Mathematical Modeling of Reverse Osmosis System Design and Performance

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Abstract:

Reverse Osmosis (RO) is one of the most effective technologies for water desalination. However, the performance of the RO system is very sensitive to its design parameters and operating conditions. In this study, a computational model for RO desalination performance prediction was developed. The study compares the performance parameters of the RO system using different types of membranes with the developed model using one pressure vessel and seven membrane elements inside the pressure vessel. Two different feed water concentrations were investigated in this study. The first one is for seawater at a concentration of 40,000 mg/L, and the other one is at a concentration of 32,000 mg/L. By using WAVE software, the recovery ratio, feed pressure, salt rejection, and permeate concentration of every membrane element inside the pressure vessel were compared with the results obtained from the developed model.

1. Introduction:

Due to the increasing popularity of reverse osmosis technology, it is widely used in the desalination industry [1,2]. This process involves the use of semipermeable membranes designed to remove organic chemicals, proteins, and ions from water [3]. RO has many advantages such as a small footprint, compact design, and automatic process control capabilities [4]. Furthermore, it offers many advantages over traditional thermal processes such as multi-stage flashing (MSF) and multi-effect distillation (MED), most importantly the lower energy requirements of RO compared to thermal processes [5-8]. For brackish water, the RO process is probably the most widely used desalination technology using low-energy BWRO membranes [9]. The salt removal rate of RO systems is high, reaching 99.8% for seawater desalination and over 99% for brackish water [10].

The physical phenomenon of osmosis has been known for many years [11]. Osmosis term can be defined as a natural process in which water molecules spontaneously move from a low concentration (low osmotic pressure) to a higher concentration (high osmotic pressure) across a semipermeable membrane as shown in Figure (1a, 1b, and 1c)[12]. The semi-permeable membrane rejects the solutes and only allows water molecules to pass through. This process continues until a state of osmotic equilibrium is reached where the chemical potentials across the membrane become equal Figure [1b]. The flow process of water molecules can be reversed by applying external pressure on the solution of higher concentration (feed solution). In this case, the applied pressure difference is greater in magnitude than the osmotic pressure difference across the membrane. Hence, the water molecules are forced to flow in a direction opposite to that of the natural osmosis phenomenon. Correspondingly, the process occurring is known as RO and is depicted in Figure [1c].

To design a new RO membrane plant, it needs the evaluation of the membrane performance to estimate how many RO elements will be used and the type of membrane which is appropriate for a particular feed water concentration and recovery rate required to be obtained from this plant. Besides, the permeate concentration and flow rate also have to be estimated. Therefore, a special computational model is required to get fairly reliable results about the membrane performance. There are different types of software that have been developed by membrane manufacturing companies that are extensively used in research and industries for estimating the performance of membrane systems. However, most of this software cannot be coupled with other software or used with different RO membranes manufactured by a different company. As a result, the use of this software is limited by the specifications that the manufacturers determined regarding the characteristics of the membrane they are producing. Therefore, this study aims to develop a model and compare it with three types of membranes under two different feed water concentrations.

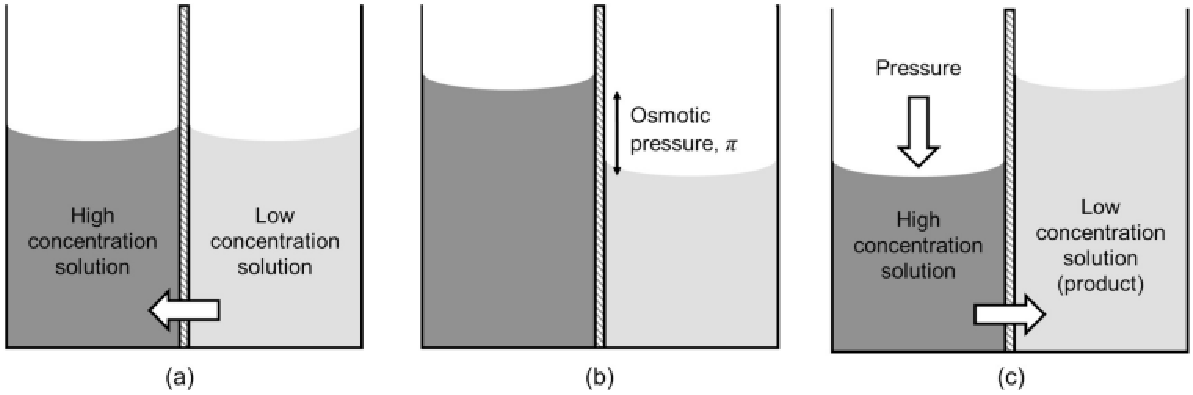

Figure 1, Osmotic pressure of RO system

Literature Review:

Many researchers have done in-depth studies on the modeling and optimization of the process of RO systems. K. Jamal et al. [13] investigated a small-scale reverse osmosis system to model a seawater desalination system. This study only focused on modeling and analyzing flux and salt rejection of a single element. Moreover, K. Jamal ignored the effect of concentration polarization in his model.

A. Alexiadis et al. [14] from the university of new south Wales conducted a CFD (Computational Fluid Dynamics) modeling and experimental validation of reverse osmosis membrane. Like K. Jamal, A. Alexiadis conducted the study on a single flat sheet reverse osmosis membrane module. The experiments were conducted by using a solution of salt (NaCl) at 2 g/L concentration. The feed solution was delivered to the membrane at a maximum pressure of 15 bars. The results he obtained showed good agreement between experiments and calculations, especially for ΔP less 1198.7 kPa.

A. Altaee [15] developed a computational model to predicate the performance of RO systems using four membrane elements with two different feed water salinity (35,000 mg/L and 38,000 mg/L). Altaee compared the results he obtained from the model with results obtained by ROSA software. The results from his study showed very good agreement with ROSA reaching up to 95%.

J.S. Choi et al. [16] performed a design method based on a simulation technique that has been developed for optimizing two-pass RO desalination systems. Choi focused on his study on the maximization of the permeate throughput (overall recovery), energy consumption minimization, and boron concentration in permeate. The results of the study of the two passes are that the flux for the 1st RO ranges from 9.6 L/m^2.h to 22 L/m^2.h with the ratio between 0.6 and 0.9 and that for the 2nd RO ranges from 8.1 L/m^2.h to 27 L/m^2.h with the ratio between 0.6 and 0.9. The total energy consumption ranges from 4 kWh/m^3 to 6.5 kWh/m^3, and boron rejection is low at normal operation conditions (pH = 7 and T = 25 8C), but it can be controlled by adjusting the PH of the second flow depending on the target boron concentration.

In another study, B. A. Qureshi et al. [17] conducted a Sensitivity analysis on different design and performance factors of a reverse osmosis system considering the fouling effect. It was found that increasing the salinity of the feed under the range investigated almost doubled the sensitivity of permeate concentration and water permeate flux to it. The model is proposed for predicting the normalized decrease in permeate flux due to fouling with two constants with a robust interpretation. He concluded from the results obtained that the model could predict the behavior accurately.

2. Mathematical Modeling: Solution-Diffusion Model

Over the past 40 years, the solution-diffusion model has become the most widely accepted way to explain how things move in reverse osmosis membranes. In this section, we will use the solution-diffusion model to find the phenomenological equations for transport in the RO process.

In separation applications, the most important thing about membranes is that they can control how different species pass through them. This permeation process is explained by two models. The first is the solution-diffusion model, in which permeants dissolve in the membrane material and then move through the membrane along a concentration gradient. Different permeants can be kept apart because the amount of material that dissolves in the membrane and the rate at which the material moves through the membrane are not the same for each. The second is the pore flow model, which says that permeants are separated by convective flow driven by pressure through tiny pores. One of the permeants is kept out of some of the pores in the membrane through which other permeants move. This keeps the different permeants from mixing. Both models were proposed in the 1800s, but the pore-flow model was more popular until the mid-1940s because it was more like what people normally experience. In the 1940s, however, the solution-diffusion model was used to explain how gases moved through polymeric films. This use of the solution-diffusion model wasn't too controversial, but in the 1960s and early 1970s, there was a lot of debate about how water moved through reverse osmosis membranes [18].

To start modeling the RO process, we need to find out the inlet feed water pressure to the system, which will pass from the first element to the n^{th} element in the pressure vessel. To determine the feed pressure, we should identify the osmotic pressure and flux required to be produced. The water flux is the amount of water produced per unit area per unit of time. Therefore:

$$J_w = K_w * (\Delta P - \Delta \pi) \qquad (1)$$

Where Kw is the membrane permeability and is characteristic of the membrane. The water flux also can be found by:

$$J_w = \frac{Qp}{Am} \qquad (2)$$

Q_p is the quantity of water produced by the system in volume per unit of time and A_m is the total surface area of the membrane elements inside the pressure vessel.

The osmotic pressure (π) can be found by the following equation:

$$\pi = \frac{2*C(av)*Rg*T}{1000*Mol\ (NaCl)} \qquad (3)$$

C_{av} is the average concentration in the feed side and can be calculated by:

$$C_{av} = C_f * ACF \qquad (4)$$

Where C_f is the concentration of feed and ACF is the average concentration factor which is a function of the membrane recovery rate (R), where brine concentration increases with the process of recovery rate along the membrane.

$$ACF = \frac{ln ln\ (1/(1-R))}{R} \qquad (5)$$

Since NaCl is the dominant particle in the concentration of feed water, the molecular weight (Mol) is counted in order to calculate the osmotic pressure.

In the practical RO process, the concentration of feed solution on the membrane surface is higher than the bulk concentration of feed water. Consequently, the osmotic pressure at the membrane surface will be higher than the bulk stream. This phenomenon of accumulation of salt on the membrane surface can be defined as the concentration polarization factor. Figure [2] shows the effect of concentration polarization on the membrane surface. This parameter then can be calculated by the following equation:

$$\beta = \frac{Cm}{Cf} \qquad (6)$$

where β is the concentration polarization factor, and C_m is the concentration on the membrane surface. Experimentally, the concentration polarization factor can be estimated as a function of the recovery rate:

$$\beta = EXP(0.7R) \qquad (7)$$

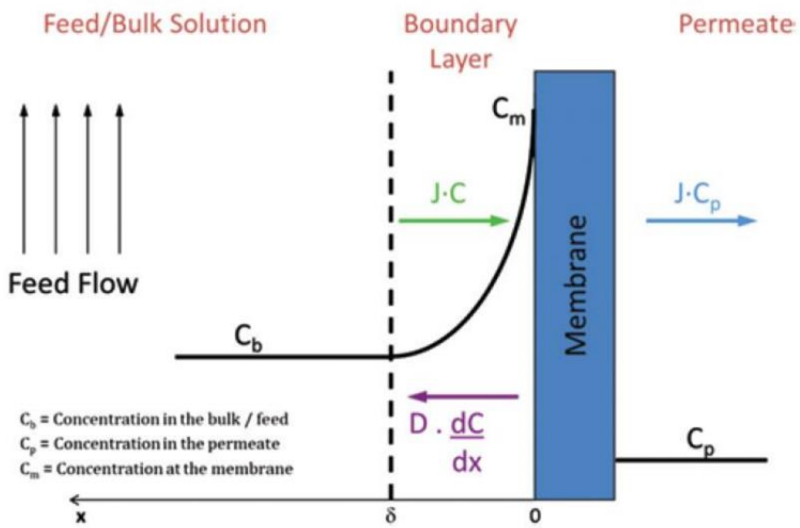

Figure 2, the effect of concentration polarization on the membrane surface.

The concentration polarization factor also can be calculated as a function of flux and mass transfer coefficient.

$$\beta = EXP\left(\frac{-Jw}{K}\right) \qquad (8)$$

where K is the mass transfer coefficient. The mass transfer coefficient depends on the physical characteristics of the system and the flow condition whether it is laminar or turbulent. Hence:

$$K = \left(\frac{Sh*D}{dh}\right) \qquad (9)$$

Where Sh is the Sherwood number depending on the type of flow and the cross-sectional area of the membrane, and d_h is the hydraulic diameter of the membrane.

The D parameter in the mass transfer equation known as the salt diffusion coefficient represents the membrane selectivity to salt transport. This value of the membrane can be determined experimentally by the manufacturer. The diffusion coefficient can be related to the membrane rejection rate:

$$D = \frac{(1-Rj)*Jw}{Rj} \qquad (10)$$

The value of D is not constant, but it is changing from one type of membrane to another. Therefore, this model estimates this value for simplicity to be (0.0014 m/d).

The rejection rate (R_j) is defined as the ratio of concentration difference between the feed concentration and permeate concentration to the feed concentration.

$$R_j = \frac{Cf-Cp}{Cf} = 1 - \frac{Cp}{Cf} \qquad (11)$$

The term C_p represents the permeate concentration which is the quality of the filtered water produced by the membrane. Therefore, the permeate has osmotic pressure and can be found by rewriting equation (1):

$$J_w = K_w * ((P_{os} - P_p) - (\beta\pi_m - \pi_p)) \qquad (12)$$

π_p is calculated by using equation (3) with the salinity of the permeate.

Therefore, the total production from the RO system can be calculated by rearranging the equation (2):

$$Q_p = A_m * K_w * ((P_{os} - P_p) - (\beta\pi_m - \pi_p)) \qquad (13)$$

The fouling effect can be applied to equation (13) because of the loss of permeability by the composition of fouling and scaling on the membrane surface and inside the pores of the membrane. Typically, the value is less than unity depending on the membrane lifetime. As a result of considering the fouling effect (FE):

$$Q_p = A_m * K_w * FE * ((P_{os} - P_p) - (\beta\pi_m - \pi_p)) \qquad (14)$$

The feed inlet pressure is calculated by applying equations [1-14]. As a sequence, the performance parameters for every membrane element can be determined using mass and salinity balance equations:

$$Q_f[n-1] = Q_p[n] - Q_c[n] \qquad (15)$$

$$(Q_f[n-1] * C_f[n-1]) = (Q_p[n] * C_p[n]) - (Q_c[n] * C_c[n]) \qquad (16)$$

Where $Q_f[n-1]$ is the feed exits from the previous element and entering the next element with concentration $C_f[n-1]$, and $Q_c[n]$ and $Q_p[n]$ are the brine exits and the permeate produced by each membrane element with salinities $C_c[n]$ and $C_p[n]$ respectively. The symbol (n) represents the number of elements inside the pressure vessel.

The feed pressure will be reduced as it is passing from one element to the other inside the pressure vessel. Thus, the drop in feed pressure should be taken into account in order to calculate the performance parameters of each element. The pressure drop is calculated by the following equation [15]:

$P_{dp} = 0.01 * n * (Q_{av})^{0.17}$ (17)

And $Q_{av} = \frac{Qf+Qc}{2}$ (18)

Using the above equations, the performance parameters for every membrane element can be calculated. It is necessary to mention that the performance of RO membranes is affected by the feed temperature. In case the temperature of the feed is changed, simulation results have to be adjusted by a factor known as the temperature correction factor (TCF). This is due to the variation in fluid and membrane polymer characteristics at different temperatures.

3. Results and Discussion:

Tables [1] show the specification of the membranes that are used to compare the results of the model. Some parameters in the design need to be assumed to make the comparison between the membranes in this study. The permeability (Kw), the diffusion coefficient (D), and the membrane surface area in the model calculations are assumed to be constant. These values are 0.9 L/m^2.h.bar, 0.0014 m/d, and 38 m^2 per membrane element respectively. Figure [3] shows the layout of the system which consists of one pass membrane system with seven elements in the pressure vessel.

Membrane Type	Symbol	Area (m2)	Comment
SW30XLE-440i	A	40.857	Applications less than 35 C
SW30XFR-400/34i	B	37.14	-
SW30HRLE-440i	C	40.857	Applications less than 35 C
SW30HR-380	D	35.286	-

Feed Water	Cf (mg/L)	Temperature ()	R %	Qf (m3/h)
NaCl	32,000	25	45	6
NaCl	40,000	25	45	6

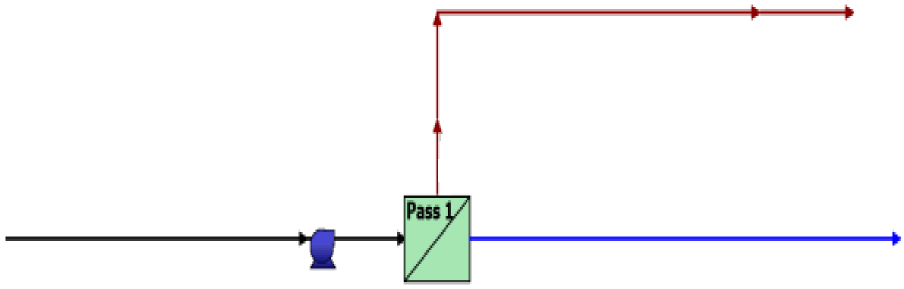

Table [2] shows the two different cases that were simulated in the study and the results were compared with those from WAFE software. The feed water temperature was assumed to be 25 °C. The rest of simulating experiment parameters are listed in Table [2].

From the results obtained by the simulation, it was found there was a good similarity between the membranes results and model results. Figure [4a, 4b] shows the variation of pressure drop across the membrane elements between the simulation and the types of membranes. The model results show approximately 97% agreement of the pressure drop of the model and the results obtained by WAVE at the two concentrations studied (32,000 mg/L and 40,000 mg/L). furthermore, figure [5a, 5b] shows the results of the recovery rates. It can be noticed that the model results show good agreement that can be 90% for the concentration of 32,000 mg/L and about 83% for the concentration of 40,000 mg/L. These percentages are the average between the simulation results and the results obtained by WAVE for the different membranes. Similarly, figure [6a, 6b] illustrates the results for the permeate flow rates from the elements in the pressure vessel. The model results show approximately 90% similarity for the concentration of 32,000 mg/L and about 86% for the concentration of 40,000 mg/L. Lastly, the permeate concentrations from each membrane element from this study were slightly higher than that from WAFE, especially from membranes B, C, and D as shown in figure [7a, 7b]. Overall, the permeate concentrations are approximately 86% similar for the concentration of 32,000 mg/L and 81% for the concentration of 40,000 mg/L.

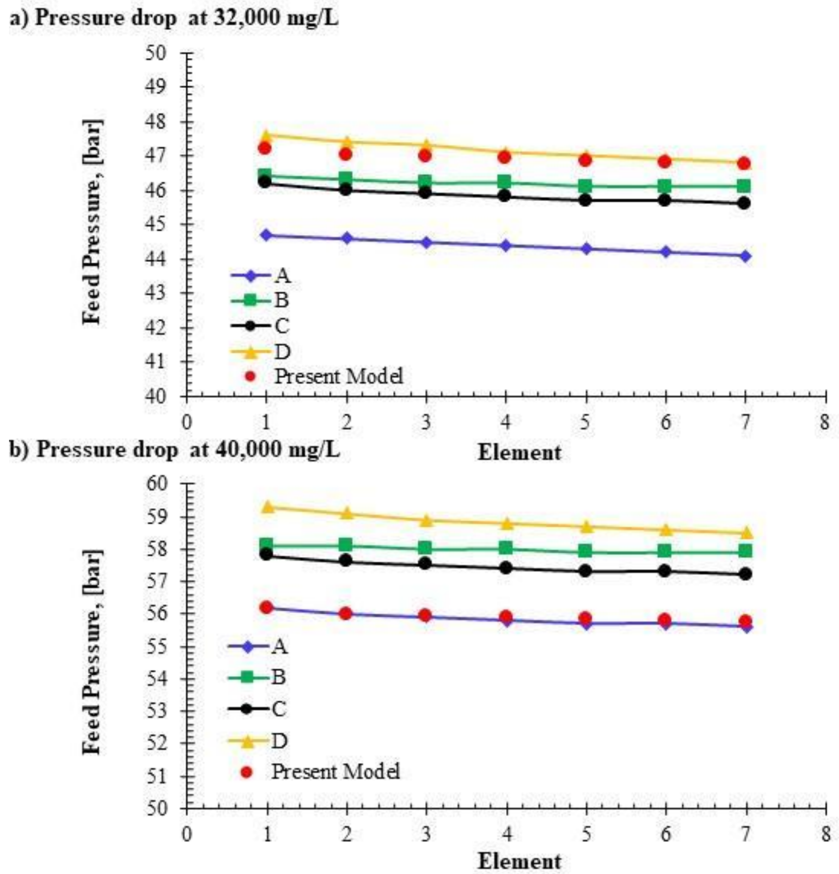

Figure 4, a) feed pressure at each membrane element at a concentration of 32,000 mg/L, b) feed pressure at each membrane element at a concentration of 40,000 mg/L.

The slight variation between the results doesn't mean that the values are less reliable, but a marginal error can be expected even between the software results and the real RO system performance.

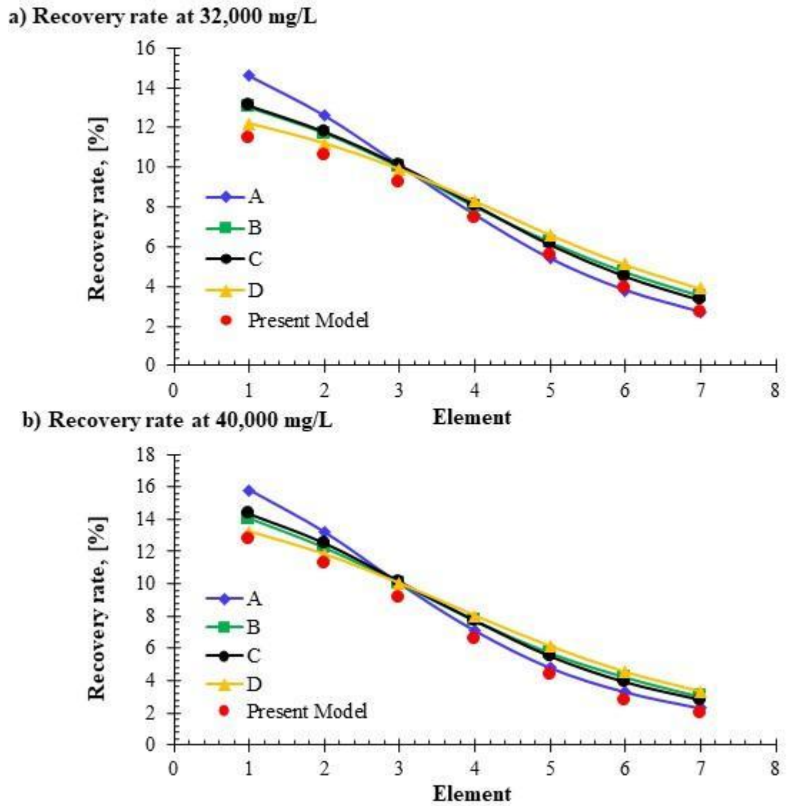

Figure 5, a) recovery rate at each membrane element at a concentration of 32,000 mg/L, b) Recovery rate at each membrane element at a concentration of 40,000 mg/L.

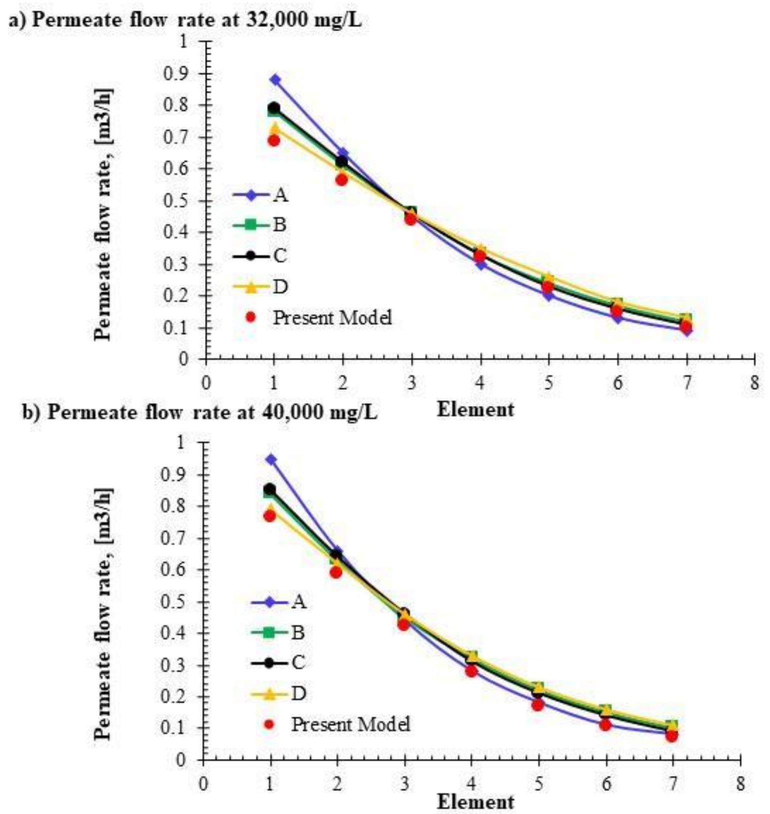

Figure 6, a) Permeate flow rate at each membrane element at a concentration of 32,000 mg/L, b) Permeate flow rate at each membrane element at a concentration of 40,000 mg/L.

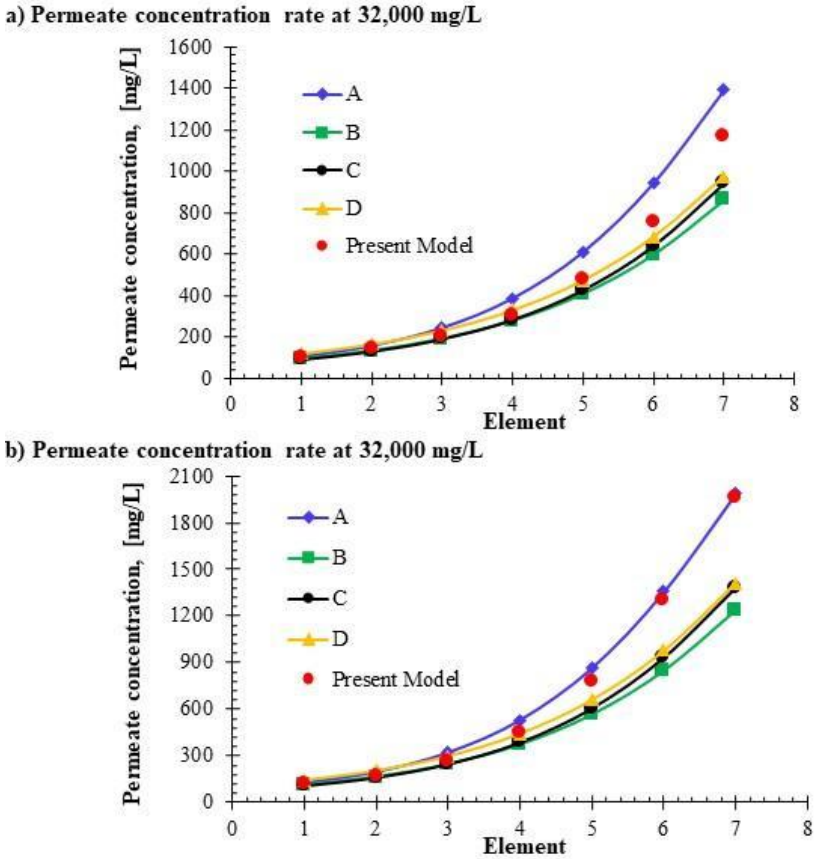

Figure 7, a) Permeate concentration at each membrane element at a concentration of 32,000 mg/L, b) Permeate concentration at each membrane element at a concentration of 40,000 mg/L.

5. Conclusion:

In this study, the performance of the RO system was calculated using a computational model that can predict the performance parameters of different membranes. These results from the model were compared with WAVE software and it was shown that they were in good agreement. The main parameters of the RO system such as the feed pressure, the concentration of permeate, the recovery rate and permeate flow rate for each element in the RO system were compared with the software results as shown in figures []. It found that only a small discrepancy was found between the model and WAFE. Hence, it can be indicated that the model is good accuracy in estimating the performance of the RO system for pretreated feed solution using different membranes by different manufacturers. As a result, the present model is open to prediction with any type of RO membrane regardless of the manufacturing company.

7. Nomenclature:

J_w	water flux L/ m^2. h
K_w	water permeability constant L/m^2.h.bar
A	Surface Area of the membrane element m^2
A_m	Surface Area of membranes in the pressure vessel m^2
β	Concentration Polarization Factor
ACF	average concentration factor
Q_p	permeate flow rate m^3/h
Q_f	Feed flow rate m^3/h
Q_c	concentrate flow rate m^3/h
R	Recover rate %
R_g	universal gas constant 0.081345 kg.m^2/h^2.K
C_m	concentration at the membrane surface mg/L
C_f	concentration of Feed flow mg/L
K	Mass transfer coefficient m/s
D	Salt diffusion coefficient m/d
R_j	Rejection factor %
P_{dp}	Pressure drop across the membrane element bar
FE	Fouling effect
n	Number of elements
π_m	Osmotic pressure on membrane surface bar
π_p	Permeate osmotic pressure bar

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