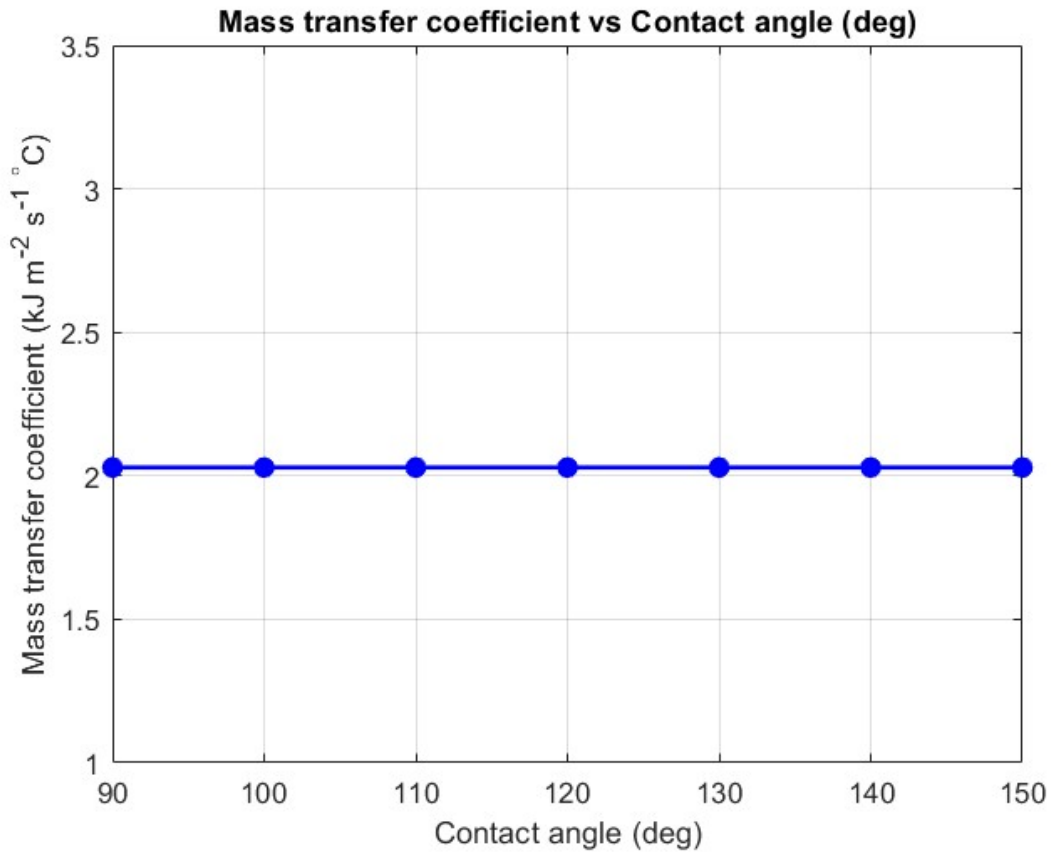


Figure 4.9: Mass Transfer Coefficient vs Contact Angle

Figure 4.9 depicts the relationship between the contact angle and mass transfer coefficient in the membrane distillation system. Furthermore, it depicts the influencing nature of the contact angle on the mass transfer coefficient in the membrane distillation system. As shown in Figure 4.9, the mass transfer coefficient remains constant when the contact angle changes from 90 degrees to 150 degrees. It establishes that the contact angle does not have any impact on freshwater production. Moreover, the contact angle can't change anything in the system when water vapor moves through the surface of the membrane. However, the contact angle doesn't make any difference in the mass transfer coefficient on the system; it directly affects the wetting tendency of the membrane. A higher contact angle makes the membrane surface more hydrophobic, which aids in protecting the pores from water penetration. Furthermore, it helps to improve the wetting resistance of the membrane. Although the contact angle does not have any direct impact on the mass transfer coefficient, it protects the membrane from

wetting and makes the membrane more durable. Therefore, a higher contact angle enhances the performance of the membrane distillation system by protecting the membrane from wetting, which makes the membrane more durable, but doesn't have any influence on the freshwater production.

This section discusses the influence of membrane properties, such as membrane thickness, pore size, porosity, and contact angle, on the mass transfer coefficient. Next, this section is planned to identify the relationship between the membrane properties and mass transfer coefficient by illustrating the plot, which aids in understanding with insightful ideas. Now, starting with presenting the relationship between the Liquid Entry Pressure and Membrane Thickness, which is given below:

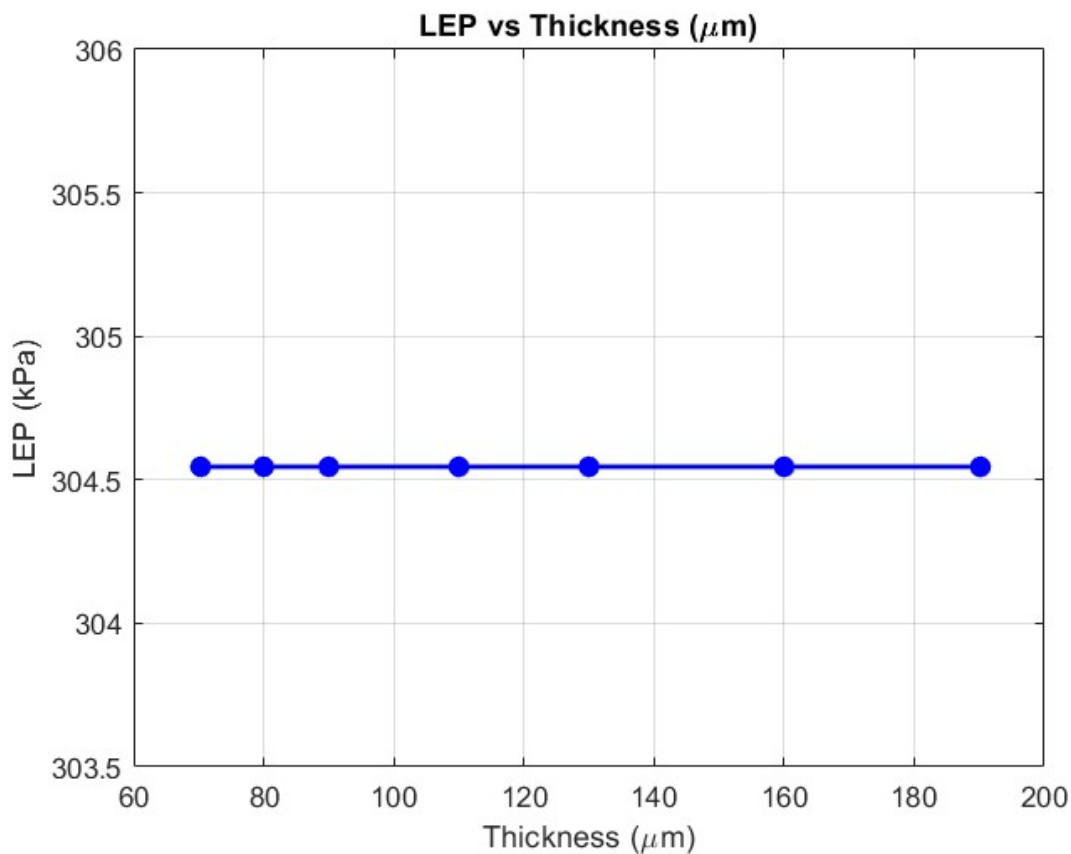


Figure 4.10: LEP vs Membrane Thickness

Figure 4.10 depicts the relationship between the membrane Thickness and Liquid Entry Pressure in the membrane distillation system. Furthermore, it illustrates the influence of

membrane thickness on Liquid Entry Pressure in the membrane distillation system. It is shown in Figure 4.10 that the membrane thickness remains Liquid Entry Pressure when the membrane thickness changes from 70 micrometres to 190 micrometres. It establishes that the membrane thickness does not have any impact on Liquid Entry Pressure. Moreover, the membrane thickness can't change anything about the Liquid Entry Pressure. However, the membrane thickness doesn't make any difference in the LEP in the system; it directly affects the permeate flux and mass transfer coefficient [50].

In short, it is shown in Figure 4.10 that membrane thickness doesn't have any impact on the Liquid Entry Pressure on the system.

Next, this part discusses the influence of the porosity on the Liquid Pressure Entry, which is presented below:

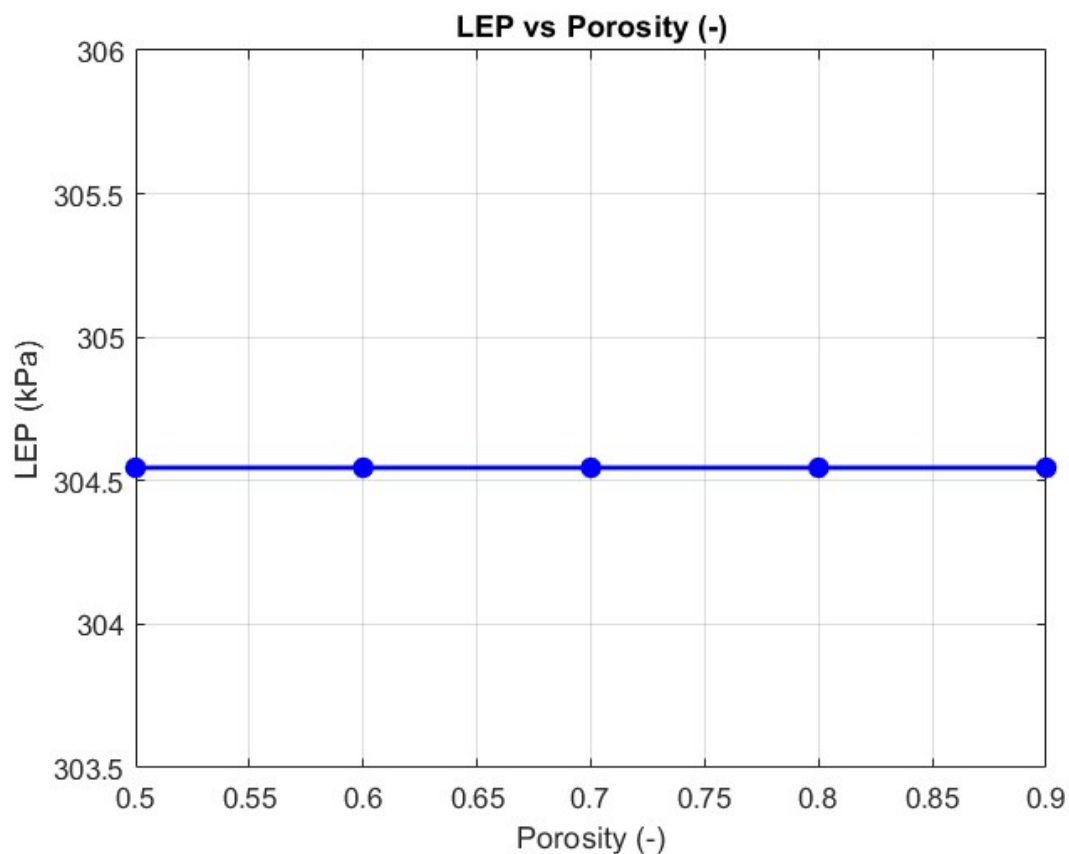


Figure 4.11: Liquid Entry Pressure vs Porosity

Figure 4.11 depicts the relationship between the Porosity and Liquid Entry Pressure in the membrane distillation system. Furthermore, it illustrates the influence of Porosity on Liquid Entry Pressure in the membrane distillation system. It is visible in Figure 4.11 that porosity remains the Liquid Entry Pressure when the liquid Entry Pressure changes from 0.5 to 0.9. It establishes that the porosity does not have any impact on Liquid Entry Pressure. Moreover, the Porosity can't change anything about the Liquid Entry Pressure. In short, the Porosity doesn't make any difference in the LEP in the system; it directly affects the permeate flux and mass transfer coefficient [51]. Next, this section will discuss the influence of the pore diameter on Liquid Entry Pressure. Now, it's time to present the relationship between Pore Diameter and Liquid Entry Pressure, which is shown below:

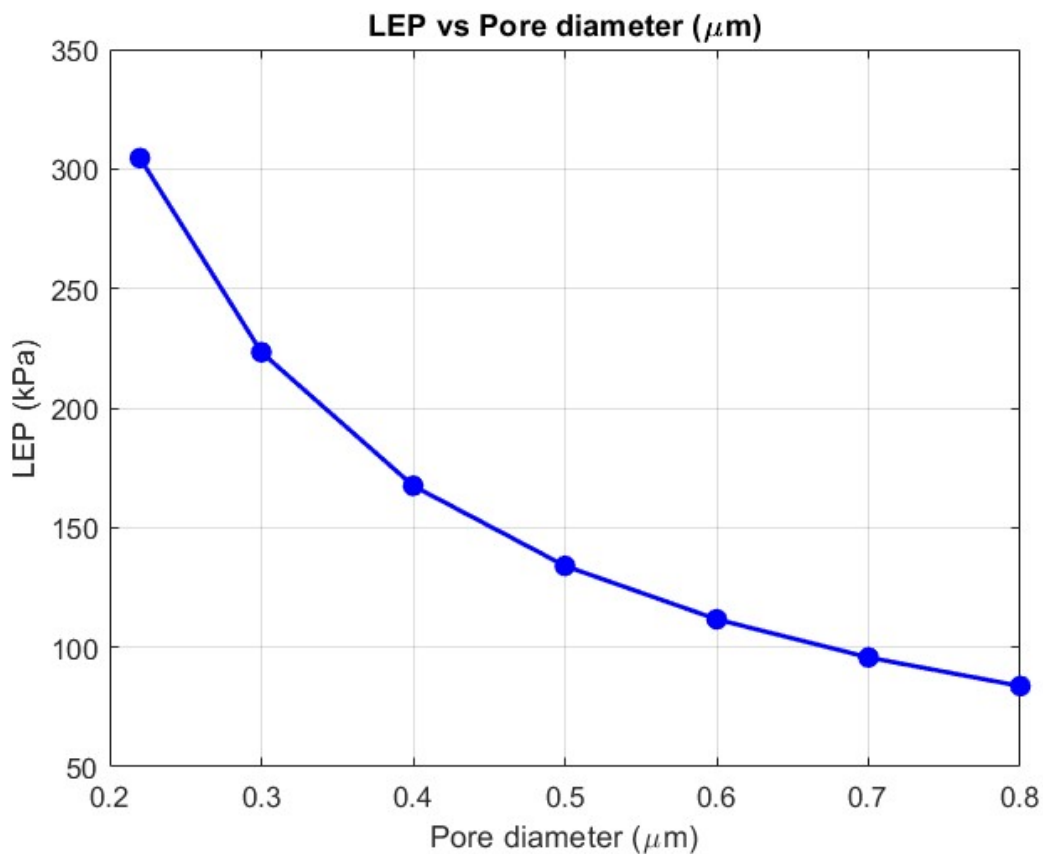


Figure 4.12: Liquid Entry Pressure vs Pore Diameter

Figure 4.12 depicts the relationship between the Pore Diameter and Liquid Entry Pressure. Moreover, it explains how well the pore diameter responds to the Liquid Entry Pressure in

the membrane distillation system. It is visible in Figure 4.12 that a larger pore diameter drop in the Liquid Entry Pressure because the membrane with a larger pore diameter allows more water vapor to go through the surface of the membrane, leading to lower resistance for liquid penetration, resulting in a drop in the LEP. In contrast, the lower pore diameter makes it difficult for water vapor to go through the surface of the membrane due to restricting the water vapor from traveling, leading to higher resistance for water vapor to travel, which increases the Liquid Entry Pressure. On the other hand, a larger pore diameter has the advantage for travel through the membrane because it opens more ways for water vapor to go through the surface of the membrane, also easier to produce more fresh water due to having fewer restrictions, reducing the Liquid Entry Pressure. A lower pore diameter restricts the way for the vapor to travel through the membrane surface due to having a smaller number of open pores, which results in an increase in the Liquid Entry Pressure [52]. On the other hand, a higher pore diameter creates more scope for mass transfer through the open pores, which lowers the resistance to mass transfer and enhances vapor transportation across the membrane surface, resulting in reducing the Liquid Entry Pressure. Although a higher pore diameter reduces the resistance of water vapor, it weakens the membrane and increases the likelihood of membrane wetting. Therefore, it's crucial to determine the optimum value of pore diameter for enhancing the Liquid Entry Pressure while maintaining the durability and stability of the membrane distillation system [53]. Now, this section discusses the influence of the contact angle on the Liquid Entry Pressure, which is presented below:

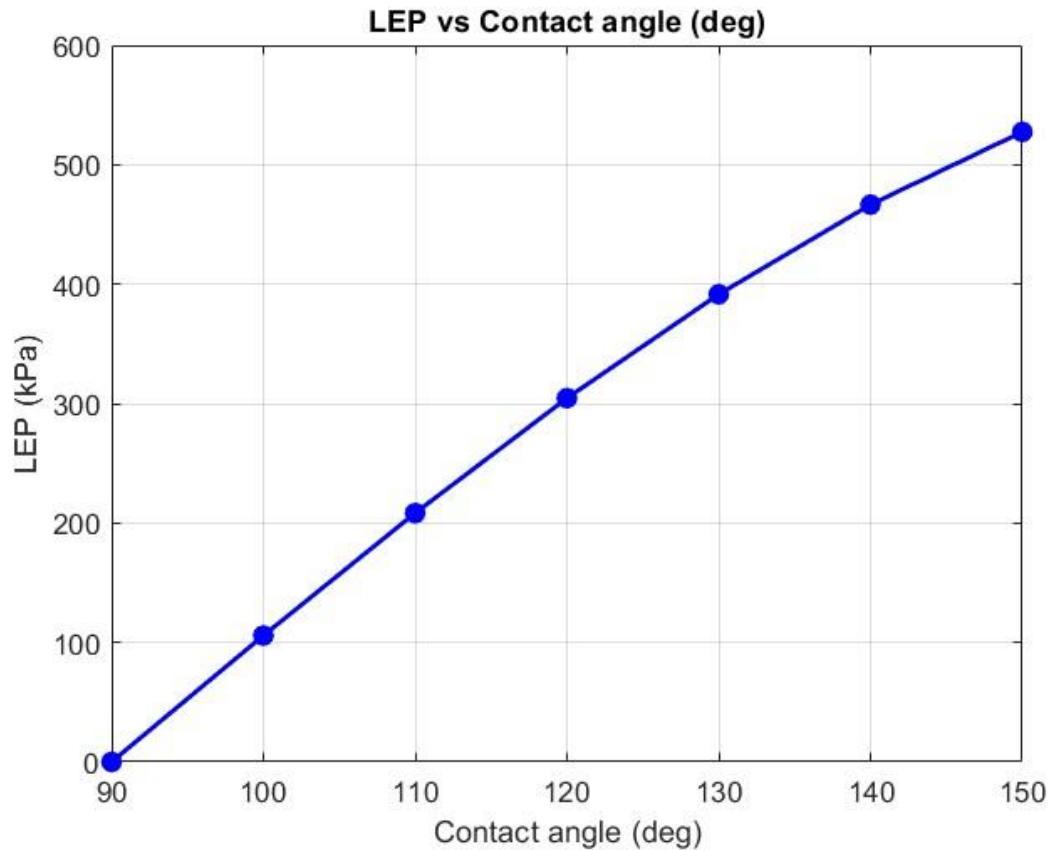


Figure 4.13: Contact Angle vs LEP

Figure 4.13 illustrates the relationship between the Contact Angle and Liquid Entry Pressure. Moreover, it describes how well the contact angle responds to the Liquid Entry Pressure in the membrane distillation system. It is visible in Figure 4.13 that a higher contact angle increases the Liquid Entry Pressure because the membrane with a higher contact angle creates more resistance to water vapor from going through the surface of the membrane, leading to higher resistance for liquid penetration, resulting in an increase in the LEP. Furthermore, the higher contact angle makes it difficult for water vapor to go through the surface of the membrane due to restricting the water vapor from traveling, leading to higher resistance for water vapor to travel, which increases the Liquid Entry Pressure. On the other hand, a lower contact angle makes it easier for water vapor to go through the surface of the membrane because of less restricts the water vapor from traveling, leading to lower resistance for water vapor to travel, which reduces the Liquid Entry Pressure. A higher

contact angle restricts the way for the vapor to travel through the membrane surface, which increases the Liquid Entry Pressure. On the other hand, a lower contact angle creates more scope for mass transfer through the open pores, which lowers the resistance to mass transfer and enhances vapor transportation across the membrane surface, resulting in reducing the Liquid Entry Pressure. A lower contact angle reduces the resistance of water vapor, weakens the membrane, and increases the likelihood of membrane wetting. A higher contact angle makes the membrane surface more hydrophobic, which aids in protecting the pores from water penetration. Furthermore, it helps to improve the wetting resistance of the membrane because a higher contact angle only allows water vapor to go through the pores. Moreover, the contact angle has a direct impact on the Liquid Entry Pressure; it protects the membrane from wetting and makes the membrane more durable. Therefore, a higher contact angle enhances the performance on the Liquid Entry Pressure of the membrane distillation system by protecting the membrane from wetting, which makes the membrane more durable, but doesn't have any influence on the freshwater production and mass transfer coefficient. Therefore, it's crucial to determine the optimum value of contact angle for enhancing the Liquid Entry Pressure while maintaining the durability and stability of the membrane distillation system.

4.5 EQUATIONS REVIEW FOR OPTIMIZATION

The performance metrics of the MD system mostly rely on the structure and properties of the membrane, which can present four variables:

$$x = [\varepsilon, d, \delta, \theta]^T$$

Here,

ε = membrane porosity (no dimension)

d = pore diameter (μm)

δ = membrane thickness (μm)

θ = contact angle ($^{\circ}$)

Each variable has been limited by some practical bounds, which are shown below:

$$\varepsilon \in [\varepsilon_{min}, \varepsilon_{max}], d \in [d_{min}, d_{max}], \delta \in [\delta_{min}, \delta_{max}] \quad \& \quad \theta \in [\theta_{min}, \theta_{max}]$$

Here,

$$H_{fg} = \text{latent heat of vaporization } (J \cdot kg^{-1})$$

$$R_{const} = \text{specific gas constant for water vapor } (J \cdot kg^{-1} \cdot K^{-1})$$

$$T_{hi}, T_{ci} = \text{hot/cold bulk temperatures } (^{\circ}C)$$

$$\text{Mean Temperature, } T_m = \frac{T_{hi} + T_{ci}}{2}$$

$$\Delta T = T_{hi} - T_{ci}$$

$$P_m = \text{mean pore pressure } (Pa)$$

$$\gamma = \text{surface tension } (N \cdot m^{-1})$$

$$\tau = \text{tortuosity}$$

Permeate Flux:

Permeate Flux illustrates how much vapor is going through the surface of the membrane, and turns the vapor into fresh water in the permeate tank.

$$J_p(\varepsilon, d, \delta) = C_w(\varepsilon, d, \delta) \left(\frac{H_{fg}}{(R_{const} \times (T_m + 273) \times P_m)} \right) (T_{hi} - T_{ci}) \quad [kg \cdot m^{-2} \cdot s^{-1}]$$

$$C_w(\varepsilon, d, \delta) \propto \frac{\varepsilon d}{\tau \delta}$$

Here,

J_p = Permeate Flux, C_w = Mass Transfer Coefficient, H_{fg} = Latent Heat Vaporization, R_{const} = Specific Gas Content, T_m = Mean Temperature, P_m = Mean Pressure, T_{hi} = Inlet Heat Temperature, T_{ci} = Inlet Cold Temperature

Liquid Entry Pressure:

Liquid Entry Pressure measures the pressure difference before the water enters the hydrophobic membrane. The equation below is obtained from the Laplace equation:

$$LEP(d, \theta) = \left[\frac{-2 \times y_i}{r_{memb}} \right] \times \cos \theta$$

Here,

y_i = sea water surface tension

θ = Contact angle between water and the membrane surface

r_{memb} = largest pore size

A larger contact angle and smaller pore diameter increase LEP, improving resistance to pore wetting. The combination of a higher contact angle and a smaller diameter of the pore increases the liquid entry pressure and enhances the performance of resistance for membrane wetting.

Mass Transfer Coefficient:

The mass transfer coefficient works on the movement of the vapor transfer inside the membrane.

$$K_m(J_p) = \left[\frac{J_p \times H_{fg}}{T_{hi} - T_{ci}} \right] \times 1$$

Desirability Functions:

This study focuses on identifying the ideal design for a membrane distillation system by converting three performance metrics, such as Permeate Flux, Mass Transfer Coefficient, and Liquid Entry Pressure, into a desirability function, which responds 0 for unacceptable performance, and responds 1 for the ideal value.

For each response $y_i \in \{J_p, K_m, LEP\}$ define lower acceptable bound L_i , target T_i ($T_i > L_i$), and shape exponent $r_i > 0$: _

$$d_i(y_i) = \begin{cases} 0, & y_i \leq L_i \\ \left(\frac{y_i - L_i}{T_i - L_i}\right)^{r_i}, & L_i < y_i < T_i \\ 1, & y_i \geq T_i \end{cases}$$

- d_1 for J_p , d_2 for K_m , d_3 for LEP
- $r_i > 1$ emphasizes values near the target; $r_i < 1$ rewards modest gains
- $LEP \geq 300 \text{ kPa}$

$$\theta_0 = 1$$

$$-2.25 \theta_1 + \theta_2 = -1$$

$$\theta_1 - 2.25 \theta_2 + \theta_3 = 0$$

$$\theta_2 - 2.25 \theta_3 + \theta_4 = 0$$

$$2\theta_3 - 2.25 \theta_4 = 0 \quad \text{for } i = M \text{ [Tip]}$$

Desirability to maximize:

The combined performance is measured using a weighted geometric mean:

The combination of the optimized performance metric is measured by using the geometric mean.

Here, w_i are the weights of the substances.

Assign importance weights $w_i > 0$ (e.g., equal $w_1 = w_2 = w_3$). The overall desirability is the weighted geometric mean:

$$D(x) = (d_1(x)^{w_1} d_2(x)^{w_2} d_3(x)^{w_3})^{\frac{1}{w_1+w_2+w_3}} \in [0,1]$$

The final goal is to find the membrane configuration that maximizes

The main aim is to identify the behavior of the membrane properties, which maximizes the value of $D(x)$

Now, the objective is to get the maximum values for $\max D(x)$ because it will help to identify the best combinations of the membrane properties.

$x \in X$

$s.t. \varepsilon_{min} \leq \varepsilon \leq \varepsilon_{max}, d_{min} \leq d \leq d_{max}, \delta_{min} \leq \delta \leq \delta_{max}, \theta_{min} \leq \theta \leq \theta_{max}$

$, (optional\ Safety) LEP(d, \theta) \geq L_{req} (e.g., 300\ kPa)$

Outputs: the optimal $x = [\varepsilon, d, \delta, \theta]$ and the corresponding J_p, K_m, LEP [35]

4.6 BUILDING UP OPTIMIZATION MODELS ON MATLAB

All procedures are implemented to work on the MATLAB Software. For instance, profound knowledge of membrane distillation has been gained from the peer-reviewed articles. Next, it was documented in the literature review section, which helped to identify the goals of the research. Next, the objective is to identify the equations that align with the target of the research. Then, it's necessary to have profound knowledge of the parameters of the equation, as well as needs to consider boundary conditions and assumptions. For instance, a steady-state operation environment is considered for the membrane distillation system, where the temperatures for the inlet are constant for two separate sides of the membrane surface. Moreover, Heat loss is considered negligible to the environment, and Pore size is considered uniform.

Once the equation is set and already documented about the fixed and variable parameters, it is the perfect time to start the MATLAB coding to get the prediction model.


```

clear; clc; close all; rng(1); % for reproducibility

%% ----- Constants (unchanged physics) -----
Hfg = 2.406e6; % J/kg (latent heat)
Rconst = 461.5; % J/(kg.K) (water vapor)
Thi = 66; % °C (feed hot)
Tci = 44; % °C (permeate cold)
Tm = (Thi + Tci)/2; % °C (mean)
dT = Thi - Tci; % °C (bulk ΔT)
Pm = 1.013e5; % Pa (mean pore pressure ~ 1 atm)
gamma = 0.067; % N/m (surface tension)
tau = 2; % (-) tortuosity (assumed constant)

%% ----- Design bounds (from your PDFs) -----
eps_lb = 0.48; eps_ub = 0.91; % porosity (-)
d_lb = 0.21; d_ub = 0.98; % pore DIAMETER (μm)
th_lb = 70.31; th_ub = 190.18; % thickness (μm)
th0 = th_lb; % baseline thickness used in calibration
th_units = '\num';
theta_lb = 90; theta_ub = 150; % contact angle (deg)

%% ----- Baseline (for Cw scaling to match your PDF) -----
% Baseline from your validated figures:
eps0 = 0.80; d0 = 0.22; theta0 = 120; % (deg); LEP uses theta only
Jp_baseline_h = 66.79; % kg m^-2 h^-1
% Membrane coefficient Cw α (ε * d) / (τ * δ)
Cw_raw = @(eps, d_um, th_um) (eps .* (d_um*1e-6)) ./ (tau .* (th_um*1e-6));
% Calibrate a scale so baseline reproduces Jp = 66.79 kg m^-2 h^-1
Cw_base = Cw_raw(eps0, d0, th0);
scaleFact = (Jp_baseline_h/3600) / (Cw_base * (Hfg/(Rconst*(Tm+273)*Pm)) * dT);
Cw = @(d_um, th_um) scaleFact .* Cw_raw(eps, d_um, th_um);

%% ----- Finalized performance models (unchanged) -----
% Permeate flux Jp (kg m^-2 h^-1)
Jp_h = @(eps, d_um, th_um) 3600 .* Cw(eps, d_um, th_um) .* (Hfg./(Rconst*(Tm+273)*Pm)) .* dT;
% Mass transfer coefficient (kJ m^-2 s^-1 °C^-1)
Km = @(Jp_h_val) ((Jp_h_val/3600) .* Hfg ./ dT) ./ 1000;
% Liquid Entry Pressure (kPa) using pore DIAMETER (μm)
LEP = @(d_um, theta_deg) (2*gamma*abs(cosd(theta_deg))) ./ (d_um*1e-6) ./ 1000;

%% ----- Desirability setup (Derringer-Suich, larger-is-better) -----
% Choose engineering lower bounds (acceptable) and targets (desired)
% If you have specific specs, set them here. Otherwise auto-set from achievable min/max.
% Auto compute achievable extrema at corners (Jp and Km are monotone in eps,d,th; LEP in d,theta)
Jp_min_auto = Jp_h(eps_lb, d_lb, th_ub);
Jp_max_auto = Jp_h(eps_ub, d_ub, th_lb);
Km_min_auto = Km(Jp_min_auto);
Km_max_auto = Km(Jp_max_auto);
LEP_min_auto = LEP(d_ub, theta_lb); % worst LEP at largest d, smallest |cosθ| (near 90°)
LEP_max_auto = LEP(d_lb, theta_ub); % best LEP at smallest d, largest |cosθ| (150° in your range)
% ---- User-specifiable desirability thresholds (edit if you have specs) ----
L1 = Jp_min_auto; T1 = Jp_max_auto; r1 = 1; % Jp (kg m^-2 h^-1)
L2 = Km_min_auto; T2 = Km_max_auto; r2 = 1; % Km (kJ m^-2 s^-1 °C^-1)
% Safety requirement example: enforce LEP >= 300 kPa by setting L3 = 300
LEP_min_req = 300; % kPa (set [] or NaN to disable)
L3 = max(LEP_min_auto, LEP_min_req); T3 = LEP_max_auto; r3 = 1; % LEP
% Weights (importance) for overall desirability (equal by default)
w1 = 1; w2 = 1; w3 = 1;
% Individual desirability, larger-is-better
d_lob = @(y, L, T, r) (y<=L).*0 + (y>=T).*1 + ...
(y>L & y<T).*((y-L)./(T-L)).^r);
% Overall desirability (weighted geometric mean)
D_overall = @(d1,d2,d3) (d1.^w1 .* d2.^w2 .* d3.^w3).^^(1/(w1+w2+w3));

%% ----- Optimization (Monte-Carlo search + optional local refine) -----
Nsamp = 25000; % number of random samples
eps_s = eps_lb + (eps_ub-eps_lb).*rand(Nsamp,1);
d_s = d_lb + (d_ub-d_lb).*rand(Nsamp,1);
th_s = th_lb + (th_ub-th_lb).*rand(Nsamp,1);
tht_s = theta_lb + (theta_ub-theta_lb).*rand(Nsamp,1);
% Evaluate performance
Jp_s = Jp_h(eps_s, d_s, th_s);
Km_s = Km(Jp_s);
LEP_s = LEP(d_s, tht_s);
% Desirabilities
d1_s = d_lob(Jp_s, L1, T1, r1);
d2_s = d_lob(Km_s, L2, T2, r2);
d3_s = d_lob(LEP_s, L3, T3, r3);
D_s = D_overall(d1_s, d2_s, d3_s);
% Pick best sample
[~, idx_best] = max(D_s);
eps_opt = eps_s(idx_best);
d_opt = d_s(idx_best);
th_opt = th_s(idx_best);
theta_opt = tht_s(idx_best);

```

Figure 4.14: MATLAB CODE GENERATION I

```

% Compute optimal performance
Jp_opt = Jp_h(eps_opt, d_opt, th_opt);
Km_opt = Km(Jp_opt);
LEP_opt = LEP(d_opt, theta_opt);
D_opt = D_s(idx_best);

%% ----- Results printout -----
fprintf('\n===== Desirability Optimization Result =====\n');
fprintf('Porosity (ε) = %.4f (-)\n', eps_opt);
fprintf('Pore diameter (d) = %.4f μm\n', d_opt, th_units);
fprintf('Thickness (δ) = %.4f μm\n', th_opt, th_units);
fprintf('Contact angle (θ) = %.1f °\n', theta_opt);
fprintf('Permeate flux = %.2f kg m-2 h-1\n', Jp_opt);
fprintf('Mass transfer coefficient = %.2f kJ m-2 s-1 °C-1\n', Km_opt);
fprintf('LEP = %.2f kPa\n', LEP_opt);
fprintf('Overall desirability (D) = %.4f (0-1)\n', D_opt);

%% ----- Visualizations -----
% 1) Trade-off across pore diameter at optimal ε, δ, θ
d_grid = linspace(d_lb, d_ub, 400);
Jp_g = Jp_h(eps_opt, d_grid, th_opt);
Km_g = Km(Jp_g);
LEP_g = LEP(d_grid, theta_opt);
d1_g = d_lob(Jp_g, L1, T1, r1);
d2_g = d_lob(Km_g, L2, T2, r2);
d3_g = d_lob(LEP_g, L3, T3, r3);
D_g = D_overall(d1_g, d2_g, d3_g);
figure('color','w');
yyaxis left; plot(d_grid, Jp_g, 'b-', 'LineWidth',1.6); ylabel('Permeate flux (kg m-2 h-1)', 'Interpreter','tex');
yyaxis right; plot(d_grid, LEP_g, 'r--', 'LineWidth',1.6); ylabel('LEP (kPa)', 'Interpreter','tex');
xlabel('Pore diameter (μm)', 'Interpreter','tex'); grid on; hold on;
yyaxis left; plot(d_opt, Jp_opt, 'bo', 'MarkerFaceColor','b');
yyaxis right; plot(d_opt, LEP_opt, 'ro', 'MarkerFaceColor','r');
title('Trade-off across pore diameter at optimal \epsilon,\delta,\theta', 'Interpreter','tex');
legend({'Permeate flux','LEP','Optimum'}, 'Location','best');
% 2) Overall desirability vs pore diameter (others fixed at optimum)
figure('color','w');
plot(d_grid, D_g, 'k-', 'LineWidth',1.6); grid on; hold on;
plot(d_opt, D_overall(d_lob(Jp_opt,L1,T1,r1), d_lob(Km_opt,L2,T2,r2), d_lob(LEP_opt,L3,T3,r3)), ...
'ko', 'MarkerFaceColor','k');
xlabel('Pore diameter (μm)', 'Interpreter','tex');
ylabel('Overall desirability, D (0-1)', 'Interpreter','tex');
title('Overall desirability across pore diameter', 'Interpreter','tex');
% 3) Bar chart of optimal design variables
figure('color','w');
cats = categorical({'epsilon (-)', 'd (μm)', '\delta (μm)', '\theta (°)'});
vals = [eps_opt, d_opt, th_opt, theta_opt];
bar(cats, vals); grid on;
ylabel('Value', 'Interpreter','tex');
title('Optimized membrane properties', 'Interpreter','tex');
% 4) Desirability components at optimum
figure('color','w');
d1_opt = d_lob(Jp_opt, L1, T1, r1);
d2_opt = d_lob(Km_opt, L2, T2, r2);
d3_opt = d_lob(LEP_opt, L3, T3, r3);
bar(categorical({'d_1 (Flux)', 'd_2 (Km)', 'd_3 (LEP)', 'D overall'}), [d1_opt, d2_opt, d3_opt, D_opt]);
ylim([0,1]); grid on;
ylabel('Desirability (0-1)', 'Interpreter','tex');
title('Desirability at the optimum', 'Interpreter','tex');

%% ----- (Optional) Local refinement using fmincon -----
% Convert to maximization by minimizing -D; keep bounds.
% Requires Optimization Toolbox. Comment out if not available.
try
    x0 = [eps_opt, d_opt, th_opt, theta_opt];
    lb = [eps_lb, d_lb, th_lb, theta_lb];
    ub = [eps_ub, d_ub, th_ub, theta_ub];
    D_neg = @(x) -D_overall( ...
        d_lob(Jp_h(x(1), x(2), x(3)), L1, T1, r1), ...
        d_lob(Km(Jp_h(x(1), x(2), x(3))), L2, T2, r2), ...
        d_lob(LEP(x(2), x(4)), L3, T3, r3) );
    opts = optimoptions('fmincon','Display','none','Algorithm','sqp');
    [x_ref, fval] = fmincon(D_neg, x0, [], [], [], lb, ub, [], opts);
    % Update if improved
    if -fval > D_opt
        eps_opt = x_ref(1); d_opt = x_ref(2); th_opt = x_ref(3); theta_opt = x_ref(4);
        Jp_opt = Jp_h(eps_opt, d_opt, th_opt);
        Km_opt = Km(Jp_opt);
        LEP_opt = LEP(d_opt, theta_opt);
        D_opt = -fval;
        fprintf('\n(Local refine) Improved overall desirability D = %.4f\n', D_opt);
    end
catch
    % If no Optimization Toolbox, skip refinement
end

```

Figure 4.15: MATLAB CODE GENERATION 2

The objective of this MATLAB code is to identify the optimized value for the membrane properties, such as membrane thickness, porosity, pore size, and contact angle, which offers the best performance in water production with the stability of the system. It focuses on finding out the optimal value of the four membrane properties to identify the combination of

membrane properties that can provide the best outcome of the performance metrics, such as permeate flux, mass transfer coefficient, and Liquid Entry Pressure.

Initially, the MATLAB code starts with introducing fixed parameters, such as temperature, pressure, and tension of the surface, which explains the environment of the operating conditions. Then the ranges are set for the variable parameters, like membrane properties, from which the ideas of ranges are taken from the peer-reviewed articles. The MATLAB CODE uses some equations to measure the permeate flux, mass transfer coefficient, and liquid entry pressure.

This MATLAB code works on the desirability function, which is a method to identify the ideal design for a membrane distillation system by converting three performance metrics, such as Permeate Flux, Mass Transfer Coefficient, and Liquid Entry Pressure, into a desirability function and then returns 0 for unacceptable performance and returns 1 for the ideal value. The desirability function created more than 25000 combinations of membrane properties and tried to identify which combination offers the highest score. At the end, it comes up with the best combination of membrane properties.

In short, the MATLAB code behaves like a real-world experiment, which tries to identify the best possible combination of membrane properties that can produce freshwater while avoiding membrane wetting.

Now, this section will discuss the influence of pore diameter on permeate flux, mass transfer coefficient, and Liquid Pressure Entry. This section will explain the relationship between the pore diameter and the combination of performance metrics by illustrating the plot, which aids in understanding with clear ideas. First, starting with presenting the relationship between pore diameter and the combination of performance metrics, which is given below:

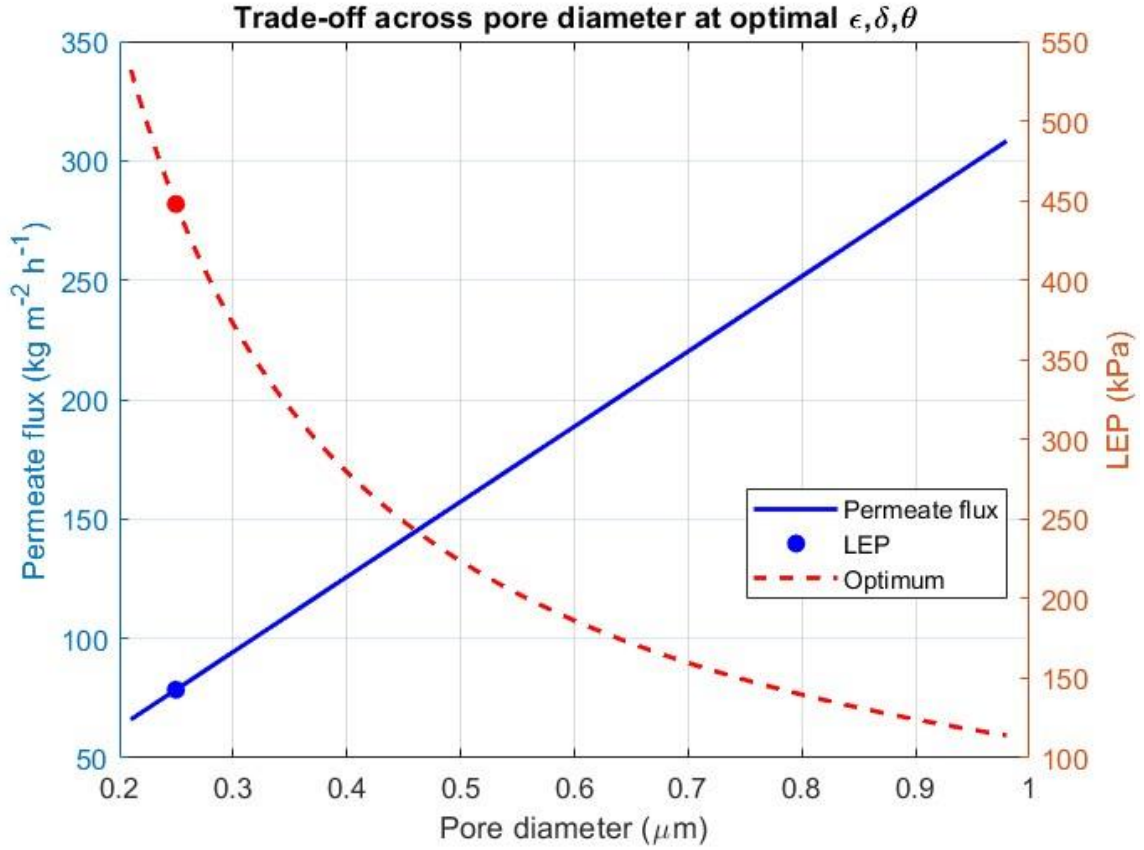


Figure 4.16: Determination of Optimal Value for Pore Diameter

Figure 4.16 represents the relationship between the pore diameter, Liquid Entry Pressure, and permeate flux. Moreover, it depicts how the Liquid Entry Pressure and permeate flux respond to the change in the pore diameter in the direct contact membrane distillation system, emphasizing the balance between water productivity and stability of the system. In Figure 4.16, the permeate flux is denoted by the blue line, which shows that it is increasing with the larger pore diameter because a larger pore diameter allows more vapor to go through the membrane surface. Although a larger pore diameter is an advantage for producing more water, there is a risk of membrane wetting as it allows more water vapor to travel, which may lead to liquid penetration in the membrane. In Figure 4.16, the Liquid Entry Pressure is denoted by the red dashed line, which indicates that it is going down with the larger pore diameter because it allows more water vapor to go through the surface of the membrane, leading to lower resistance for liquid penetration, resulting in a drop in the LEP. In contrast,

the lower pore diameter makes it difficult for water vapor to go through the surface of the membrane due to restricting the water vapor from traveling, leading to higher resistance for water vapor to travel, which increases the Liquid Entry Pressure but drops in freshwater production. In Figure 4.16, the optimal value for pore diameter is denoted by the red dot, which presents an optimal balance between permeate flux and liquid entry pressure. In the red dot point, the system produces the maximum amount of fresh water by maintaining the stability of the system. The trade-off between permeate flux and liquid entry pressure ensures higher permeate flux by maintaining the durable and stable operation of the membrane distillation system. Now, it's time to present the overall desirability across Pore Diameter to maintain the balance between the performance output and durability, which is shown below:

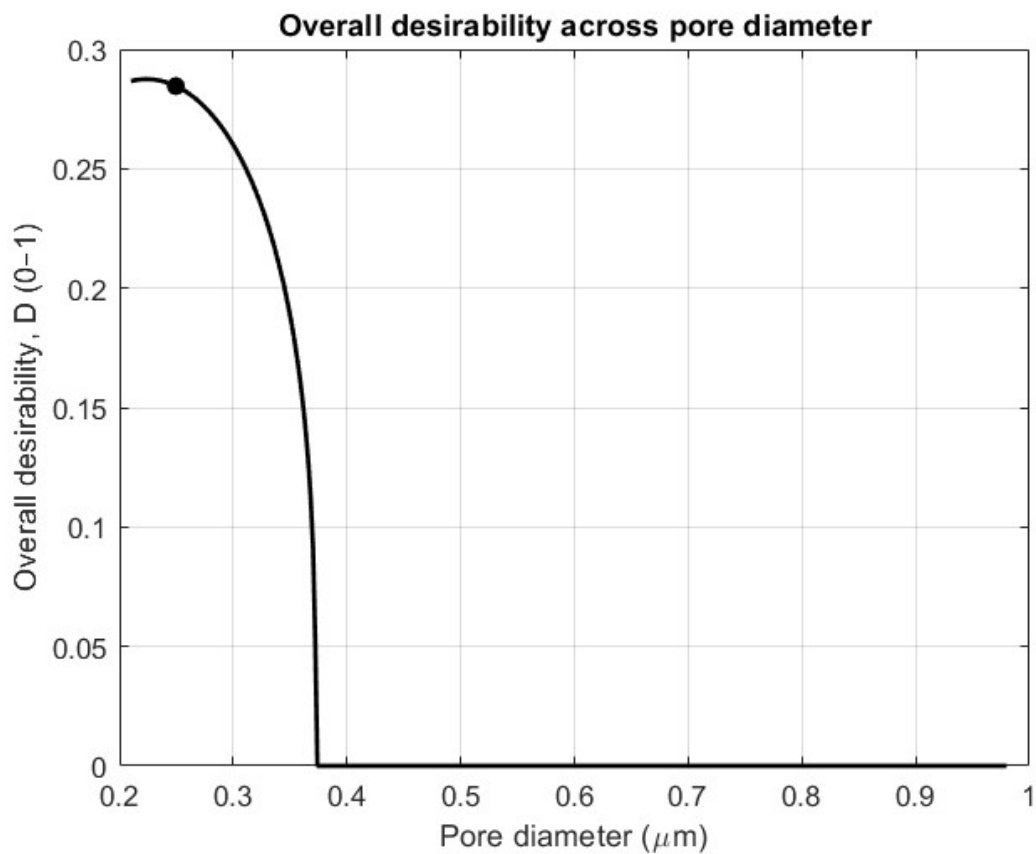


Figure 4.17: Overall Desirability across Pore Diameter

Figure 4.17 represents the value of the overall desirability function for the performance of the membrane distillation system with a change of pore diameter. Desirability tries to

identify the best combination of membrane properties such it can meet the goals of the membrane design to get the maximum water production while avoiding membrane wetting. In Figure 4.17, it is visible that the value of desirability increases with the lower pore diameter, which is preferred around 0.25 micrometres for getting a better value of desirability. In contrast, larger pore diameter drops in the desirability rapidly and shows that desirability reaches zero when the pore diameter is around 0.4 micrometres. This is occurring because the larger pore diameter allows more water vapor to travel, less restricted for water vapor to go through the membrane surface, which may lead to a higher chance of membrane wetting. After all, a larger pore diameter reduces the value of Liquid Entry Pressure, which makes the chances higher for membrane wetting. In Figure 4.17, the optimal pore diameter is denoted by a black dot, which is around 0.25 micrometres, offering the best performance of the system. Figure 4.17 illustrates a trade-off between the durability and permeability of the membrane distillation system and recommends that a lower pore diameter is enough to maintain the balance between the performance metrics and stability.

Now, this section will show the optimized value of the membrane properties, such as membrane thickness, pore diameter, porosity, and contact angle, by plotting the bar chart. This section will explain the reasoning for the optimized value of membrane properties, which aids in understanding with clear ideas. First, starting with presenting the optimized value of the membrane properties, such as membrane thickness, pore diameter, porosity, and contact angle, which is given below:

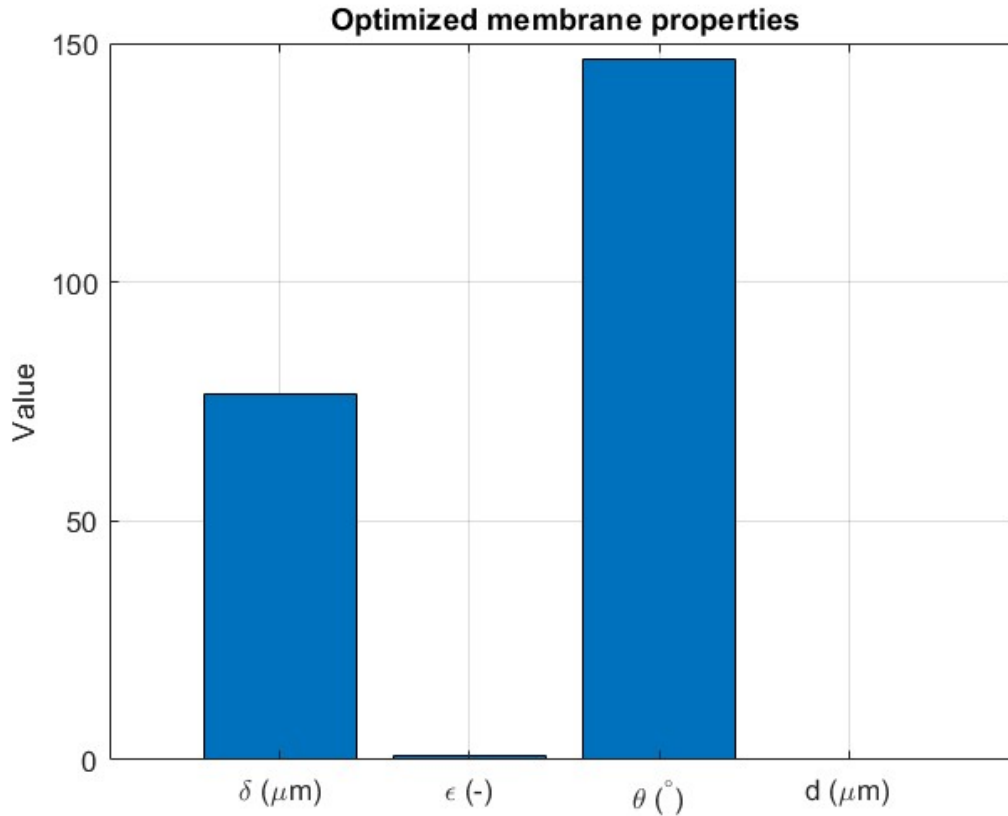


Figure 4.18: Optimized Value of Membrane Properties

Figure 4.18 illustrates the optimized value of the membrane properties, such as membrane thickness, pore diameter, porosity, and contact angle, and represents the value by plotting the bar chart. It is visible in Figure 4.18 that it offers an optimized design of the membrane by identifying the best combinations of the membrane properties, such as membrane thickness, pore size, porosity, and contact angle. Moreover, the recommended properties of the membrane ensure a higher production rate of fresh water with stronger resistance to membrane wetting. Figure 4.18 only shows the bar chart with the optimized value of membrane properties, but the values are not clear every time. So, Figure 4.19 is generated to show the exact value of optimal membrane properties and the value of the output parameters.

```

1  %% ===== MD Optimization via Desirability (Finalized Physics) =====
2  clear; clc; close all; rng(1); % for reproducibility
3
4  %% ----- Constants (unchanged physics) -----
5  Hfg = 2.406e6; % J/kg (latent heat)
6  Rconst = 461.5; % J/(kg.K) (water vapor)
7  Thi = 66; % °C (feed hot)
8  Tci = 44; % °C (permeate cold)
9  Tm = (Thi + Tci)/2; % °C (mean)
10 dT = Thi - Tci; % °C (bulk ΔT)
11 Pm = 1.013e5; % Pa (mean pore pressure ~ 1 atm)
12 gamma = 0.067; % N/m (surface tension)
13 tau = 2; % (-) tortuosity (assumed constant)
14
15 %% ----- Design bounds (from your PDFs) -----
16
Command Window

===== Desirability Optimization Result =====
Porosity (ε) = 0.9021 (-)
Pore diameter (d) = 0.2496 μm
Thickness (δ) = 76.5204 μm
Contact angle (θ) = 146.5 °
Permeate flux = 78.51 kg m-2 h-1
Mass transfer coefficient = 2.39 kJ m-2 s-1 °C-1
LEP = 447.77 kPa

```

Figure 4.19: The value variable and output parameters

Figure 4.19 is taken from the screenshot of the MATLAB Code. The primary objective is to present it because it shows the value of optimized membrane properties and the output parameter after changing the membrane design.

It is shown in Figures 4.18 & 4.19 that the value of porosity is 0.9021, which means that 90 percent of the membrane has open pores to allow the vapor to go through the membrane surface and increases the chance higher to enhancing freshwater production. Figures 4.18 & 4.19 also depict the bar chart for pore diameter, which presents the optimal value for pore diameter, which is around 0.2496 micrometers. Optimal Pore diameter ensures higher permeate flux and higher restriction for the penetration of liquid. It is visible in Figures 4.18 & 4.19 that the optimal membrane thickness is 76.52 micrometers, which is perfectly thin to permit the water vapor transport efficiently and maintain the stability of the system. Figures 4.18 & 4.19 present the optimal contact angle, which is around 146.5 degrees, meaning that the surface of the membrane is hydrophobic. Although it doesn't have any impact on the permeate flux and mass transfer coefficient, it has a significant impact on the Liquid Entry

Pressure. Moreover, it is important to protect the membrane from wetting and maintain the stability of the system.

After using these optimized values of membrane properties, an enhanced permeate flux is recorded, which is $78.51 \text{ kg/m}^2\text{h}$, as shown in Figure 4.19, indicating that the membrane can generate a huge amount of fresh water per hour. The enhanced performance of the mass transfer coefficient is detected, which is around $2.39 \text{ kJ/m}^2\text{s}^\circ\text{C}$, as shown in Figure 4.19, meaning that vapor has been transferred efficiently from the system. The optimal value of Liquid Entry Pressure is 447.77 kPa , as shown in Figure 4.19, indicating that the membrane can tolerate a vast amount of pressure without the penetration of liquid.

In short, the membrane is supposed to be thin, hydrophobic, highly porous, optimal pore diameter can ensure a huge amount of freshwater production with the durability, sustainability, and stability of the system.

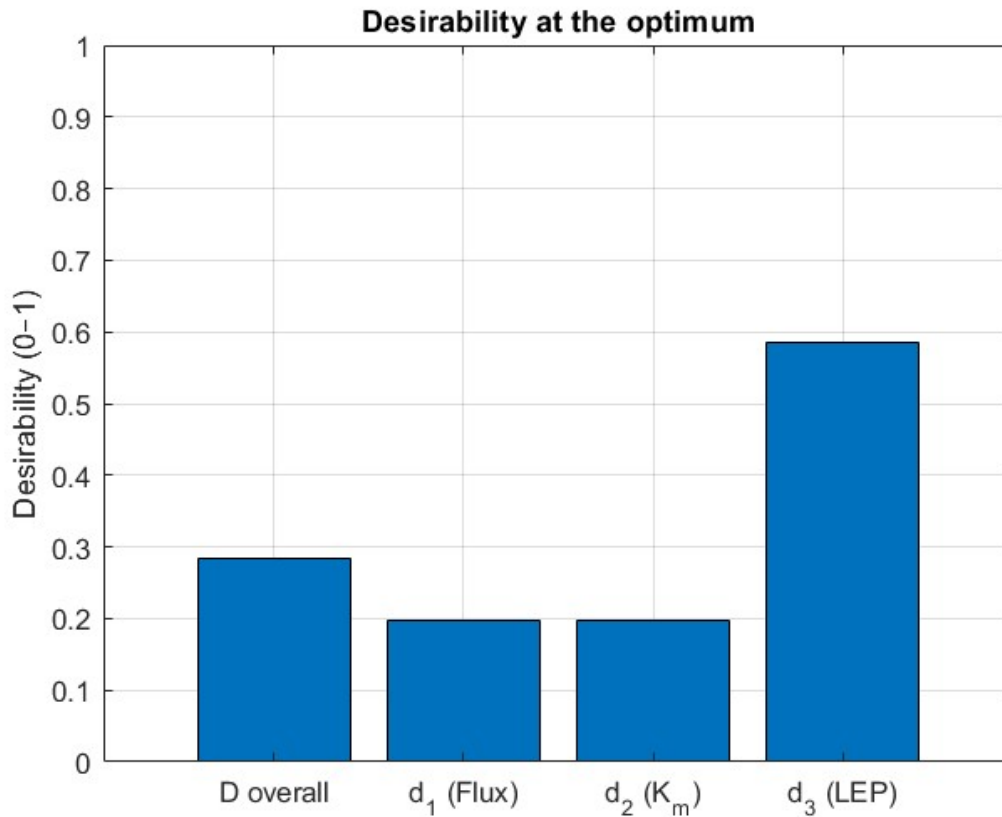


Figure 4.20: Optimum Desirability

Figure 4.20 represents the bar chart, which depicts the values of desirability for performance metrics, such as permeate flux, mass transfer coefficient, and liquid entry pressure in the membrane distillation system. Figure 4.20 shows the performance of 3 individual outputs and one overall desirability, which are given below:

- d_1 bar presents the permeate flux, and the value is close to 0.2, indicating that the permeate flux performs well but still needs to improve to reach an ideal value.
- The Mass Transfer Coefficient is indicated by d_2 bar, which is around 0.2, meaning that mass transfer coefficient is functioning relatively well, but it still needs to improve to achieve the ideal value.
- Liquid Entry Pressure is denoted by d_3 bar, which is around 0.6, and reaches a higher level than the permeate flux and mass transfer coefficient. It indicates that this proposed distillation system has stronger resistance to water penetration, ensuring the stability of the system.
- D overall represents the mean desirability of the system, which is around 0.28, combining the performance of three other performance metrics.

In short, Figure 4.20 depicts the performance of the optimized design of the membrane, which performs best in the Liquid Entry Pressure, ensuring stability, durability, and sustainability of the system by maintaining an enhanced mass transfer coefficient and permeate flux.

4.7 RESULT COMPARISON

This section will discuss comparing the results of optimized values of membrane properties with the membrane properties data from the peer-reviewed article [35], and then compare the results of the permeate flux, mass transfer coefficient, and liquid entry pressure with the data from the peer-reviewed articles. The analysis has been done by MATLAB software, and the code is given below:

```

%% ===== MD: Compare Optimized Design vs PDF Reference (units fixed) =====
clear; clc; close all;

%% ---- Physics constants ----
Hfg = 2.406e6; % J/kg (latent heat)
Rconst = 461.5; % J/(kg.K) (water vapor)
Thi = 66; % °C (feed hot)
Tci = 44; % °C (permeate cold)
Tm = (Thi + Tci)/2; % °C (mean temperature)
dT = Thi - Tci; % °C (temperature difference)
Pm = 1.013e5; % Pa (mean pore pressure)
gamma = 0.067; % N/m (surface tension)
tau = 2; % (-) tortuosity

%% ---- Governing relations ----
Cw_raw = @(eps, d_um, th_um) (eps .* (d_um*1e-6)) ./ (tau .* (th_um*1e-6));
Jp_h = @(Cw) 3600 .* Cw .* (Hfg./(Rconst*(Tm+273).*Pm)) .* dT;
Km_fun = @(Jp_h_val) ((Jp_h_val/3600) .* Hfg ./ dT) ./ 1000; % kJ.m^-2.s^-1.°C^-1
LEP_fun = @(d_um, theta_deg) (2*gamma*abs(cosd(theta_deg))) ./ (d_um*1e-6) ./ 1000; % kPa

%% ---- Calibration ----
eps0 = 0.80; d0 = 0.22; th0 = 70.31; Jp_baseline_h = 66.79; % kg.m^-2.h^-1
Cw_base = Cw_raw(eps0, d0, th0);
scaleFact = (Jp_baseline_h/3600) / (Cw_base * (Hfg./(Rconst*(Tm+273).*Pm)) * dT);
Cw = @(eps, d_um, th_um) scaleFact .* Cw_raw(eps, d_um, th_um);

%% ===== 1) Optimized Design =====
eps_opt = 0.9021;
d_opt = 0.2496;
th_opt = 76.5204;
theta_opt = 146.5;
Jp_opt = Jp_h(Cw(eps_opt, d_opt, th_opt));
Km_opt = Km_fun(Jp_opt);
LEP_opt = LEP_fun(d_opt, theta_opt);

%% ===== 2) PDF Reference =====
eps_pdf = 0.80;
d_pdf = 0.30;
th_pdf = 70.0;
theta_pdf = 130;
Jp_pdf = 75.34; % updated as requested
Km_pdf = Km_fun(Jp_pdf);
LEP_pdf = LEP_fun(d_pdf, theta_pdf);

%% ---- Print results ----
fprintf('\n===== Comparison (Optimized vs PDF Ref) =====\n');
fprintf('Porosity ε : %7.4f vs %7.4f (-)\n', eps_opt, eps_pdf);
fprintf('Pore diameter d : %7.4f vs %7.4f μm\n', d_opt, d_pdf);
fprintf('Thickness δ : %7.4f vs %7.4f μm\n', th_opt, th_pdf);
fprintf('Contact angle θ : %7.1f vs %7.1f deg\n', theta_opt, theta_pdf);
fprintf('Permeate flux Jp : %7.2f vs %7.2f kg m^-2 h^-1\n', Jp_opt, Jp_pdf);
fprintf('Mass transfer coeff K_m : %7.2f vs %7.2f kJ m^-2 s^-1 °C^-1\n', Km_opt, Km_pdf);
fprintf('LEP : %7.2f vs %7.2f kPa\n', LEP_opt, LEP_pdf);

%% ---- Plot 1: Design variables ----
figure('Color','w');
cats = categorical({'ε','d','δ','θ'},{'\epsilon (-)','\delta (\mu m)','\theta (\circ)'});
bar(cats, [eps_opt d_opt th_opt theta_opt; eps_pdf d_pdf th_pdf theta_pdf], 'grouped');
ylabel('Value','Interpreter','tex'); grid on;
legend({'Optimized','PDF ref'}, 'Location','best');
title('Membrane properties: Optimized vs PDF reference','Interpreter','tex');

%% ---- Plot 2: Performance metrics ----
figure('Color','w');
cats2 = categorical({'Jp (kg m^-2 h^-1)','Km (kJ m^-2 s^-1 °C^-1)','LEP (kPa)'});
bar(cats2, [Jp_opt Km_opt LEP_opt; Jp_pdf Km_pdf LEP_pdf], 'grouped');
ylabel('Value','Interpreter','tex'); grid on;
legend({'Optimized','PDF ref'}, 'Location','best');
title('Performance: Optimized vs PDF reference (units fixed)','Interpreter','tex');

```

Figure 4.21: MATLAB CODE GENERATION

Figure 4.21 illustrates the comparison of the results of optimized values of membrane properties with the membrane properties data from the peer-reviewed article, and then compares the results of the permeate flux, mass transfer coefficient, and liquid pressure with the data from the peer-reviewed articles. MATLAB Code works on building the graph

to show the comparison between them visually. First, starting with the comparison of membrane properties between optimized data and the data from the journal article, which is presented below:

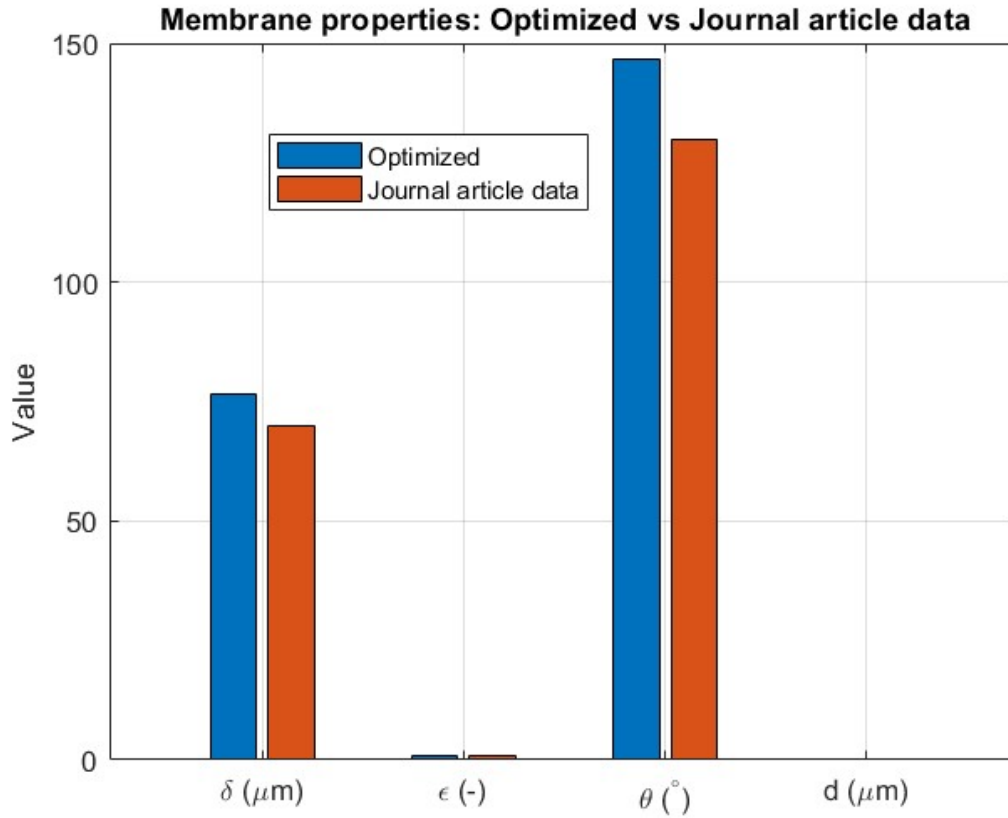


Figure 4.22: Membrane Properties: Optimized vs Journal Article Data

Figure 4.22 illustrates the membrane properties, such as membrane thickness, porosity, pore size, and contact angle, between the optimized model and the data from the peer-reviewed articles. In Figure 4.22, the values are not clearly visible. So, Figure 4.22 is taken from the common window of the MATLAB software and shows the clear value of the membrane properties between the optimized model and the journal article data.

- It is shown in Figures 4.22 & 4.24 that the value of optimized porosity is 0.9021, which means that 90 percent of the membrane has open pores to allow the vapor to go through the membrane surface and increase the chance of enhancing freshwater production. On the other hand, the value of porosity is 0.8, which is taken from the

journal article data, indicating that 80 percent of the membrane has open pores to permit the molecules of water vapor to travel and reduce the chance of water production than the optimized model.

- Figures 4.22 & 4.24 also depict the bar chart for pore diameter, which presents the optimal value for pore diameter, which is around 0.2496 micrometers. Optimal Pore diameter ensures higher permeate flux and higher restriction for the penetration of liquid. In contrast, the pore diameter from the journal article data is 0.3 micrometres, meaning that it allows more water vapor to go through the membrane surface and reduces the resistance for water vapor to travel, which can affect the stability of the system.
- It is visible in Figures 4.22 & 4.24 that the optimal membrane thickness is 76.52 micrometres, which is perfectly thin to permit the water vapor transport efficiently and maintain the stability of the system. On the other hand, the value of membrane thickness from the journal article is 70 micrometers, which is thicker than the optimized design, increasing the resistance to travel in the membrane surface, and increasing the chance of affecting the stability of the system.
- Figures 4.22 & 4.24 present the optimal contact angle, which is around 146.5 degrees, meaning that the surface of the membrane is hydrophobic. Although it doesn't have any impact on the permeate flux and mass transfer coefficient, it has a significant impact on the Liquid Entry Pressure. Moreover, it is important to protect the membrane from wetting and maintain the stability of the system. In contrast, the contact angle from the peer-reviewed article is around 130 degrees, indicating a hydrophobic surface, but the proposed optimized model offers better hydrophobicity due to having a higher contact angle.

In short, the optimized design of the membrane is thinner, more hydrophobic, highly porous, larger pore diameter, ensuring an enhanced permeate flux with the durability, sustainability, and stability of the system.

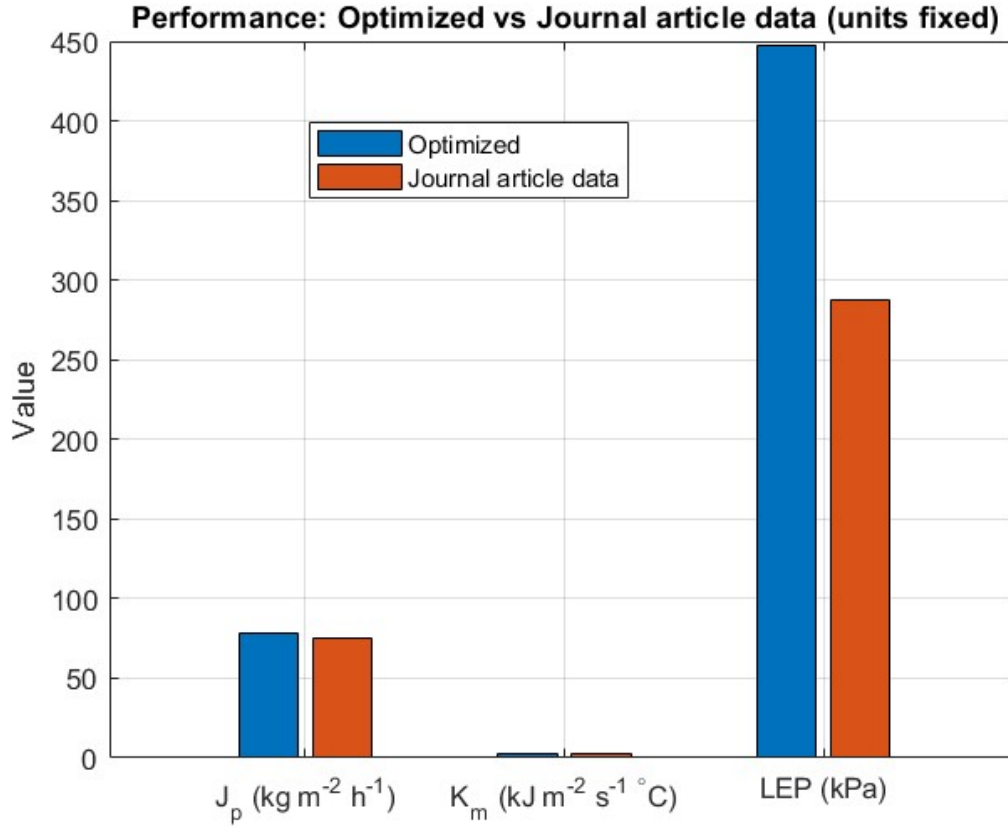


Figure 4.23: Performance: Optimized vs Journal Article Data

Figure 4.23 illustrates the performance metrics, such as permeate flux, mass transfer coefficient, and Liquid Entry Pressure, between the optimized model and the data from the peer-reviewed articles. In Figure 34, the values are vague. So, Figure 35 is obtained from the command window of the MATLAB software and depicts the value of the performance metrics between the optimized model and the journal article data [35].

Figures 4.23 & 4.24 depict that the permeate flux is $78.51 \text{ kg/m}^2\text{h}$ for the optimized design model, where the obtained permeate flux from the journal article data is $75.34 \text{ kg/m}^2\text{h}$, which means that the optimized design membrane can generate better permeate flux than the

journal article data. The enhanced performance of the mass transfer coefficient is detected for the optimized membrane, which is around $2.39 \text{ kJ}/\text{m}^2\text{s}^\circ\text{C}$, where the mass transfer coefficient from the journal data is $2.29 \text{ kJ}/\text{m}^2\text{s}^\circ\text{C}$, indicating that vapor has been transferred more efficiently than the data from the journal article.. The optimal value of Liquid Entry Pressure is 447.77 kPa, which is far better than the value of the Liquid Entry Pressure, which is obtained from the peer-reviewed article [35], which is around 287.11 kPa, indicating that the optimized membrane has better tolerance to handle a vast amount of pressure without the penetration of liquid.

```

1      %% ===== MD: Compare Optimized Design vs Journal Article Data (units fixed)
2      clear; clc; close all;
3      %% ---- Physics constants ----
4      Hfg = 2.406e6;           % J/kg (latent heat)
5      Rconst = 461.5;         % J/(kg.K) (water vapor)
6      Thi = 66;               % °C (feed hot)
7      Tci = 44;               % °C (permeate cold)
8      Tm = (Thi + Tci)/2;     % °C (mean temperature)
9      dT = Thi - Tci;         % °C (temperature difference)
10     Pm = 1.013e5;           % Pa (mean pore pressure)
11     gamma = 0.067;          % N/m (surface tension)
12     tau = 2;                % (-) tortuosity
13     %% ---- Governing relations ----
14     Cw_raw = @(eps, d_um, th_um) (eps .* (d_um*1e-6)) ./ (tau .* (th_um*1e-6));
15     Jp_h = @(Cw) 3600 .* Cw .* (Hfg./(Rconst*(Tm+273).*Pm)) .* dT;
16

```

Command Window

```

===== Comparison (Optimized vs Journal Article Data) =====
Porosity ε           : 0.9021 vs 0.8000 (-)
Pore diameter d       : 0.2496 vs 0.3000 μm
Thickness δ           : 76.5204 vs 70.0000 μm
Contact angle θ       : 146.5 vs 130.0 deg
Permeate flux Jp      : 78.51 vs 75.34 kg m^-2 h^-1
Mass transfer coeff K_m : 2.39 vs 2.29 kJ m^-2 s^-1 °C^-1
LEP                   : 447.68 vs 287.11 kPa

```

Figure 4.24: The value of Membrane Properties and Performance Metrics

The outcome of optimization shows the clear enhancements of performance and the combination of membrane properties, while it compares to the data from the peer-reviewed article [35]. Optimized membrane offers better porosity and hydrophobicity, smaller pore diameter, which aids in improving the stability of the system and enhancing the permeate flux with improved mass transfer coefficient. Furthermore, thicker membranes enhance the

mechanical strength and ensure the durability of the system by increasing the mass transfer coefficient and permeate flux. This optimized design improves the performance of hydrophobicity, mechanical strength, durability, and enhancement in water production.

5.0 CRITICAL EVALUATION

This context explores the critical evaluation of the outcomes of optimized design for the membrane distillation system, also examines the objectives of the research, and what can be obtained from comparing the optimized membrane design and data from the journal articles. The main objective is to understand the outcome of the results, integrating the knowledge into the relevance of Engineering, generating insightful ideas from earlier research, and implementing them in the practical field.

5.1 OBJECTIVE EVALUATION

The objective of this study is to obtain an optimized design of a membrane that can be capable of producing higher amounts of freshwater, higher Liquid Entry Pressure, and an enhanced mass transfer coefficient with the structural integrity, durability, and sustainability of the system. According to the results, it has been proven that the optimized design performs better than the membrane design from the peer-reviewed article. The optimized membrane design obtained a higher porosity, smaller pore diameter, thicker membrane thickness, and higher contact angle.

These characteristics of the optimized membrane properties suggests more open pores with better hydrophobicity, where the membrane properties, which found in the journal has lower porosity, larger pore diameter, thinner membrane thickness, lower contact angle, which are still good for a membrane to produce freshwater with stability of the system, but the higher porosity, higher contact angle makes the optimized membrane easier to produce more freshwater with the better durability and sustainability of the system.

The optimized membrane design obtained a better permeate flux, which is $78.51 \text{ kg/m}^2\text{h}$, where the obtained permeate flux from the journal article data is $75.34 \text{ kg/m}^2\text{h}$, indicating that the optimized design membrane can produce better freshwater than the journal article data. The optimized membrane design obtained a better mass transfer coefficient of

2.39 $\text{kJ}/\text{m}^2\text{s}^\circ\text{C}$, where the mass transfer coefficient from the journal data is 2.29 $\text{kJ}/\text{m}^2\text{s}^\circ\text{C}$, indicating that the water vapor has been transferred more efficiently than the journal article data. The optimal value of Liquid Entry Pressure is 447.77 kPa, which is far better than the value of Liquid Entry Pressure of the peer-reviewed article data, which is around 287.11 kPa, meaning that the optimized membrane has better tolerance to handle a vast amount of pressure without the penetration of liquid.

Optimized membrane design has significant implications in real-world applications for the membrane distillation system. In general, it's important to enhance the permeate flux with stability in industrial applications and desalination procedures. Higher LEP can ensure that the membrane can tolerate huge amounts of pressure without membrane wetting and protects the membrane distillation system from contamination of the freshwater with impurities. So, the optimized membrane design is important for durability with a higher volume of water production.

The enhancement in hydrophobicity is noticeable in the membrane distillation system, which is confirmed by a higher contact angle in the membrane distillation system, indicating that the surface of the membrane can resist water penetration effectively, ensuring better separation of impure materials from saline water.

In addition, the mass transfer coefficient tries to maintain a balance between mechanical strength and stability with a higher permeate flux. In practical Engineering, it's preferred to maintain a lower permeate flux with higher durability, rather than having a higher permeate flux with lower durability. In engineering terms, this optimized membrane design is the better one due to offering better stability with higher permeate flux.

5.2 COMPARISON WITH INDUSTRIAL STANDARD AND JOURNAL ARTICLE

The outcomes of the optimized membrane design illustrate realistic values when it's compared to the existing study. The optimized membrane design offers a permeate flux of $78.51 \text{ kg/m}^2\text{h}$, mass transfer coefficient of $2.39 \text{ kJ/m}^2\text{s}^\circ\text{C}$, and Liquid Entry Pressure of 447.77 kPa , exhibiting better performance in maintaining stability and durability in the applications of the membrane distillation system. Optimized membrane design matches the performance metrics with the journal article and industrial standard. This journal article has conducted a MATLAB with experimental data, and later, verified it with industrial standards. The results of the optimized membrane design have a range of values, which closely align with the industrial standard and the journal article data.

In literature, it is suggested that a thinner membrane thickness, a higher contact angle, a highly porous membrane with a larger pore diameter have a higher tendency to produce a huge amount of freshwater with stability and integrity of mechanical strength in the membrane distillation system. In the same way, the optimized membrane design offers a thinner, more hydrophobic, highly porous, larger pore diameter, ensuring an enhanced permeate flux with the durability, sustainability, and stability of the system.

The result of optimization shows the clear improvements in performance and the combination of membrane properties, while comparing to the data from the peer-reviewed article. Optimized membrane offers better porosity and hydrophobicity, smaller pore diameter, which aids in improving the stability of the system and enhancing the permeate flux with improved mass transfer coefficient. Furthermore, thicker membranes enhance the mechanical strength and ensure the durability of the system by increasing the mass transfer coefficient and permeate flux. This optimized design improves the performance of hydrophobicity, mechanical strength, durability, and water production.

5.3 STRENGTHS AND LIMITATIONS OF THIS STUDY

The primary strength of this study is its comprehensive strategy for optimizing the variable parameters. The MATLAB software seamlessly integrates the equations of performance metrics, such as permeate flux, mass transfer coefficient, and Liquid Entry Pressure. The desirability function aids in identifying the combination of optimized membrane properties, which ensures higher permeate flux, efficient mass transfer coefficient, and better Liquid Entry Pressure. Another primary strength of this study is that the optimized membrane design offers stability, durability, with high performance. Optimized Membrane Design provides enhanced hydrophobicity, offering a more stable structure with the protection of membrane wetting. The optimized model is not focused on maximizing the performance of the output to the system, but also ensuring the stability, sustainability, and durability of the membrane configuration.

Though this study shows advantages, it still has some drawbacks. The optimized model is based on the assumptions of a steady state, indicating that it doesn't rely on the effects of time-dependent factors, such as polarization, temperature, and fouling, which impact the performance over time. Furthermore, the optimized model works on uniform properties of the membrane, but the membranes could have minor variations in pore diameter. Moreover, the surface is assumed to be uniform, but it can be rough over time, which can affect the performance of the system. In addition, experimental data is taken from only one journal article, where more datasets can strengthen the comparison of the research work.

In short, the optimization process aids in understanding how small changes in membrane properties can affect the performance metrics, such as permeate flux, mass transfer coefficient, and Liquid Entry Pressure. For instance, the optimized model offers a better combination of membrane properties than the journal article data, where there are slight differences between them, but it still enhances the performance metrics. The study provides

an insightful idea about the necessity of a trade-off between the parameters to improve performance. For instance, higher porosity enhances the Permeate flux, but it still has detrimental effects on the mechanical strength of the membrane. Moreover, a Lower pore diameter reduces the production of fresh water but enhances the Liquid Entry. Therefore, the desirability function plays a vital role in the trade-off between the parameters. This study aids in understanding the importance of working on prediction models, which saves time, cost, and resources, and provides complete ideas about the design, which is beneficial for working on the experimental setup. Moreover, MATLAB uses equations to find the best combinations of the membrane properties, ensuring design and performance before creating the membrane, which saves time, cost, and resources.

6.0 CONCLUSION

This study aims to identify the combination of membrane properties, such as membrane thickness, porosity, pore size, and contact angle, and suggest an optimized membrane design to get the maximum output with stability. The study is successful to reach on the target. The study totally relies on a computational framework via MATLAB software, by governing equations to calculate the optimal value of permeate flux, mass transfer coefficient, and Liquid Entry Pressure. Different approaches have been conducted based on different datasets from the peer-reviewed articles. This approach aids in achieving the optimal membrane design with better performance and ensures the durability, stability, and sustainability of the system.

This study shows how significantly the computation framework can optimize the design of the membrane, excluding reliance on lab experiments. At first, it was challenging to come up with equations and modify the equations of the optimization model. But after trial and error, the equations were generated perfectly for the MATLAB Software. A computational approach using MATLAB examines performance metrics, such as permeate flux, mass transfer coefficient, and LEP, with improved stability. Moreover, this process is cost-effective and time-saving compared to the traditional method. Furthermore, it offers engineers a cost-effective and easy-to-use tool to design the membrane with optimized performance and durability. This study helps to connect the theoretical knowledge and the development of a practical membrane.

Risk Management of this project prioritizes finding possible challenges in the early stage and identifying pathways to minimize their effect. The main risk of this study is inaccurate data, an unstable model, and modelling mistakes in MATLAB. The optimized model and

the values of variables have been verified by a peer-reviewed article for the accuracy of the system. To ensure a feasible outcome, testing regularly and validation assist in avoiding calculation errors. Time management is highly prioritized to avoid delays in the project. This risk management shows how important proper planning, validation, and alternative strategies are to get risk risk-free research project.

The output of the research offers significant potential for desalination in the real world and impactful water treatment. This improved design of the membrane can be used in the Direct Contact Membrane Distillation System to get optimized recovery rates of water with minimal input of energy. This model can be used in those areas where resources are limited and fresh water can hardly be obtained, or a shortage of freshwater. Therefore, the optimized model helps to design the membrane by reducing the industry waste and the reliance on experiments.

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