

The Influence of water permeability, solute resistance and mass transfer coefficient on water flux behavior in forward osmosis

Abdulrahman Alalawi¹, Ibrahim S. Al-mutaz^{*2}, Nawaf Bin Darwish¹, Ibrahim A. Alsayer³

¹Desalination Technologies Institute, King Abdulaziz City for Science and Technology, Saudi Arabia

²Chemical Engineering Dept., College of Engineering, King Saud University,
P.O. Box 800, Riyadh 11421, Saudi Arabia

³Department of Chemical Engineering, Northern Border University, Arar, Saudi Arabia

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Abstract. Forward osmosis (FO) is an innovative membrane process with growing potential. Mathematical models for predicting water flux in forward osmosis (FO) are valuable for understanding the system behavior and helpful in optimizing the performance. This work explores the relationship between water flux key governing parameters, namely water permeability, solute resistance and mass transfer coefficient which affect the water flux behavior. The influence of these parameters on water flux behavior is analyzed, highlighting how water permeability governs the water transport capacity, solute resistance dictates the rejection of solutes, and the mass transfer coefficient reflects the impact of external boundary layers. For both orientations the membrane active layer faces the feed solution (AL-FS) and the membrane active layer faces the draw solution (AL-DS), water flux increases with an increase in water permeability since water flux is directly proportional to the membrane water permeability as given by the basic flux equations. The mass transfer coefficient, whether on the feed side (AL-FS mode) or on the draw side (AL-DS mode), does not significantly influence the enhancement of water flux associated with increased membrane water permeability. On the other hand, solute resistance has a pronounced effect on the water flux with an increase in water permeability. At higher values of solute resistance, the increase in water flux resulting from enhanced water permeability becomes progressively limited, due to the intensified internal concentration polarization that diminishes the effective osmotic driving force.

Keywords: forward osmosis; mass transfer coefficient; solute resistance; water flux; water permeability

1. Introduction

Forward osmosis (FO) is a membrane process of water separation and purification. The movement of water from the feed solution (low concentration) to the draw solution (high concentration) through a selectively permeable membrane without any external energy is called forward osmosis.

Water flux describes the water movement across the membrane, and it is a key element to determine the efficiency of the FO membrane process. High flux is an important criterion for scaling up the FO process for industrial applications. Optimizing the FO membrane flux can be achieved by fabricating a high-flux membrane and by improving the operating conditions of FO

*Corresponding author, Professor, E-mail: almutaz@ksu.edu.sa; ialmutaz@gmail.com

[1]. Mathematical modeling is often used to evaluate the performance of FO systems [2]. It infers the effects of various parameters on the FO performance. Also, it helps in designing the FO system and optimizing the operating conditions. The methodologies used in current water flux models require extensive knowledge of FO membrane properties and system hydrodynamics. The performance of the FO process is linked to the properties of membranes and draw solutions [3]. The osmotic pressure generated by the draw solution (DS) has a significant impact on the FO water flux [4]. Membrane properties also have important role in the FO performance. There are several parameters governing the membrane performance. Water permeability, solute resistance, and mass transfer coefficient are crucial factors affecting water flux behavior in forward osmosis systems. Water permeability governs the rate at which water molecules flow across the membrane. Solute resistance refers to the impediment created by solute molecules in the feed solution. Mass transfer coefficient affects effectiveness of water transport across the membrane.

The FO water flux increases almost proportionally with the membrane water permeability at low permeability values when other parameters are not changed. Water flux is enhanced by high water permeability. However, concentration polarization modifies the osmotic pressure gradient to offset this enhancement. Concentration polarization can be divided into two categories: internal concentration polarization (ICP) and external concentration polarization (ECP) based on the developed concentration gradient. In ECP concentration gradient occurs at the membrane surface in the laminar boundary layer between the bulk stream and the membrane while in ICP the concentration gradient happens within the porous support layer [5]. When the FO membrane is operating at a high-water flux or using high salinity draw solutions, the ECP effect is significant [6].

The internal concentration polarization (ICP) is likely less important at a relatively low flux level. The increase in water flux will be associated with severe internal concentration polarization. Concentrative and dilutive are the two types of ICP depending on the forward osmosis mode orientation [7]. Concentrative ICP happens when the membrane active layer faces the draw solution (AL-DS) configuration. While the dilutive ICP occurs when the membrane active layer faces the feed solution (AL-FS) configuration. For (AL-DS) configuration, more severe ICP was observed compared to (AL-FS) as a result of dilutive ICP in the FO support layer [8].

Higher membrane water permeability cannot completely eliminate the impact of internal concentration. It may maintain reasonable water flux despite the reduction in the driving force caused by the concentration gradient within the support layer. However, very high membrane water permeability might also allow for increased draw solute back diffusion, reducing the overall performance. A combination of high membrane water permeability, a well-designed support layer, and optimized process conditions is key to minimize ICP's impact on water flux.

Solute resistance or solute resistivity is a function of the membrane characteristics, such as membrane porosity, tortuosity, and thickness and draw solution diffusion coefficient [9]. These properties increase the resistance to the water transport through FO membrane. Solutes that resist diffusion more readily create a concentrated zone near the membrane, weakening the osmotic pressure difference and hindering water flow. Solutes with high resistance to diffusion (low diffusivity) can exacerbate ICP and significantly hinder water flux in FO. Larger solutes generally have lower permeability through the membrane. Lower molecular weight solutes have higher diffusion coefficient and may promote higher water fluxes across the membrane nevertheless they exhibit high reverse salt diffusion (RSF) too [10]. While charged solutes can interact with the membrane's charge, affecting their passage. Hydrophobic solutes tend to have lower affinity for water and the membrane, hindering their passage. Increasing the temperature will reduce the

resistivity to solute diffusion due to the increase in diffusivity and reduction in viscosity [11]. Draw solution with a high diffusion coefficient will readily diffuse through the membrane support layer and thus decrease the ICP effects [12].

The mass transfer coefficient is a function of system geometry, fluid velocity, and fluid properties. It is commonly correlated using the dimensionless Sherwood, Reynolds, and Schmidt numbers as proposed by [7]. The majority of the Sherwood relations proposed in the literature were derived for mass transfer in smooth, non-porous systems or through heat transfer-mass transfer analogies [13]. On the other hand, FO membranes are often rough on a microscopic scale and semipermeable. The mass transfer coefficient varies with the direction of flow, as does the mass transfer, which is also dependent on the fluid characteristics and flow rate [14].

Fundamentally, the mass transfer coefficient is defined as the ratio of the molecular diffusivity constant to the thickness of the solute boundary layer. To date, limited efforts have been made to gain a better understanding of boundary layer phenomena in forward osmosis processes [15]. According to the film theory, the mass transfer coefficient dictates the severity of the external concentration polarization (ECP). Any small inaccuracy in the mass transfer coefficient value can generate significant error because the concentration profile in the boundary layer is exponential. Therefore, it is essential to determine the proper correlation of the mass transfer coefficient for each particular membrane process having specific hydrodynamic channel and membrane characteristics in order to construct a rigorous model for the FO process.

Despite the significant progress in FO membrane development and system design, several challenges remain that hinder the widespread adoption of forward osmosis in large-scale applications. One of the main obstacles is the complex interplay between membrane properties and operational parameters, which can lead to suboptimal performance if not properly understood and controlled. For instance, while increasing water permeability is desirable for higher flux, it can also result in elevated reverse solute flux, potentially contaminating the feed solution and reducing the efficiency of the separation process. Furthermore, the selection of an appropriate draw solution is crucial, as it must provide a sufficient osmotic driving force while maintaining low toxicity, high diffusivity, and ease of regeneration or recovery [16, 6].

Recent advancements in mathematical modelling have provided valuable insights into the mechanisms governing water and solute transport in FO systems. These models enable researchers and engineers to predict the effects of various parameters on system performance, facilitating the design of more efficient membranes and optimized operating conditions. By incorporating factors such as concentration polarization, solute resistance, and mass transfer limitations, these models can simulate real-world scenarios with greater accuracy. Consequently, a thorough understanding of the fundamental transport phenomena and their interdependencies is essential for overcoming existing limitations and advancing the practical implementation of forward osmosis technology in water treatment, desalination, and resource recovery applications [16, 17].

The objective of this study is to explore the influences of water permeability, solute resistance and mass transfer coefficient on water flux behavior in Forward osmosis process. The mathematical model used in this work was derived using the modified film theory and diffusion transport coupled with balance equations.

Unlike our previous study, which focused on model derivation and validation, the present work provides a systematic parametric analysis that isolates the individual and coupled effects of water permeability, solute resistance, and mass transfer coefficients on forward osmosis water flux. This analysis offers new mechanistic insight into flux-limiting behavior under different membrane orientations and operating regimes.

2. Prediction of water flux in forward osmosis

The mathematical models for the prediction of water flux in forward osmosis were developed recently [18]. Internal and external concentration polarization were taken into consideration in both cases, i.e., active layer facing the feed solution (AL-FS) and active layer facing the draw solution (AL-DS).

In this theoretical study, the feed and draw solutions were assumed to be aqueous NaCl solutions. The feed solution concentration was fixed, while the draw solution concentration was varied to investigate its influence on water flux behavior. The osmotic pressures of the feed (π_{Fb}) and draw (π_{Db}) solutions were calculated using the van't Hoff equation and used as input parameters in the model. The water flux expressions employed in this study are closed-form analytical equations that are implicit with respect to the water flux due to the exponential terms associated with concentration polarization. These equations were derived from modified film theory and diffusion transport principles and do not require coupling with additional transport equations.

The developed model for the prediction of water flux in forward osmosis based on the effect of internal and external concentration polarization in the feed side for active layer facing the feed solution (AL-FS) is as follows.

$$J_w = A \left(\pi_{Db} e^{(-J_w K)} - \pi_{Fb} e^{\left(\frac{J_w}{k_F}\right)} \right) \quad (1)$$

where A is the pure water permeability coefficient (m/atm.d), π_{Db} is the osmotic pressure of the draw solution (atm), K is the solute resistance inside the porous support layer (d/m), k_F mass transfer coefficient on the feed side of the membrane (m/d), and π_{Fb} is the osmotic pressure of the feed solution (atm). The mathematical model was solved numerically using a custom-developed MATLAB code, where the governing equations were solved using a numerical root-finding scheme implemented in MATLAB. The mathematical model for predicting water flux in forward osmosis, accounting for internal and external concentration polarization for the active layer facing the draw solution (AL-DS), is given below.

$$J_w = A \left(\pi_{Db} e^{\left(-\frac{J_w}{k_D}\right)} - \pi_{Fb} e^{J_w K} \right) \quad (2)$$

where A is the pure water permeability, π_{Db} is the osmotic pressure of the draw solution., K is the solute resistance inside the porous support layer, k_D mass transfer coefficient on the draw side of the membrane (m/d), and π_{Fb} is the osmotic pressure of the feed solution. Because the water flux appears on both sides of Eqs. (1, 2), the equations were solved numerically using a root-finding algorithm implemented in MATLAB. Convergence was achieved rapidly for all parametric cases considered, ensuring numerical stability and reproducibility of the results. The governing equations used in this work were previously validated against independent experimental data reported by [7]. Detailed quantitative comparisons demonstrating good agreement between predicted and experimental water flux values are presented in Tables 2, 3 of [18]. Accordingly, the present study builds upon a validated theoretical framework.

3. Factor affecting water flux in forward osmosis

Water flux in forward osmosis (FO) is influenced by a range of interrelated factors that govern

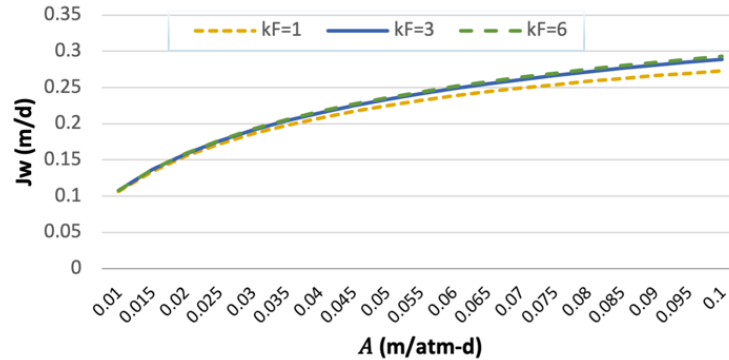


Figure 1. Plot of water flux (J_w) vs. water permeability coefficient (A) at constant solute resistance (K) of 4.53 (d/m) and different values of feed mass transfer coefficient (k_F) expressed in (m/d)

the efficiency of water transport across the semi-permeable membrane. Key determinants include the osmotic pressure gradient between the draw and feed solutions, which serves as the primary driving force for water movement. The nature and concentration of solutes in both solutions influence external concentration polarization and reverse solute diffusion, which can hinder water transport.

The forward osmosis (FO) performance is different when the feed solution is against the two different layers of the membrane. The FO membrane can be used in either orientation such as AL-FS mode, in which the membrane active layer is facing the feed solution and AL-DS mode, in which the membrane active layer is facing the draw solution.

In the following sections, the effect of water permeability (A), solute resistance (K) and mass transfer coefficient (k_F) on water flux in forward osmosis in AL-FS mode will be studied.

3.1 Forward osmosis with AL-FS mode

3.1.1 Effect of water permeability (A)

Water permeability (A) is a critical parameter influencing water flux in forward osmosis (FO) processes. It reflects the membrane's intrinsic ability to allow water molecules to pass through under an osmotic pressure gradient. Water permeability describes the amount of water that can pass through the membrane per unit-time. High water permeability would lead to higher flux, while a low water permeability will have the opposite effect. However, its effect is closely linked to membrane structure and the extent of internal concentration polarization, which can diminish the effective driving force. Therefore, optimizing water permeability, while minimizing structural resistance and solute back diffusion, is essential for achieving high-performance FO membranes and maximizing water recovery efficiency [19].

Fig. 1 shows the change in water flux with increasing the water permeability at different feed mass transfer coefficient (k_F) and constant solute flux. From this figure, water flux increases with increasing the water permeability. This behavior is expected, as water flux is directly proportional to the membrane water permeability as given by the basic flux equations. The effect of mass transfer coefficient on the water flux is minimal. Small increase in water flux with increasing in the mass transfer coefficient is observed. This is attributed to the decrease in the back diffusion as

the mass transfer coefficient increases.

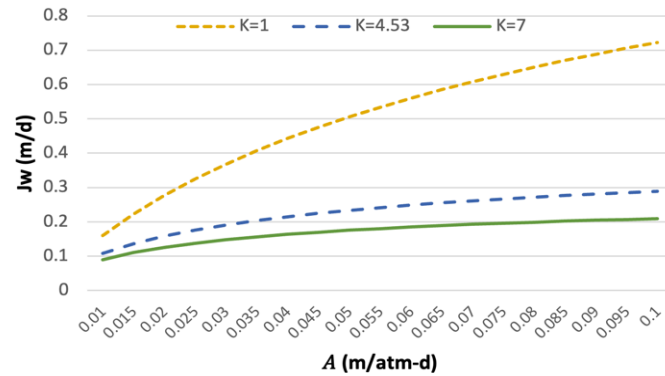


Figure 2. Plot of water flux (J_w) vs. water permeability coefficient (A) at constant feed mass transfer coefficient (k_F) of 3.0 (m/d) and different values of solute resistance (K) expressed in (d/m)

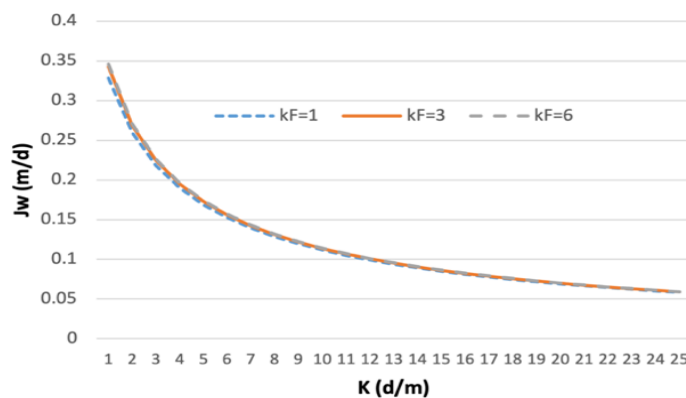


Figure 3. Plot of water flux (J_w) vs. solute resistance (K) at constant water permeability coefficient (A) of 0.027 (m/atm-d) and different values of feed mass transfer coefficient (k_F) expressed in (m/d)

On the other hand, Fig. 2, shows the effect of water permeability coefficient (A) on water flux at different constant values of solute resistance (K) while holding value of mass transfer coefficient (k_F) at constant value of 3.0 (m/d). The variation of water flux with water permeability is shown in Fig. 2. Water flux increases with the increasing in the water permeability, since the water flux is directly proportional to the membrane water permeability as mentioned before. The effect of solute resistance on water flux is pronounced especially at low values of solute resistance. As shown Fig. 2, for example at $A=0.07$ (m/atm-d), water flux at $K=1$ increases 132.8% from that at $K=4.53$ (m/d) and 215.6% from that at $K=7$ (m/d). This means the lower the solute resistance, the higher the water flux.

Moreover, at high values of solute resistance, the increase of the water flux with the water permeability is limited. This indicates that high solute resistance values play a major role in the water transport across the FO membrane.

3.1.2 Effect of Solute Resistance (K)

Solute resistance (K) describes the resistance to solute diffusion across the membrane support

layer. Solute resistance in forward osmosis (FO) significantly impacts water flux by influencing

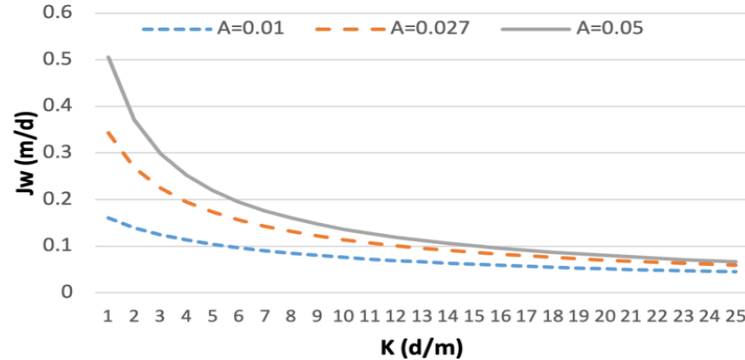


Figure 4. Plot of water flux (J_w) vs. solute resistance (K) at constant feed mass transfer coefficient (k_F) of 3.0 (m/d) and different values of water permeability coefficient (A) expressed in (m/atm.d)

the extent of concentration polarization within and outside the membrane. Higher solute resistance leads to better separation but lower flux, while low solute resistance would lead to the opposite. Additionally, solute resistance can hinder the back diffusion of draw solutes, further intensifying ICP. Therefore, minimizing solute resistance through optimized membrane design and material selection is essential for enhancing FO performance and sustaining high water flux [19]. Fig. 3 exhibits the same behavior as Fig. 2, the lower the solute resistance, the higher the water flux. So, water flux decreases as the solute resistance increases. The solute resistance is a function of draw solution diffusion coefficient, membrane thickness, tortuosity, and porosity. These properties increase the resistance to the water transport through FO membrane.

From Fig. 4, water flux decreases as the solute resistance increases at constant water permeability coefficient as expected. However, at lower values of solute resistance, water flux changes significantly with the change in the water permeability coefficient, as displayed on Fig. 4. Higher values of solute resistance diminished the effect of water permeability coefficient on the water flux.

3.1.3 Effect of Mass Transfer Coefficient (k_F)

The mass transfer coefficient plays a vital role in determining water flux in forward osmosis (FO) by governing the rate at which solutes are transported across the boundary layers adjacent to the membrane surfaces. A higher mass transfer coefficient enhances the removal of solutes from the membrane surface, thereby reducing external concentration polarization (ECP) and maintaining a stronger effective osmotic driving force. Conversely, a low mass transfer coefficient leads to solute accumulation near the membrane, diminishing the osmotic gradient and reducing water flux [20]. Optimizing flow conditions and membrane module design to improve mass transfer is therefore essential for maximizing FO efficiency. Mass transfer coefficient is a diffusion rate constant. It relates the mass transfer rate, mass transfer area, and the change in concentration. The effect of mass transfer coefficient (k_F) on water flux at different constant values of water permeability coefficient (A) while holding value of solute resistance (K) constant at 4.53 (d/m) is shown in Fig. 5. Water flux increases with the increase in feed mass transfer coefficient at different values of water permeability as shown in Fig. 5. Then water flux reaches a constant value where any increase in feed mass transfer coefficient does not cause significant change in the water flux. The

process is not in the mass transfer control region.

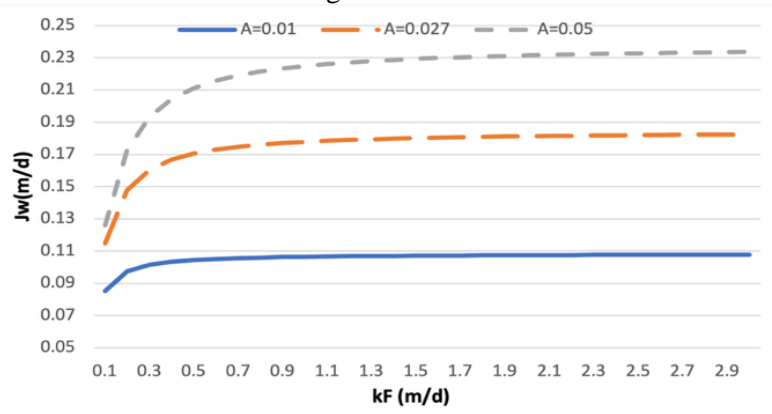


Figure 5. Plot of water flux (J_w) vs. feed mass transfer coefficient (k_F) at constant solute resistance (K) of 4.53 (d/m) and different values of water permeability coefficient (A) expressed in (m/atm.d)

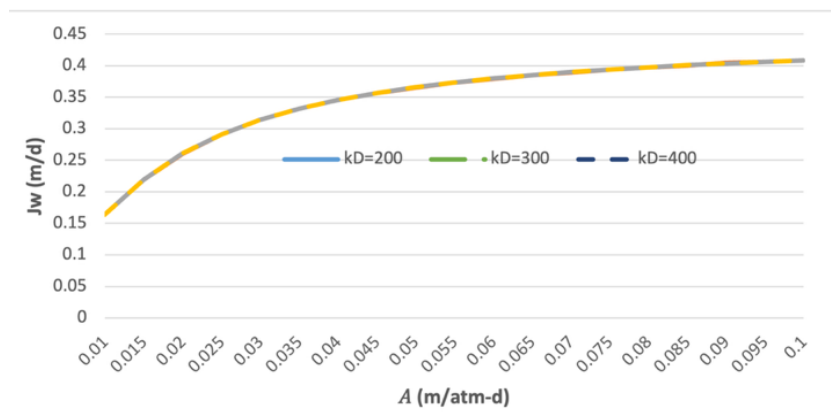


Figure 7. Plot of water flux (J_w) vs. water permeability coefficient (A) at constant solute resistance (K) of 4.53 (d/m) and different values of draw mass transfer coefficient (k_D) expressed in (m/d)

The effect of feed mass transfer (k_F) on water flux (J_w) was studied at different solute resistance (K). The results obtained are presented in Fig. 6 which shows that water flux increases when feed mass transfer increases. Higher values of water flux are obtained at lower solute resistance. Higher values of solute resistance limited the effect of water permeability coefficient on the water flux.

3.2 Forward Osmosis with AL-DS Mode

3.2.1 Effect of Water Permeability (A)

Fig. 7 shows the change in water flux with increasing the water permeability at different draw mass transfer coefficient (k_D) and constant solute flux. From this figure, water flux increases with increasing the water permeability. Moreover, there is no significant effect on the water flux when the draw mass transfer (k_D) increases with increasing water permeability (A).

On the other hand, Fig. 8 shows the effect of water permeability coefficient (A) on water flux at

different constant values of solute resistance(K) while holding value of draw mass transfer

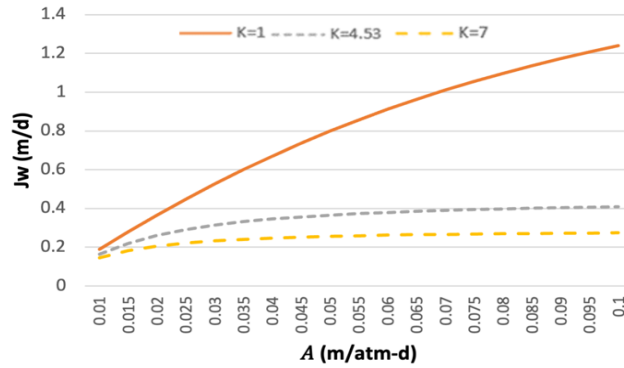


Figure 8. Plot of water flux (J_w) vs. water permeability coefficient (A) at constant draw mass transfer coefficient (k_D) of 300 (m/d) and different values of solute resistance(K) expressed in (d/m)

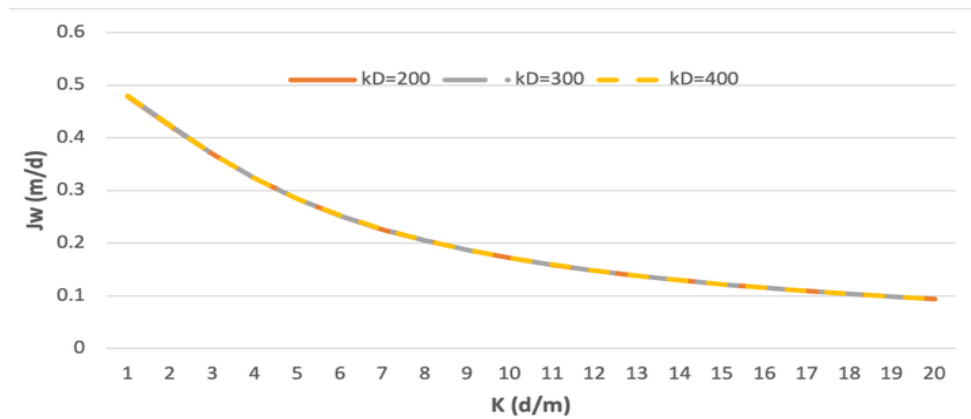


Figure 9. Plot of water flux (J_w) vs. solute resistance(K) at constant water permeability coefficient (A) of 0.027 (m/atm-d) and different values of draw mass transfer coefficient (k_D) expressed in (m/d)

coefficient (k_D) at constant value of 300 (m/d). The variations of water flux versus water permeability are shown in Fig. 8. Water flux increases with the increasing in the water permeability, since the water flux is directly proportional to the membrane water permeability as mentioned before. The effect of solute resistance on water flux is pronounced especially at low values of solute resistance. This means the lower the solute resistance, the higher the water flux. Moreover, at high values of solute resistance, the increase of the water flux with the water permeability is limited. This indicates that high solute resistance values play a major role in the water transport across the FO membrane.

3.2.2 Effect of Solute Resistance

Fig. 9 exhibits the same behavior expel from Fig. 8, the lower the solute resistance, the higher the water flux. So, water flux decreases as the solute resistance increases. The solute resistance is a function of draw solution diffusion coefficient, membrane thickness, tortuosity, and porosity. These properties increase the resistance to the water transport through FO membrane.

Fig. 10 shows the effect of solute resistance (K) on water flux at different constant values of

water permeability coefficient (A) while holding value of draw mass transfer coefficient (k_D)

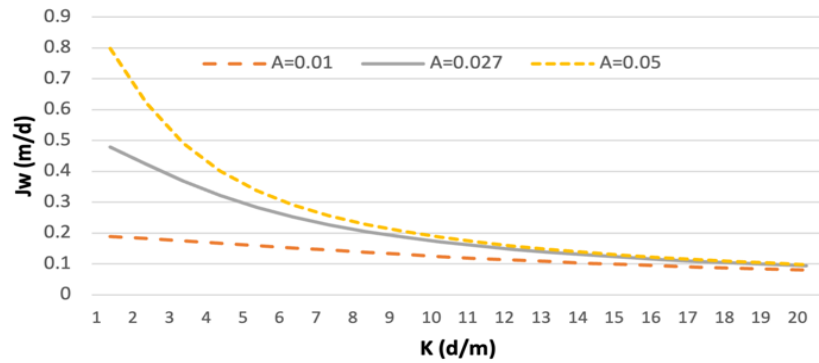


Figure 10. Plot of water flux (J_w) vs. solute resistance (K) at constant draw mass transfer coefficient (k_D) of 300 (m/d) and different values of water permeability coefficient (A) expressed in (m/atm.d)

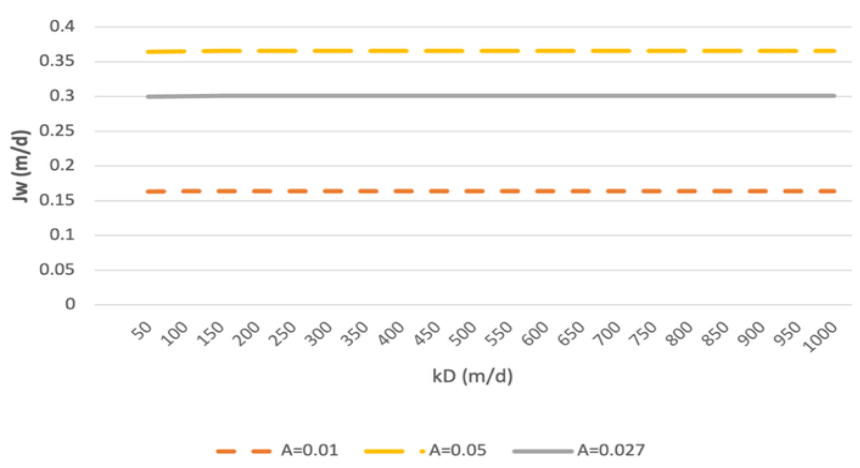


Figure 11. Plot of water flux (J_w) vs. draw mass transfer coefficient (k_D) at constant solute resistance (K) of 4.53 (d/m) and different values of water permeability coefficient (A) expressed in (m/atm.d)

constant at 300 (m/d). From Fig. 10, water flux decreases as the solute resistance increases at constant water permeability coefficient as expected. However, at lower values of solute resistance, water flux changes significantly with the change in the water permeability coefficient, as displayed on Fig.10. Higher values of solute resistance diminished the effect of water permeability coefficient on the water flux.

3.2.3 Effect of Mass Transfer Coefficient (k_D)

The effect of draw mass transfer coefficient (k_D) on water flux at different constant values of water permeability coefficient (A) while holding value of solute resistance (K) constant at 4.53 (d/m) are shown in Fig. 11. Water flux increases with the increase in draw mass transfer coefficient at different values of water permeability as shown in Fig. 11. Then water flux reaches a constant value where any increase in draw mass transfer coefficient does not cause significant change in the water flux. The process is not in the mass transfer control region.

The effect of draw mass transfer (k_D) on water flux (J_w) was studied at different solute

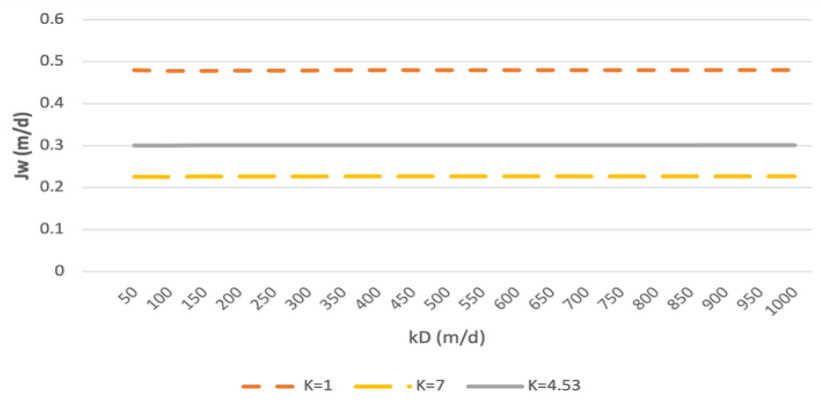


Figure 12. Plot of water flux (J_w) vs. draw mass transfer coefficient (k_D) at constant water permeability coefficient (A) of 0.027 (m/atm-d) and different values of solute resistance (K) expressed in (d/m)

resistance (K). The results obtained are presented in Fig. 12 which shows that water flux increases when draw mass transfer increases. Higher values of water flux are obtained at lower solute resistance. Higher values of solute resistance limit the effect of water permeability coefficient on the water flux.

4. Conclusions

The influence of various variables on the water flux in the forward osmosis process was studied to demonstrate their effects. The study examined the influence of water permeability on the water flux. For both orientations (AL-FS and AL-DS), water flux increases with an increase in water permeability since water flux is directly proportional to the membrane water permeability as given by the basic flux equations. Mass transfer coefficient on the feed side (AL-FS mode) or on the draw side (AL-DS mode) has no significant effect on the increase of water flux with an increase in water permeability. On the other hand, solute resistance has a pronounced effect on the water flux with an increase in water permeability. At higher solute resistance values, the increase in water flux with increasing water permeability becomes limited. This indicates that high solute resistance minimizes the effect of increase in the water permeability.

Also, the study examined the impact of solute resistance on the flux. For both orientations (AL-FS and AL-DS), water flux decreases as the solute resistance increases since solute resistance restricts the diffusion through the membrane. The solute resistance is a function of draw solution diffusion coefficient, membrane thickness, tortuosity, and porosity. Mass transfer coefficient on the feed side (AL-FS mode) or on the draw side (AL-DS mode) has no significant effect on the decrease of water flux with an increase in water solute resistance. At low solute resistance values, water flux increases as the water permeability increases. However, the higher values of solute resistance diminished the effect of water permeability on the water flux.

The effect of mass transfer coefficient on the water flux was also examined. For AL-FS orientation, the increase in the mass transfer coefficient on the feed side of the membrane increases the water flux in particular at low water permeability and solute resistance. In the AL-DS

orientation, the mass transfer coefficient on the draw side of the membrane almost has no observable effect on water flux at every level of water permeability and solute resistance. For AL-FS, when water permeability is low, the feed side mass transfer coefficient plays a more crucial role in mitigating concentration polarization and boosting water flux. While for AL-DS, the strong driving force from the draw solution minimizes the influence of the feed side mass transfer coefficient on water flux, regardless of water permeability or solute resistance. High solute resistance strengthens the rejection of solutes by the membrane, reducing the impact of concentration polarization on water flux. This can contribute to a less pronounced effect of mass transfer coefficient on water flux, especially for the AL-DS orientation.

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