CHEMICAL ENGINEERING TRANSACTIONS
VOL. 112, 2024
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it
Guest Editors: Selena Sironi, Laura Capelli

ISBN 979-12-81206-13-7; **ISSN** 2283-9216
DOI: 10.3303/CET24112043

Prediction of Membranes Distillation Performance for Desalination Process using MATLAB-Simulink Numerical Modelling

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While experimental studies indicate that concentration, temperature, and membrane properties have significant impact on membrane distillation (MD) performances, a systematic numerical modelling linking all variables with operation condition is lacking. With such model, we can quantitatively analyze, optimize, and predict how variations in membrane properties affect the process performance under varied operational conditions. In this study, a simulation model was created using MATLAB-Simulink to analyze the influence of membrane properties specifically membrane thickness, porosity, pore size, and contact angle on MD performance over a wide variety of operational settings. The simulation result showed a decrease in permeate flux from 66.79 to 24.61 kg/m².h as membrane thickness increased from 60 µm to 180 µm, while greater porosity from 0.5 to 0.9 led to around five times greater permeate flux. However, both properties had no effect on liquid entry pressure (LEP) value. Next, bigger pore size was found to enhance the permeate flux and mass transfer coefficient but lessened the LEP. Contact angle was discovered to be critical for LEP as it rose from zero to 529.8 kPa for contact angle 90 to 150°, but it had no effect on permeate flux and mass transfer coefficient. Overall, the study proves the suitability of using programmable MATLAB model in predicting MD performance.

1. Introduction

Desalination describes a process which discards salts and minerals from water, normally rendering seawater into fresh water. The output water from such operations then shall be applicable for human consumption, agriculture and commercial purposes (Zolghadr-Asli et al., 2023). There are two significant technologies in desalination process that are primarily used namely thermal desalination and membrane distillation (MD). In the former, feed saline water is heated at appropriate operating temperatures and pressures, causing water vapor to condense as pure water. The latter sees semi-permeable membranes filter salt mineral from water (Liu et al., 2024). MD is a thermally induced membrane separation technique with promising impact as it is capable of eliminating salts and mineral from highly saline waters (Yao et al., 2020). While MD has a large amount of salt rejection, it consumes minimum amount of energy and minimal operational requirements (normal pressure and lower temperature) compared to other separation methods, making it an attractive solution in desalination technology. The drawbacks of the current MD technology in desalination process are its low water flux and slow recovery process. There is the risk of pore wetting and liquid penetration during continuous MD operation which could result in a selectivity loss of the membrane (McGaughey et al., 2020). MD also consumes a lot of space relative to other membrane methods. When applied inefficiently, it could consume considerable energy throughout the operation because of the required temperature polarization.
MD performance would suffer when one of these issues arises during the process. As a response, many researchers attempted to improve the performance of MD by exploring factors such as saline water concentration, MD temperature, membrane properties namely liquid entry pressure (LEP), contact angle, pore size, porosity, thickness, and thermal conductivity (Kebria and Rahimpour, 2020). As there are plethora of factors involved, not all parameters are considered during experiment.

Paper Received: 27 May 2024; Revised: 14 June 2024; Accepted: 12 August2024
Please cite this article as: Mat Shayuti M.S., Razak N.A., Othman N.H., Marpani F., Alias N.H., 2024, Prediction of Membranes Distillation Performance for Desalination Process using MATLAB-Simulink Numerical Modelling, Chemical Engineering Transactions, 112, 253-258 DOI:10.3303/CET24112043

Numerical simulation could be the solution to this problem. Systematic mathematical modelling for MD processes may be performed to simultaneously account for all the factors involved. It plays a crucial role in understanding the complex transport phenomena and optimizing the design and operation of MD system, but simulating MD is a web of complex tasks involving coupled heat and mass transfer equations within membrane module. The robust computational capabilities and vast library of MATLAB make it possible for it to simulate complex transport phenomena by incorporating models of heat and mass transfer in MD processes. Furthermore, it could be used for system optimization and prediction of performance under specific conditions. For instance, MATLAB was employed for direct contact membrane distillation (DCMD) process and the feed temperature and membrane thickness were found to massively impact the permeate flux (Ameen et al., 2020). Among other studies performed in MATLAB include the impact of operating conditions such as feed temperature, flow rate, vacuum pressure (Zhang et al., 2022), membrane materials & configurations (Zuo et al., 2024), and energy efficiency (Alam et al., 2023).

Other numerical approaches using finite element method (FEM), finite volume method (FVM), and computational fluid dynamics (CFD) were also observed. Some researchers predicted the temperature and concentration polarizations effects (Ullah et al., 2023), membrane material and configuration for instance flat sheet and hollow fiber (Ali et al., 2023), MD integration with other techniques such as reverse osmosis and solar (Elhenawy et al., 2023), and energy efficiency (Christie et al., 2020). Notwithstanding the numerical methods, the selection of factors in analysis is vital for mathematical simulation.

To date, the effect of membrane thickness, porosity, pore size, and contact angle have not been studied in extensive simulation studies, especially when all parameters are simultaneously considered. Hence, this research aimed to analyze the influence of the said factors on MD performance under broad practical operational settings using MATLAB-Simulink. Simulink is an environment in MATLAB that utilizes block diagram to model systems with multiple domains. Its graphical programming can be utilized for simulating and analyzing multidomain dynamical systems, which is the case of desalination process using MD.

2. Methodology

2.1 Process Modelling

Figure 1 shows a schematic diagram of the experimental DCMD process. This work utilized a mathematical dynamic model for the DCMD process which described the heat and mass transfer mechanisms. The MD model then was created on Simulink block in MATLAB as shown in Figure 2, containing commands and definition of variables involved in the process. In this study, we focused on the mass transfer mechanism that took place inside the DCMD module. The model allowed for investigation of the process performance in terms of membrane properties (membrane thickness, porosity, pore size, and contact angle), thereby contributing to a thorough understanding of the process, particularly when dealing with varying membrane property values. The output from the simulation would then be compared and validated with recent findings and theories.

2.2 Governing equations

The mass transfer coefficient, K_m was calculated using equation 1 (Alklaibi and Lior, 2005)

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

where J_p, H_{fg}, T_{hi} and T_{ci} are the permeate flux, latent heat vaporization, inlet hot and inlet cold temperatures, respectively. Next, liquid entry pressure (LEP) value was calculated using Laplace (Cantor) Equation (Alklaibi and Lior, 2005)

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

where γ_i and θ represent the sea water surface tension and contact angle between the sea water and the membrane surface, respectively, while r_{memb} is the largest pore size. Lastly, permeate flux, J_p, was computed using the equation 3 (Alklaibi and Lior, 2005)

$$J_p = C_w\left(\frac{H_{fg}}{(R_{const} \times (T_m + 273) \times P_m)}\right)(T_{hi} - T_{ci}) \tag{3}$$

where C_w, R_{const}, T_m, and P_m are overall mass transfer coefficient, specific gas constant, mean temperature, and mean pressure, respectively .

2.3 Constant parameters

Several parameters in this model were held constant as shown in Table 1. The membrane area was 0.2×10 m^2, with a thermal conductivity of 0.19 w/m.k, while permeate (T_P) and feed (T_f) temperatures were 45 °C and 60 °C, respectively. Seawater salinity was 35000 ppm and the product salinity that represented the fresh water was 500 ppm. The minimum pump efficiency chosen for this model was 0.75.

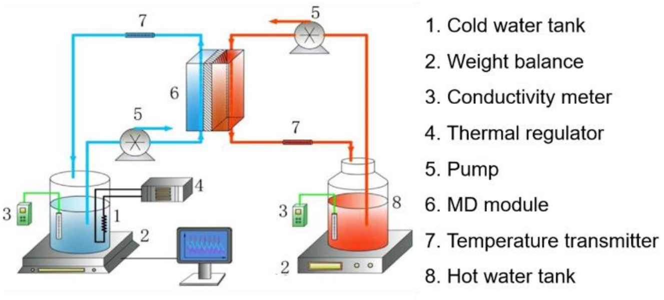

Figure 1: Schematic diagram of the experimental DCMD process

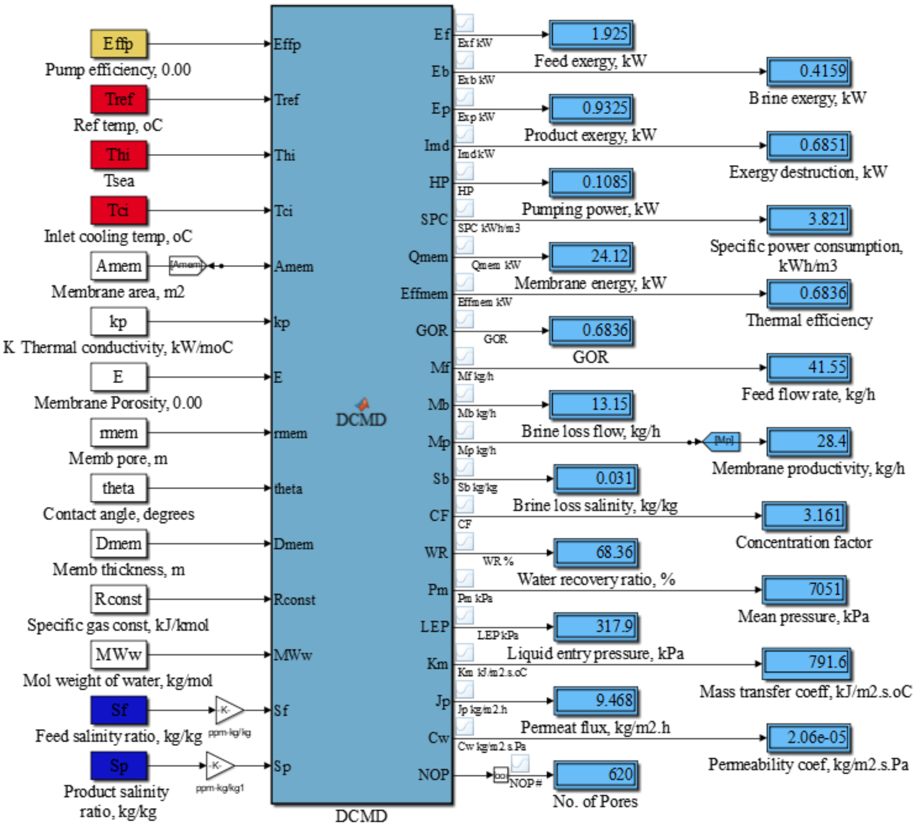

Figure 2: MATL*AB-Simulink block involving comprehensive parameters in the DCMD*

Table 1: Fixed input

Constant Parameters	Value
Membrane area	0.2^10 m^2
Thermal conductivity	0.00019 kW/m°C
Feed salinity ratio	35000 ppm
Product Salinity ratio	500
Pump efficiency	0.75

2.4 Varied parameters

A simulation model was created in this study using MATLAB software to analyze the influence of membrane properties namely porosity, pore size, contact angle, and membrane thickness on MD performance.
The first simulation examined the impact of membrane thickness and determined the optimum thickness to achieve excellent performance. From literature, the thinnest MD was 70 µm and the thickest was 200 µm (Zhao et al., 2018). Thus, we employed an MD range of 70-190 µm in this simulation. It was expected that thicker MD will reduce the permeate flux due to increased mass transfer resistance.
It is generally accepted that the membrane porosity is one of the most important parameters in MD for flux and energy efficiency, regardless of the MD configuration. According to (El-Bourawi et al., 2006), membrane porosity in the MD system varies from 0.30 to 0.85, while (Zhang et al., 2010) mentioned that the porosity of the membranes typically is in the range of 0.60 to 0.95. Therefore, we employed a range of 0.50-0.90 in this simulation. Note that a membrane with high porosity has higher permeate flux and lower conductive heat loss.
Membrane pore size plays an important role in term of permeate flux. The normally used pore size in MD is in the range of 0.20 µm-1.0 µm (Alkhudhiri et al., 2012). Therefore, we chose a range of 0.22 µm-1.0 µm in this simulation. It was expected that the permeate flux will increase when membrane pore size becomes higher.
A contact angle above 90° is typically recommended for MD (Eykens et al., 2016). In this simulation, we employed a range of 90°-150°. Note that when contact angle increases, the liquid entry pressure also rises.

3. Results and discussion

3.1 Effect of membrane thickness

Figure 3(a) shows the results from simulation when membrane thickness was from 70-190 µm. There were declines in permeate flux and mass transfer coefficient, whereas LEP remained constant as the membrane thickness increased. The highest permeate flux recorded was 66.79 kg/m^{2}h when the membrane was the thinnest (70 µm). When the membrane was the thickest (190 µm), the lowest permeate flux was 24.61 kg/m^{2}h. This implies that if the membrane is too thick, it is difficult for the permeate to pass through and results in an increase in mass transfer resistance (Kebria and Rahimpour, 2020).
As for the mass transfer coefficient, it decreased as the membrane thickness increased. The highest value of mass transfer coefficient was 9423 kJ/m^{2}s°C when the thickness was minimum, and the lowest value was 3427 kJ/m^{2}s°C when the thickness was maximum. This was in line with the finding from literature (Berry et al., 2017). The membrane performance would be considered excellent if the MD process results in higher permeate flux and greater mass transfer coefficient. Even though the membrane thickness was increased, the LEP value was unchanged at 305.9 kPa. This suggests that membrane thickness had no effect on the LEP and did not contribute to the membrane wetting phenomenon (Alklaibi and Lior, 2005).

3.2 Effect of membrane porosity

Figure 3(b) portrays the simulation outcome with membrane porosity of 0.50-0.90. There was an increment in permeate flux and mass transfer coefficient, whereas LEP remained constant when the porosity of the membrane increased. The highest flux recorded was 100.6 kg/m^{2}h at the maximum porosity (0.90), while the lowest was 16.7 kg/m^{2}h at the minimum porosity (0.50). This means that porous membranes would allow ions and other particles to permeate more easily, corroborating earlier finding that high porosity membranes had higher permeate flux (El-Bourawi et al., 2006). However, there is possibility of membrane fouling when the membrane is too porous which could cause permeate flux to decrease over time.
The mass transfer coefficient increased as the membrane porosity increased. The highest was 14190 kJ/m^{2}s°C when the porosity was at the peak, and the lowest value 2356 kJ/m^{2}s°C was reached when the porosity was the lowest. This implies that porous membrane enhanced the rate of pollutant emission from aqueous solution. The LEP value also stayed at 305.9 kPa even when the porosity was raised, indicating that the porosity had no effect on the LEP value and did not contribute to the membrane wetting phenomenon.

3.3 Effect of membrane pore size

Figure 3(c) depicts the results of varying membrane pore size from 0.22-1.0 µm. There was an accretion towards permeate flux and mass transfer coefficient, whereas LEP value dropped as the pore size got bigger. The highest permeate flux recorded was 242.9 kg/m^{2}h when the membrane pore size was the largest (1.0µm). When the membrane pore size was minimum (0.22 µm), the smallest flux recorded was 66.79 kg/m^{2}h. This implies smaller pore size only permitted certain ions and particles to permeate. Despite larger pore size resulted in higher flux and lower fouling rate, there was a possibility of seeping. Thus, the optimum pore size should be used to get high permeate flux while minimizing the drawbacks.

It can be observed that the mass transfer coefficient improved as the membrane pore size increased, demonstrating directly proportionality. The highest mass transfer coefficient was 34260 kJ/m^{2}s°C with the largest pore size, and the lowest mass transfer coefficient was 9423kJ/m^{2}s°C with the lowest pore size. When the pore size of the membrane was increased, the LEP reduced from 305.9 to 84.12 kPa. A high LEP is preferred in MD process as it could prevent feed liquid from penetrating wetting the membrane.

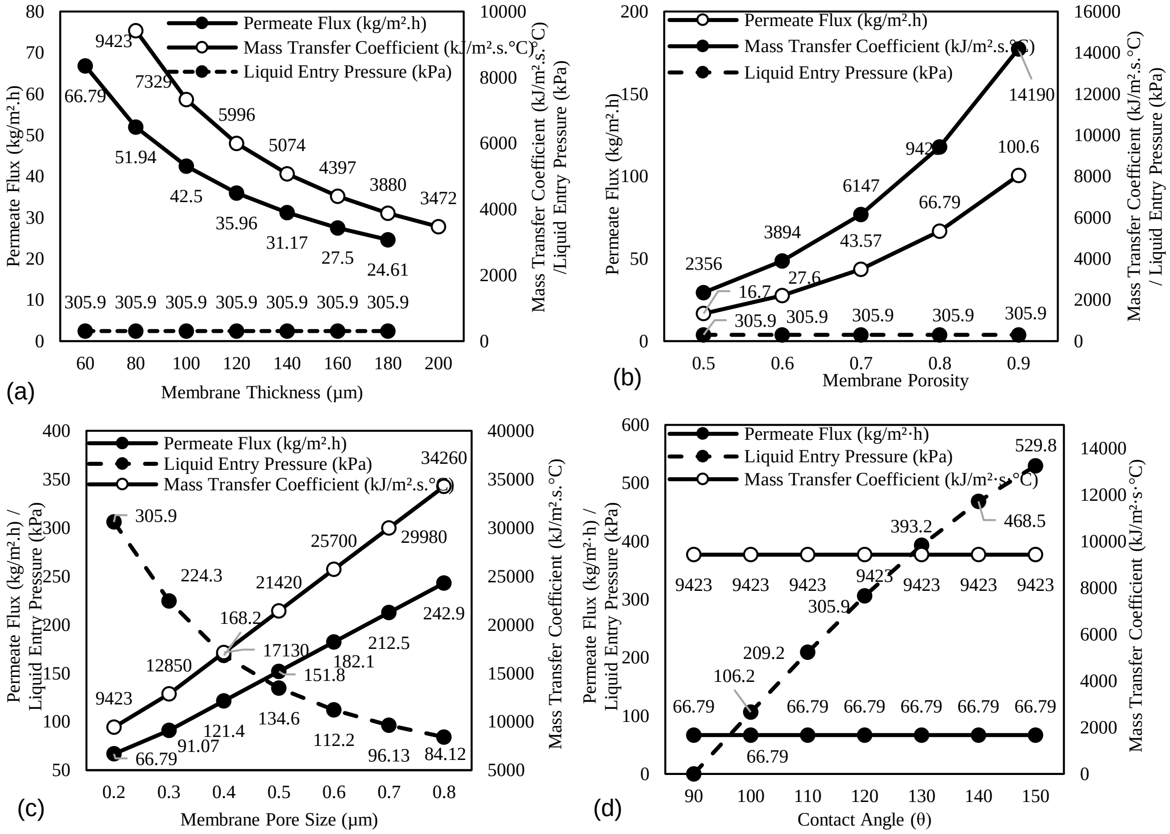

Figure 3: Effects of (a) membrane thickness, (b) porosity, (c) pore size, and (d) contact angle towards permeate flux, mass transfer coefficient, and liquid entry pressure

3.4 Effect of contact angle

Figure 3(d) displays the outcome of varied contact angle from 90°-150°. It was revealed that permeate flux and mass transfer coefficient remained constant, whereas LEP increased when the contact angle was greater. This implies that the contact angle had no effect on the permeate flux and mass transfer coefficient. This denotes that changes in the rate of pollutant emission from aqueous solution were not caused by the contact angle.

On the other hand, the LEP and membrane contact angle were directly proportional. The highest value of LEP was 529.8 kPa when the contact angle was the largest (150°) and zero when the contact angle was the smallest (90°), proving significant impact of the contact angle on LEP. Large contact angle is preferred to obtain a high value of LEP and reduce the occurrence of membrane wetting.

4. Conclusions

The simulation reveals properties that have significant impact on MD performance. A thin membrane was necessary for high permeate flux and mass transfer coefficient, with the proposed thickness was 70 µm. Porosity increment from 0.5 to 0.9 resulted in five times higher flux and enhanced mass transfer coefficient, but it could potentially lead to fouling problem. In MD process, 0.75-0.80 porosity was suggested. Pore size within 0.20-0.40 µm was beneficial towards greater permeate flux and mass transfer coefficients, but it restricted the LEP. Finally, a contact angle greater than 90° was proposed to raise the LEP up to 529.8 kPa. Permeate flux and mass transfer coefficient remained constant when contact angle was varied, indicating that contact angle had no effect on either. These validated findings are critical for understanding and optimizing MD system. However, there are limitations in oversimplification of complex physical phenomena and full variability of conditions in realworld scenario. Further progress could be achieved via multiphysics models or artificial intelligence that can incorporate chemical reactions, fouling mechanism, real-time operational data, and scale-up studies.

Acknowledgments

The authors would like to acknowledge College of Engineering, Universiti Teknologi MARA and Ministry of Higher Education Malaysia for research grant (FRGS/1/2022/TK05/UITM/02/9).

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