International Journal of Engineering and Modern Technology (IJEMT) E-ISSN 2504-8848
P-ISSN 2695-2149 Vol 10. No. 11 2024 www.iiardjournals.org Online Version

Modeling and Simulation of Reverse Osmosis Process for Boiler Feed Water Treatment

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DOI:10.56201/ijemt.v10.no11.2024.pg55.67

Abstract
The models for the description of the performance of the reverse osmosis process for the behaviour of the boiler feed water were presented. The models developed were to predict the feed solution concentration and transmembrane pressure during the treatment process as the separation would involve the diffusion of solvent from the solution with more solvent to the solution with low solvent. The diffusion takes place as the impurities in the boiler feed water are diffused through the membrane employed in reverse osmosis process for treatment of boiler feed water. The operational parameters were obtained from the plant and serve as input data for the computer program developed using MatLab software. The model results showed agreement with previous studies with minimum deviation. The simulations showed optimum separation when the transmembrane pressure was about 180Pa with the reverse osmosis process adjusted to real rejection fraction of 0.4%. Also, the impurities as at this transmembrane pressure of 180Pa had been diffused completely to clean and clear solution through the membrane. Hence, total flux been adjusted in the reverse osmosis process for boiler feed water treatment at optimum of 178Pa would be the transmembrane pressure. This means that total flux is a better sensitive parameter to be used in the purification of boiler feed water for the diffusion of impurities from the boiler feed water since the transmembrane pressure was lower when total flux was used as adjustable variable.

Key words*: Trans-membrane Pressure. Total Flux; Membrane; Diffusion; MatLab Software*

1. INTRODUCTION

Reverse osmosis treatment of boiler feed water has become a popular way to obtain fresh water for industrial use. When Loeb and Sourirajan discovered asymmetric cellulose-acetate membranes in 1962, reverse osmosis became a feasible procedure. Boiler feed water was treated by thermal operation comprising vaporizing and condensing procedure prior to the discovery of reverse osmosis. Nowadays, thermal processes only make up roughly 34% of industrial seawater desalination; at least 64% is accomplished using reverse osmosis (Henthorne, 2019). Other small-scale industrial methods for treating boiler feed water include membrane distillation, electrodialysis, and nanofiltration (Khawaji *et al.*, 2018). The thermal method's main disadvantage is that it consumes so much energy, which reduces the procedure's efficiency for commercialization of water desalting (Bagheri & Alizadeh, 2021).

Reverse osmosis is a technique for separating miscible solutions with varying concentrations using a membrane that allows the solvent to pass through but almost completely obstructs the solute (Kim *et al.*, 2020; Ligaraya *et al.*, 2020; Monjezi *et al.*, 2020). The technical definition of the procedure gives rise to the name reverse osmosis. It is the osmosis process's opposing action (Garcia-Perez *et al*., 2022). The solvent activity in the osmosis process is what propels the process forward. The direction of the solvent's diffusion is toward increased solvent activity (El-Nakla & Emam, 2022). In order to reach the zone with the higher concentration, which has a smaller solvent activity, there is diffusion of the solvent away from the zone with lower solution concentration, that has a greater solvent concentration. The osmotic pressure ($\Delta\pi$) is what drives the solvent flow from the region with smaller concentration to the region having more concentration. Solvent diffusion from the zone that is concentrated to the diluted region will occur with additional pressure increases in the concentrated solution (Asadi *et al.*, 2021; Cornelissen *et al.*, 2021). The solution's osmotic pressure, represented as ($\Delta\pi$), is the pressure needed in the area of concentration to establish zero solvent activity gradient if pure solvent is present on a membrane's side. A pressure greater than $\Delta\pi$ must be used in the dense zone so as to achieve the reverse osmosis process (Prabhakaran & Raman, 2022).

The majority of membranes employed in reverse osmosis are synthetic polymer flexible films that are made with increased permeability for only molecules of water (Choi *et al.*, 2021). Since reverse osmosis membranes are practically impermeable, they are able to filter out particles and even a large number of low molar mass species, including organics, salt ions, and other water contaminants (Ahmad *et al.*, 2007; Al-Bastaki & Abbas, 2019: Bashir *et al.*, 2020). The only molecule that can pass through the membrane is water. Chemically, they are usually composed of polysulfone or cellulose acetate wrapped with aromatic polyamides. These resources have reduced permeabilities for dissolved salts and high permeabilities for water, thus rendering them right to be applied in reverse osmosis membranes. Reverse osmosis membranes are employed as hollow fibers or maybe layers of films, which is dependent on how the desalination process is designed (Cai *et al.*, 2021; Fahmy & Ahmed, 2021). However, hollow fibers are used in industrial applications. According to reports, one stage reverse osmosis cannot effectively reject 100% of the solute (Rashid *et al.*, 2024). Only 97–99% solute rejection can be achieved in a single stage operation. In the industrial treatment of boiler feed water, multiple stage reverse osmosis systems are often utilized to attain a solute rejection rate of nearly 100%. (Cath *et al.*, 2006; Kim *et al.*, 2020).

A boiler system's operation and maintenance depend heavily on the boiler feed water being properly treated. Dissolved solids concentrate and create sediments inside the boiler as steam is produced. This results in inadequate heat transfer and lowers the boiler's efficiency. Boiler corrosion is caused by the reaction of dissolved gases, including carbon dioxide and oxygen, with the metals in the boiler system. These impurities should be managed or eliminated through internal or external treatment in order to safeguard the boiler. Thus, this study focused on the development of mathematical model for reverse osmosis process for the removal of highly toxic compounds from boiler feed water. This aim will be achieved by developing the reverse osmosis model equation from the conservation principle, application of the total flow of solvent and solute in the process for mass transfer equation, solving the developed model equations using MatLab Simulink software, comparison of model result with plant data and simulation of parameteric effects on the overall operational process efficiency

2.0 MATERIALS AND METHODS

2.1 Materials

The materials used in this study includes: MATLAB and Simulink compiler, Journals, Handbook and computer.

2.2 Method

Model equation describing the mass transfer in precise osmosis concentration process will be developed using the irreversible thermodynamic Spiegler Kedem Model. The model equation relating total flow J_V with osmotic pressure ($\Delta\pi$) and real recovery will be modeled.

2.2.1 Model Assumptions

The following assumptions are applied in modeling the reverse osmosis operational process.

i. One dimensional flow of solvent and solution transport across the membrane operation.
ii. There is complete development of the concentration polarization layer.
iii. The Spiegler-Kedem irreversible thermodynamic model is a suitably fit to describe the solute's efficiency during separation across membrane.

2.2.2 Development of Model Equation

The schematic diagram depicting the reverse osmosis process is shown in Figure 1

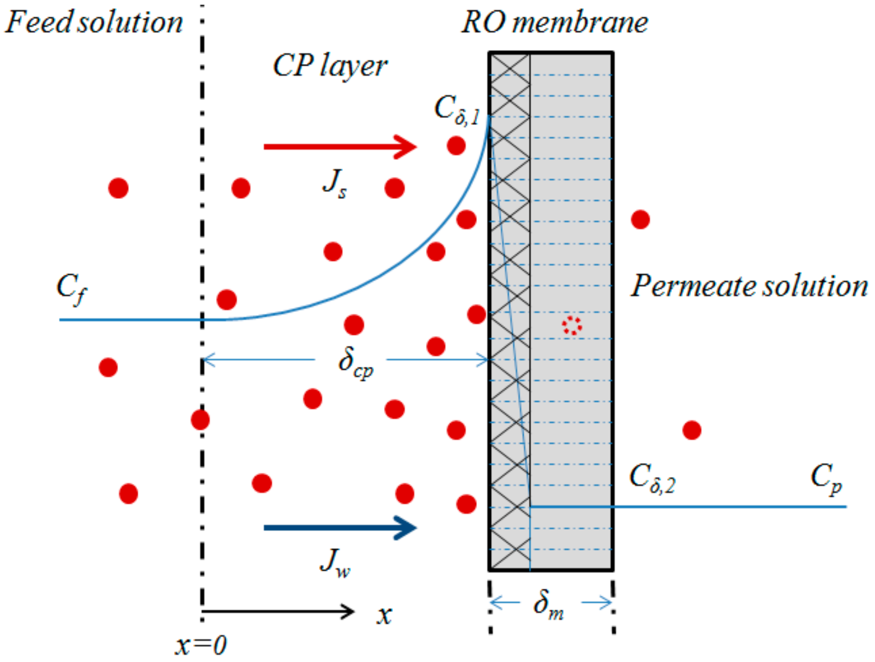

Figure 1: Mass Transfer in the Reverse Osmosis (RO) Membrane Separation Process

As shown in Figure 1 and based on the assumption above, the mass transfer equation is expressed as

$$J_w.C_p = J_w.C - D\ dc/dx \quad (1)$$

$$D\frac{dc}{dx} = J_w.C - J_w.C_p \quad (2)$$

Integrating Equation (2) and applying the boundary conditions gives

$$\frac{C_{\delta,1}-Cp}{C_f-C_p} = e^{\left(\frac{J_w}{K}\right)} \quad (3)$$

Where $K = \frac{D}{\delta C_p}$ (4)

Also, the solute flow J_s is expressed as

$$Js = B_s\left(C_{\delta,1} - C_{\delta,2}\right) = B_s\left(C_{\delta,1} - C_p\right) = J_wC_p \quad (5)$$

The volumetric flow on the permeate side of the reverse osmosis membrane, which might indicate the membrane's concentration capability, is represented by the total flow of the solvent and solute (J_v) in the reverse osmosis process.

$$J_v = J_w + J_s \approx J_w \quad (6)$$

From the principle of conservation of mass

$$Q_fC_f = Q_bC_b + Q_pC_p \quad (7)$$

$$Q_f = Q_b + Q_p \quad (8)$$

$$J_v = \frac{Q_p}{S} \quad (9)$$

The performance of the Reverse Osmosis can be expressed in terms of process recovery and rejection as expressed thus.

$$Recovery = Y = \frac{Q_p}{Q_f} \tag{10}$$

$$Rejection = R = 1 - \frac{C_p}{C_f} \tag{11}$$

The irreversible thermodynamic Spiegler-Kedem model is suitable for explaining the effectiveness of the separation of solute via membrane

$$J_v = L_p\,(\Delta p - \sigma\,\Delta\pi) \tag{12}$$

For Permeable membrane, $O < \sigma < 1$. Δπ is calculated using;

$$\Delta\pi = RT\,\left(C_{\delta,1} - C_{\delta,2}\right) = RT\,\left(C_{\delta,1} - C_p\right) \tag{13}$$

The observed membrane rejection fraction is given by

$$R_o = \frac{C_f - C_P}{C_f} \tag{14}$$

The real rejection fraction is given by

$$R_r = \frac{C_{\delta,1} - C_{\delta,2}}{C_{\delta,1}} = \frac{C_{\delta,1} - Cp}{C_{\delta,1}} \tag{15}$$

According to the Spiegler-Kedem Equation, the real rejection fraction R_V is expressed as

$$Rv = \frac{\sigma\,(1-F)}{1-\sigma F} \tag{16}$$

F is defined as

$$F = \exp\left[-J_v\frac{(1-\sigma)}{B_s}\right] \tag{17}$$

Substituting Equation (16) into Equation (17) and writing for J_v yields

$$Jv = \frac{B_s}{1-\sigma}\,ln\,\frac{\sigma\,(1-R_r)}{\sigma - R_r} \tag{18}$$

Further mathematical analysis of Equation (18) yields

$$In\,\left(\frac{1-R_o}{R_o}\right) = \frac{J_v}{K} + In\,\left(\frac{1-R_r}{R_r}\right) \tag{19}$$

Upon variable separation of Equation (19) gives

$$K = \frac{Jv}{In\frac{R_r(1-R_O)}{R_O(1-R_r)}} \tag{20}$$

Substituting Equations (3) and (13) into Equation (12) yields

$$J_v = L_p\,(\Delta p - \sigma\Delta\pi) = L_p\,\left[\Delta p - \sigma RT\,\left(C_f - C_p\right)\,e\,\left(\frac{J_v}{K}\right)\right] \tag{21}$$

Substituting Equation (20) into Equation (21) yields

$$J_v = L_p\,\left[\Delta p - \sigma RT\,\left(C_f - C_p\right)\,\frac{R_r\,(1-R_o)}{R_o\,(1-R_r)}\right] \tag{22}$$

Equation (22) is the model equation for the reverse osmosis process

2.2.3 Operating Parameters

The input parameters applied in this study are highlighted in Table 1

Table 1: Input Parameters

Input Parameters	Description	Value	Unit
R	Gas law constant	8.314	$Jmol^{-1}K^{-1}$
T	Temperature	306	K
σ	Reflection coefficient	111	
C_f	Feed solution concentration	70.17	$Mol.m^{-3}$

3.0 RESULTS AND DISCUSSION

The simulated results of the reverse osmosis model equation using MatLab software is presented in Table 2.

Table 2: Results of the Model of Reverse Osmosis Process

Real Rejection Fraction (%)	Permeate Solution Concentration (Mol/m^3)	Tans-membrane Pressure (atm)	Feed Solution Concentration (Mol/m^3)	Total Flux (m^3/m.s)
0.09	1	10100	59.33	24.54
0.1	2.	10120	62.23	24.59
0.2	2.87	10140	65.12	24.64
0.38	3.1	10160	67.19	24.69
0.4	3.76	10180	70.17	24.74
0.56	4	10200	70.2	24.78
0.6	4.12	10220	70.31	24.83
0.7	4.59	10240	70.42	24.88
0.8	4.98	10260	70.61	24.92
0.9	5.34	10280	70.74	24.96
0.99	5.86	10300	80	24.73

3.1 Validation of Model Results

The plant data applied in validating the result of the developed model equation was obtained from the works of Al-Obaidi *et al.* (2018).

Table 3: Model Validation

Parameters	Plant Data	Model Data	Deviation (%)
Real Rejection Fraction (%)	0.39	0.38	2.63
Total Flux (m^3/m.s)	2.78	2.47	11.15

Based on the percentage deviation deduced between the experimental and model results for real rejection fraction and total flux, it can be posited that the model is suitable to predict the total flux when transmembrane pressure, permeate solute concentration as well as real rejection fraction were varied for the reverse osmosis process for the boiler feed water treatment. Thus, parametric effects and sensitivity study of the reverse osmosis process can be studied.

3.2 Discussions

3.2.1 Effect Real Rejection Fraction Pressure on Total Flux

The variation or dependency of real rejection fraction against the total flux of the reverse osmosis membrane process was studied as depicted in Figure 2. It can be deduced from the Figure 2 that as real rejection fraction increases, there is corresponding increase in the total flux of the reverse osmosis process and to a maximum flux of about 24.95 m^3/m.s that depicts the total flux optimum point for reverse osmotic diffusion to take place for the separation of the solution from low concentration to the solution with high concentration.

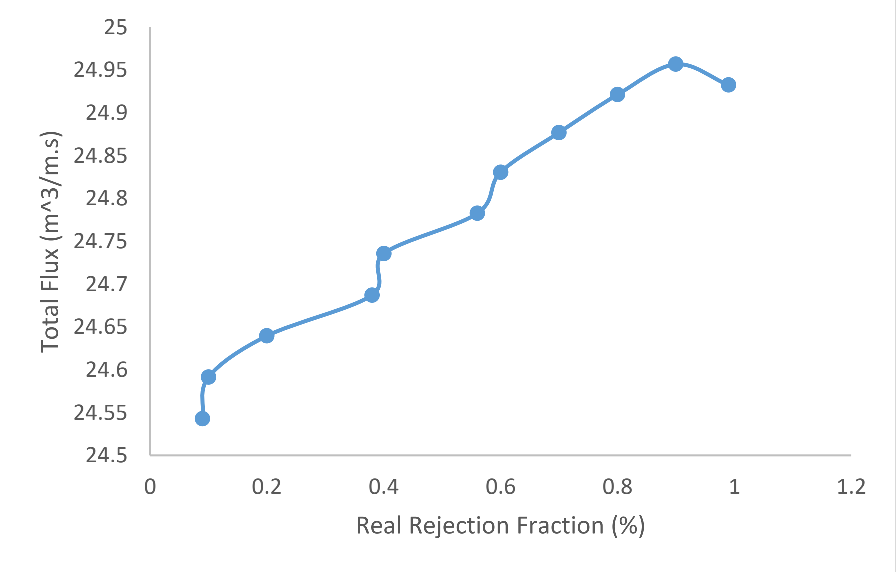

Figure 2: Effect of Real Rejection Fraction on Total Flux

However, the separation of the boiler feed water goes through osmotic diffusion were the solution with high solute diffused through the membrane to the solution with low solute. The total flux was about 24.95m^3/m.s at 0.9% real rejection fraction to achieve optimum separation of the boiler feed water. At this optimum total flux pressure, all the impurities would have been separated from the solution such that the water becomes clean and clear. This shows that after 24.95m^3/m.s, the water free from impurities may be contaminated with some impurities, thus the clean solution becomes diluted with impurities. Therefore, the separation process should be carried out at optimum total flux of 24.95m^3/m.s for appropriate separation process.

3.2.2 Effect of Permeate Solute Concentration on the Total Flux

The variations of permeate solute concentration against total flux is shown in Figure 3, as permeate solute concentration increases then the total flux increased but not in a direct or linear variation and later increased to a maximum of about 24.95m^3/m.s.

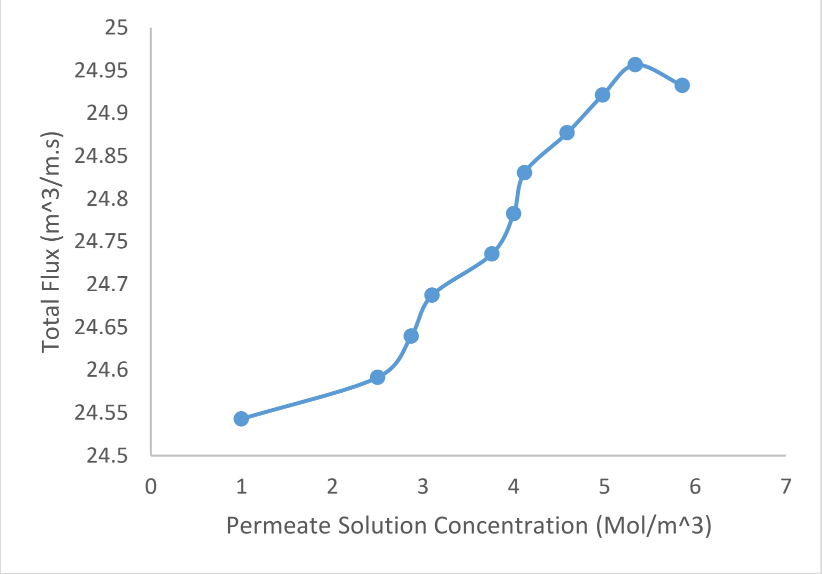

Figure 3: Effect of Total Flux on the Transmembrane Pressure

However, the total flux in the separation process ensure that the permeate solute concentration increased so that the solvent in the solution diffused through the membrane to region with less solvent and more concentrated solution. The impurities were separated at the membrane which the reverse osmotic pressure must be maintained at optimum total flux of 24.95m^3/m.s to ensure proper and good separation of the impurities in the boiler feed water.

3.2.3 Effect of Transmembrane Pressure on the Total Flux

Figure 4 shows that as transmembrane pressure increases, there is a corresponding linear increase or variation in the total flux of the reverse osmosis process to a maximum value of 24.95m^3/m.s before the total flux decline in value as highlighted.

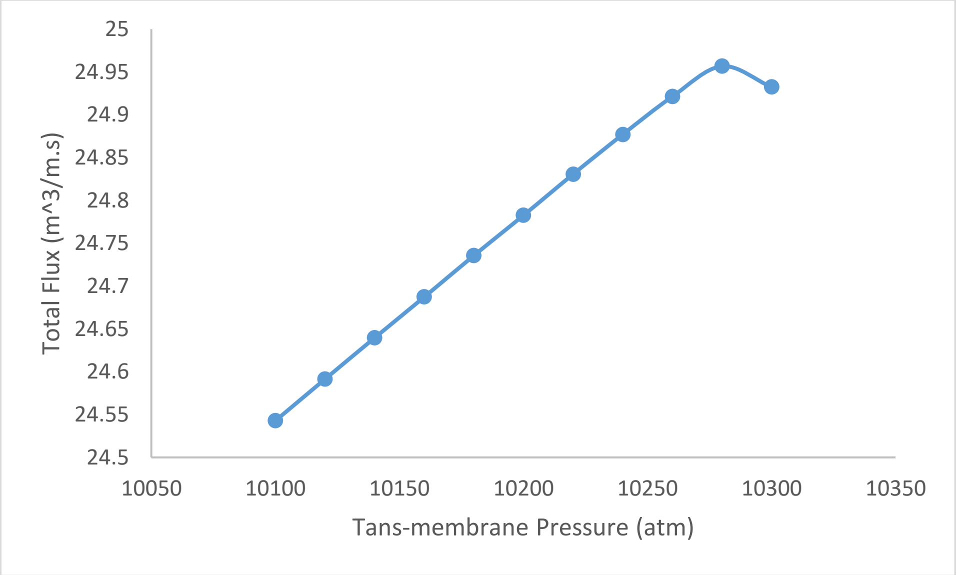

Figure 4: Effect of Transmembrane pressure on the Total Flux

Hence, with an increase in pressure of the transmembrane the total flux increased also. The reverse osmosis process used membrane to separate the boiler feed water from a solution where the solvent is more through the membrane. The solvent diffusion through the membrane separates the impurities through the membrane but when the total flux is used as a parameter for the change in the simulation of the separation process, then the fixed solution concentration could be very high to enable proper separation process. The impurities in the solution would be separated into more concentrated solution with the impurities separated at the membrane.

3.2.4 Effect of Total Flux on the Feed Solution Concentration

The variations of total flux against feed solution concentration is shown in Figure 5, as total flux increases then feed solution concentration increased as well. The graph shows that total flux is a parameter that controls the separation of the boiler feed water through the membrane. The increased in feed solution concentration shows that the membrane had separated the boiler feed water impurities to the maximum concentration.

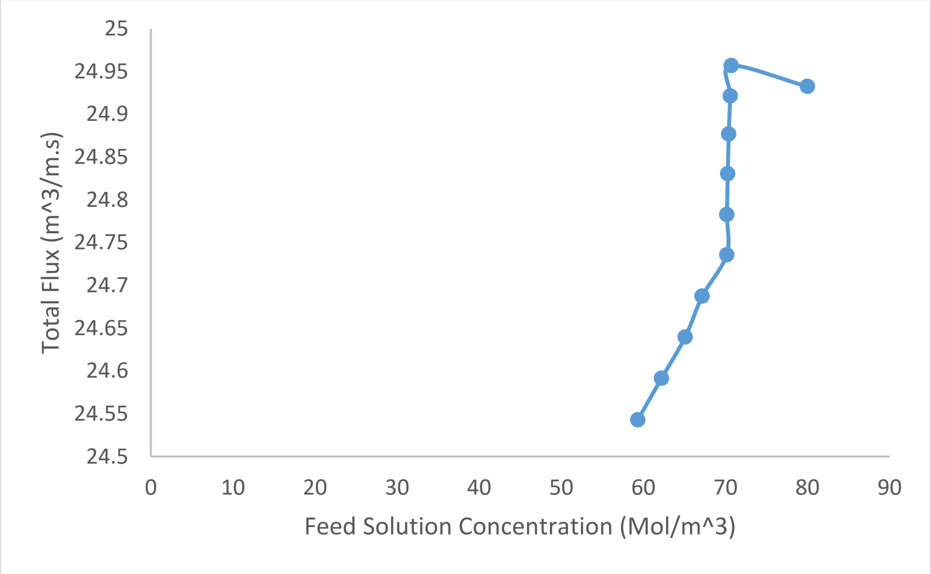

Figure 5: Effect of Feed Solution Concentration on the Total Flux

Also, the model when simulated showed that the reverse osmotic process was suitable for the separation of the boiler feed water. The treatment of the boiler feed water actually removed or separated the impurities from the solution of the boiler feed water. The boiler feed water became very suitable for industrial application, and the more the feed solution concentration then more of the boiler feed water impurities were separated since more of the solvent would diffused through the membrane to the diluted solution. This means that reverse osmosis process is a suitable method for the separation of boiler feed water.

4.0 Conclusion

Reverse osmosis was employed in the separating process to remove pollutants from the boiler feed water, which required treatment. Reverse osmosis is a membrane-based technique for removing contaminants from mixtures of varying concentrations. The membrane is permeable to the solvent but almost impenetrable to the solute. Also, the concentration solution's pressure needs to be increased to counteract the osmotic pressure in order to accomplish reverse osmosis. Osmotic diffusion slows down and eventually stops as the concentration solution's pressure rises and the activity gradient becomes zero. Solvent would diffuse from the concentrated to the diluted zone if the concentrated solution's pressure were to rise more.

Furthermore, the developed models predicted the feed solution concentration and transmembrane pressure during the treatment process as the separation would involve the diffusion of solvent from the solution with more solvent to the solution with low solvent. The diffusion takes place as the impurities in the boiler feed water are diffused through the membrane used in reverse osmosis process for treatment of boiler feed water. The operational parameters were obtained from the plant and serve as input data for the MatLab software. The MatLab software was used for the computation and simulation of the sensitive parameters of the boiler feed water treatment process, which showed a minimum deviation between the plant and model results. The simulations showed optimum separation with the total flux of 24.95m^3/m.s when the reverse osmosis process real rejection fraction was about 0.9%. Also, impurities had been diffused completely at this total flux to yield a clean solution. This means that total flux is a better sensitive parameter to be used in the treatment of boiler feed water for the diffusion of impurities from the boiler feed water.

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Nomenclature

J_w = Solvent (Water) Flow
C_p = Permanent Solution Concentration
C = Solute Concentration in the CP Layer
D = Diffusion Coefficient
x ranges from 0 to δC_p and C ranges from C_f to $C_{\delta,1}$
$C_{\delta,1}$ = Solute Concentration at Membrane Surface (Feed side)
C_f = Feed Solution Concentration
δC_p= CP Layer Thickness
K = Mass Transfer Coefficient in the CP Layer
B_s= Solute Transport Coefficient
Q_f = Feed Solution Flow
Q_b = Retentate Flow
Q_p = Permeate Flow
C_b = Retentate Solution Concentration
S = Effective RO Membrane Area
L_p = Hydraulic Permeability Constant
Δp = Trans-Membrane Pressure
$\Delta \pi$ = Difference in Osmosis Pressure across the Membrane
R = Gas Law Constant
T = Temperature
$C_{\delta,2}$ = Solute Concentration at Membrane Surface (Permeate Side).
R_r = Real Rejection Fraction
R_o = Observed Rejection Fraction
C_f = Feed Solution Concentration
C_p = Permeate Solution Concentration
σ = Reflection Coefficient which represents the Solute Separation Capacity of a Membrane
$\sigma = 0$ means No Separation
$\sigma = 1$ means Complete Separation