REPORT

ON

Mathematical modelling and Simulation of Sea Water Reverse Osmosis

BY

BHUVAN SHARMA   2019B1A10975P

Prepared in partial fulfilment of the course

Design Project

(CHE F376)

AT

BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCES, PILANI

MAY, 2023

Acknowledgement

ABSTRACT

In this study we have derived a model to analyse the performance of the membrane in two cases, one is co-current flow pattern and other is the counter flow pattern of the feed water. During this analysis we have tried to relax some assumptions on which this model was previously based on. We have tried to incorporate the effects of the chemical potential due to pressure difference across the membrane and the activity effects of the solute on the diffusion through the membrane. In this model we can see that the predicted value for the flow rate and the average permeate concentration is in good agreement with the already available literature data and concluded that counter current flow pattern is more favoured at industrial level, if we want higher efficiency of the Sea water reverse osmosis plant.

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Introduction

Reverse osmosis membranes are constructed from a membrane flat sheet. It comprises of 3 layers which are polyester Support base, microporous polysulfone layer, and 0.2-micron thick polyamide barrier layer. The very thin barrier layer that cleans the water of nutrients, pollutants, germs, and viruses is strengthened by the polysulfone layer. In order to create turbulence and provide room between the membrane sheets for the feed water, the membrane flat sheet is paired with a sheet of feed channels gaps. In order to allow the final recycling water product or permeate to flow uniformly across the entire membrane surface even under high pressure, a sheet of permeate spacer is added to the membrane sheets and feed channel spacer. The margins of the permeate spacer and the back of the membrane are entirely sealed. The membrane sheets are glued along each of the three exposed sides, and rolled around the core tube. Feed water is forced through the feed channel spacer and into the barrier layer of the membrane. The permeate channel receives water that permeates through the membrane surface. This water is the last recycled product or permeate and runs in a spiralling direction before collecting in a core tube. A pressure vessel with numerous spiral wrapped elements inserted into it can then be sealed off and feed water can be added when the end adapter is linked to the final element. High pressure feed water is pumped into the vessel; when it moves through the membrane, smaller molecules like water pass through but bigger particles like salt, bacteria, and viruses do not. The final recycled water product is collected from the end of the elements, the concentrate or the reject from that vessel flows to another stage, producing more recycled water.

Three papers were taken into consideration, including one titled "Mathematical modelling of reverse osmosis process by the orthogonal collocation on finite element method by Asian journals of applied Sciences," which used the solution diffusion mass transfer model to conduct an extensive study to predict the performance of a hollow fibre reverse osmosis. Two different scenarios—the co-current flow and the counter-current flow—were used to compare the membrane's performance. The overall recovery and purity rate were the variables used to compare the two different flow patterns. In order to construct a more tangible and realistic model to forecast the performance of the membrane, we sought to loosen some of the assumptions that were made in the original study. The paper's conclusion said that counter current is employed in series for industrial applications and is used to produce higher purity.

Mathematical Model

The assumptions used to build the model were

1. Solute and solvent were assumed to dissolve at the membrane and diffuse across it.
2. Chemical potential difference arising due to the pressure difference is assumed to be negligible.
3. The gradient for the flux is purely due to the concentration and pressure difference across the membrane.
4. The solute-solvent diffusion is assumed uncoupled.

The objective of this study is to analyse the influence of feed flow and permeate flow on the effectiveness of the membrane on the reverse osmosis systems.

Here water acts as the solvent and J_w is the corresponding mas flux. Since the flux is proportional to the Pressure gradient which is a macroscopic property of the solvent, the proportionality constant is Aw which is the water permeability constant.

$$J_w = A_w \left(\Delta P - \Delta \pi \right)$$

Where is the osmotic pressure difference across the membrane and is the Pressure difference across the membrane. can be written as the difference of individual osmotic pressures of two sides across of the membrane.

$$\cdot \Delta \pi = \pi_F - \pi_P$$

Where πF is the feed side osmotic pressure and πP is the permeate side pressure. Here we have assumed that the solute concentration is very less, which will give a linear function for π.

$$\Pi \, \alpha \, C$$

$$\Pi = KC \text{ (K is a constant)}$$

$$\Delta C = C_F - C_P$$

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Virial Equation

In statistical mechanics and thermodynamics, virial equations are a vital tool for explaining the behaviour of intricate systems of interacting particles. These equations offer a potent method for describing a system's intermolecular interactions in terms of its thermodynamic properties. When characterising the behaviour of gases at low densities, when the ideal gas law fails and intermolecular interactions are weak, the virial equation of state is particularly helpful. The virial equation offers a more precise description of the thermodynamic characteristics of gases, such as their pressure, volume, and temperature over a wide variety of conditions, by include higher-order factors in the intermolecular potential energy. A vital tool for researchers in these domains, the virial equation also has various applications in astrophysics, engineering, and materials science. The virial equation of state, its origin, and its applications in numerous academic domains will all be described in this introduction.

$$\Pi = a + bC + cC^2$$

$$\Pi_1 = a_1 + b_1C + c_1C^2$$

$$\Pi_2 = a_2 + b_2C + c_2C^2$$

$$\Pi_1 - \Pi_2 = (a_1 - a_2) + (b_1C_F - b_2C_F) + (c_1C_F^2 - c_2C_P^2)$$

Similarly, we can evaluate P and plug these variables in the above equation

$$J_w = A_w (\Delta P - \Delta \pi)$$

$$Q_w = J_w (S_a) / \rho_w$$

Pitzer-Debye Huckel Electrolyte Solution Theory

The Pitzer-Debye Huckel theory is a theoretical framework for describing the behaviour of electrolyte solutions. Charged ions, which make up electrolyte solutions, interact with one another and the solvent in their immediate environment. These interactions are intricate and strongly reliant on a variety of variables, including as the kind of ions in solution, the concentration of the electrolyte, and the system temperature.

The activity coefficients of electrolytes in solution can be computed using the Pitzer-Debye Huckel theory. For solutions of non-electrolytes, Raoult's law describes the ideal behaviour, whereas activity coefficients characterise the deviations from this behaviour. According to the Pitzer-Debye Huckel theory, an electrolyte's activity coefficient is expressed as a function of ion-solvent interactions, ion-ion interactions, and the effects of temperature and ionic strength on these interactions.

Two major presumptions form the foundation of the Pitzer-Debye Huckel theory . The first is that the activity coefficients of electrolyte solutions are mostly influenced by the e0lectrostatic interactions between ions in solution. Second, it posits that the ionic strength of the electrolyte solution may be used to represent the activity coefficients of electrolyte solutions as a power series expansion.

The comprehensive testing and validation of the Pitzer-Debye Huckel theory against experimental data makes it a trustworthy tool for researchers in a variety of domains. It is used in chemistry to simulate how electrolyte solutions behave in a variety of industrial processes, including electroplating and battery production. It is used in geochemistry to simulate how ions behave in natural streams and soils. It is employed in environmental science to simulate how contaminants behave in aqueous solutions.

The Pitzer-Debye Huckel theory has recently been expanded to take into account more intricate ion-ion and ion-solvent interactions as well as the results of ion electrostatic correlations. These advancements have increased the number of systems that the theory can accurately describe, increasing its usefulness as a research tool across numerous domains.

$$\Phi - 1 = f^{\Phi} + B_{MX}^{\Phi}m + C_{MX}^{\Phi}m^2$$

Here Φ is defined as Osmotic coefficient and f is defined as the Pitzer-Debye-Huckel electrolyte effect function. takes into account the interactions between ions in concentrated solutions, allowing for more accurate predictions of the activity coefficients.

$$f^{\Phi} = -A^{\Phi}\left(\frac{\sqrt{I}}{1 + b\sqrt{I}}\right)$$

A is defined as the Debye-Huckel slope which is evaluated graphically foe each electrolyte solution, and I is the ionic strength of the solution.

$$I = \frac{1}{2}(z_m{}^2m + z_x{}^2m)$$

B $^{\Phi}_{MX}$, C $^{\Phi}_{MX}$ are the second and third virial coefficients in the equation and m is the molality of the solution.

Osmotic coefficient can be related to the osmolality π in the following relation where v is the number of ions the compound will dissociate and m is the molality.

$$\Phi = \frac{\pi}{vm}$$

After substituting the osmotic coefficient in the virial equation, we will get the following equation which is expressing the osmolality in the virial form.

$$\pi = 2(f^{\Phi} + 1)m + 2B_{MX}^{\Phi}m^2 + 2C_{MX}^{\Phi}m^3$$

The second virial coefficient can be expanded in the following form where α is an empirical parameter and $\beta_{MX}{}^{(0)}$, $\beta_{MX}{}^{(1)}$ are constants dependent on the electrolyte solution.

$$B_{MX}^{\Phi} = \beta_{MX}{}^{(0)} + \beta_{MX}{}^{(1)}e^{-\alpha\sqrt{I}}$$

$$C_{MX}^{\Phi} = 0.00127$$

Molality is related to the Molar concentration as follows where D is the density od the solution at 25°C and M is the molar mass of the compound.

$$m = \frac{M}{(1000 \cdot D - 58.44 \cdot M)} \cdot 1000$$

After substituting the values of the molality and the osmotic coefficient in the first virial equation, we get the final equation as follows.

$$\left(\left(\left(2 - \frac{(0.782 \cdot \sqrt{m})}{1 + 1.2 \cdot \sqrt{m}}\right) \cdot m\right) + \left(0.153 + 0.5328 \cdot e^{(-2 \cdot \sqrt{m})}\right) \cdot m^2 + 0.00254 \cdot m^3 - \left(2 \cdot k - 0.0962k^2 + 0.00254k^3\right)\right) \cdot 19.3 \cdot 1000 \cdot \frac{133.322}{10^5}$$

This equation represents the osmotic pressure in mmHg units, here m is the feed side concentration and k are the permeate side concentration.

Result and Discussion
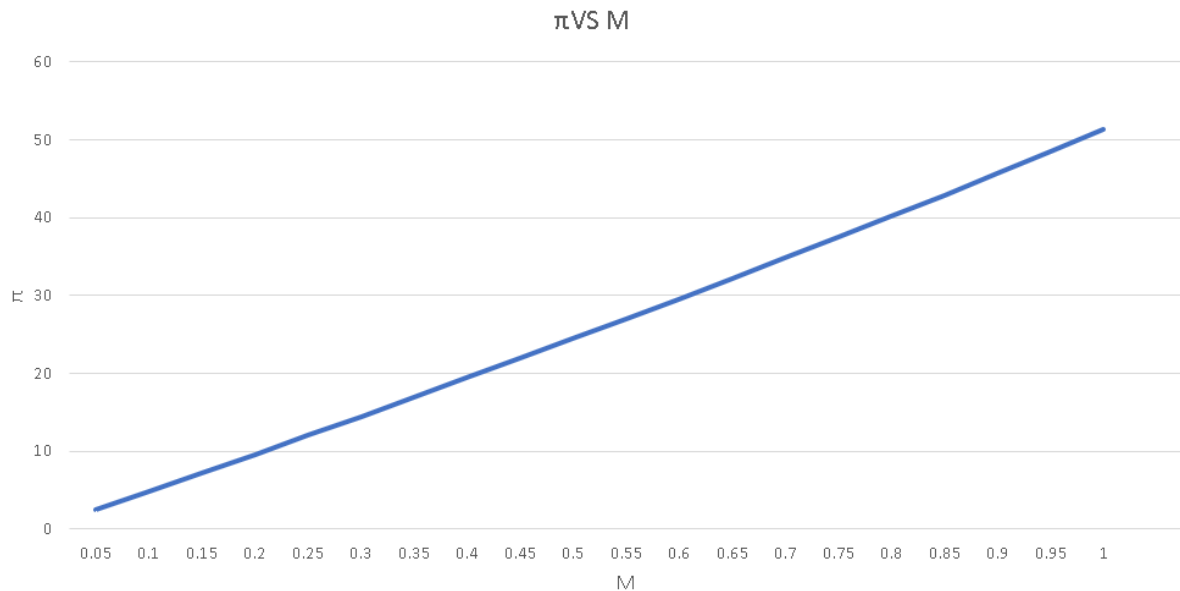
This is a trend obtained between osmotic pressure (π) and solute concentration of the feed. The trend is a non-linear curve, the value of the permeate solute concentration is kept constant, although it will increase with time as the membrane will lose its efficiency.
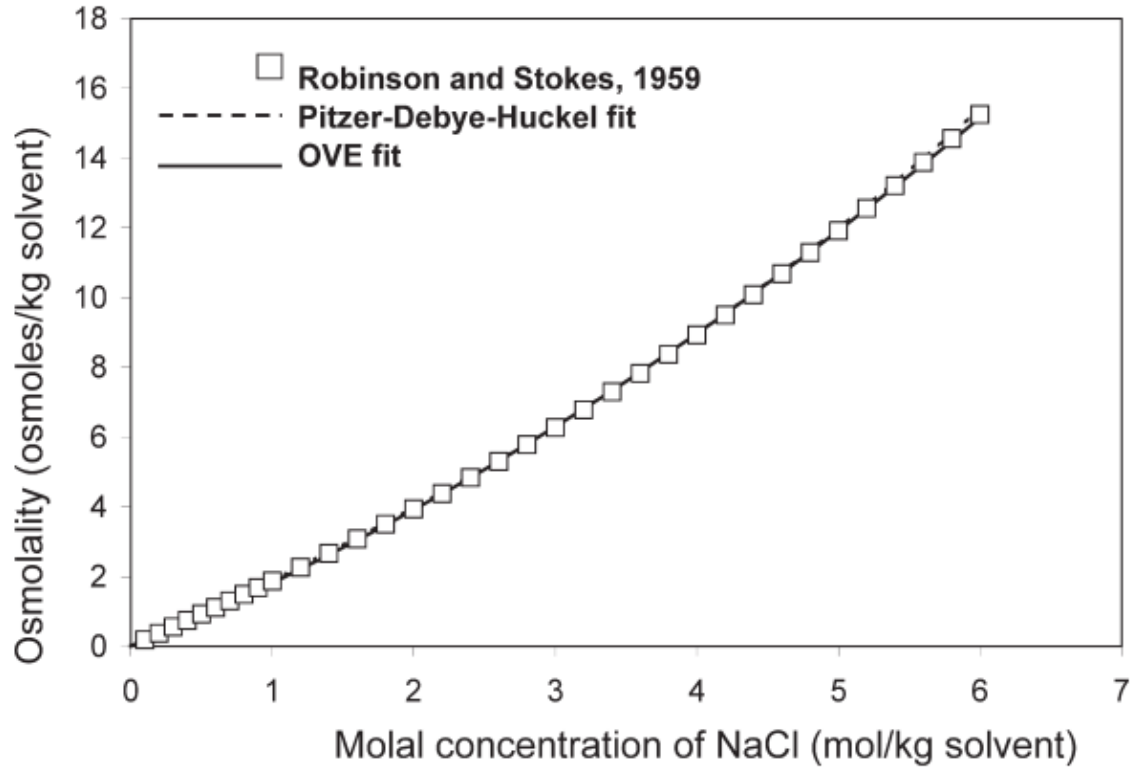
We were able to somewhat replicate the graph which was proposed by Debeye Huckel through his experiments.

Membrane Rejection

The membrane rejection represents the fraction of a specific component that is retained or rejected by the membrane. A high rejection value indicates that the membrane effectively prevents the passage of the targeted component, while a low rejection value suggests that the membrane allows significant passage of that component.

$$\frac{1}{T_R} = 1 + \frac{B_s \rho_w}{A_w} \left(\frac{1}{\Delta P - \Delta \pi} \right)$$

We have considered that we are using a high-pressure RO system where $\Delta P = 100$ atm, or above. Bs is a function of pressure difference and solute concentration.
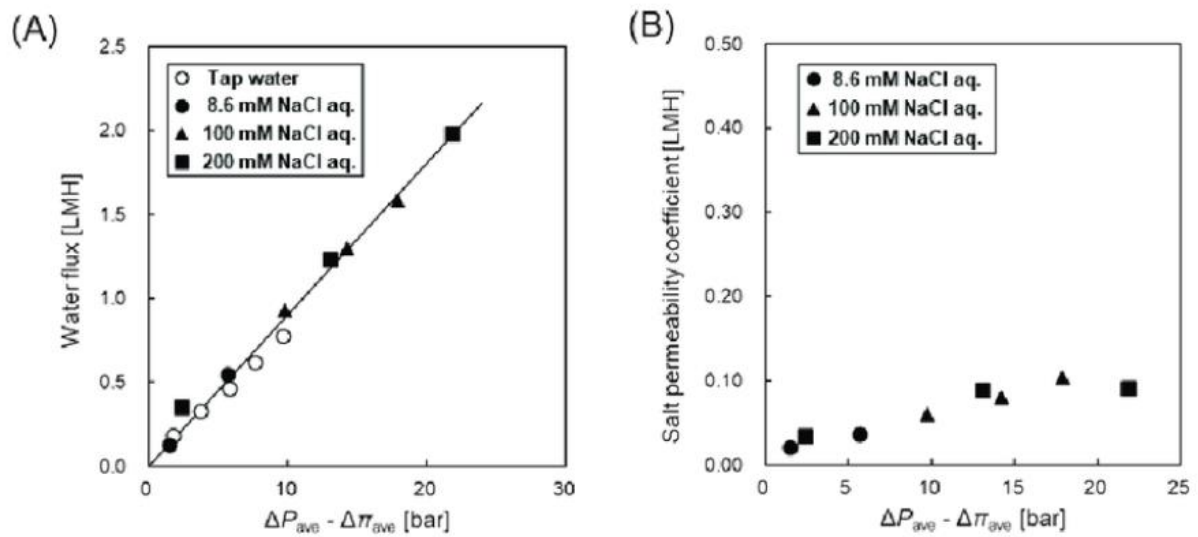
(A) Water flux and (B) salt permeability coefficient as a function of ΔP ave-$\Delta\pi$ ave with different salt concentration condition.

Taking Bs as 0.1 for 0.1 M concentration of NaCl and the water permeability A as follows.
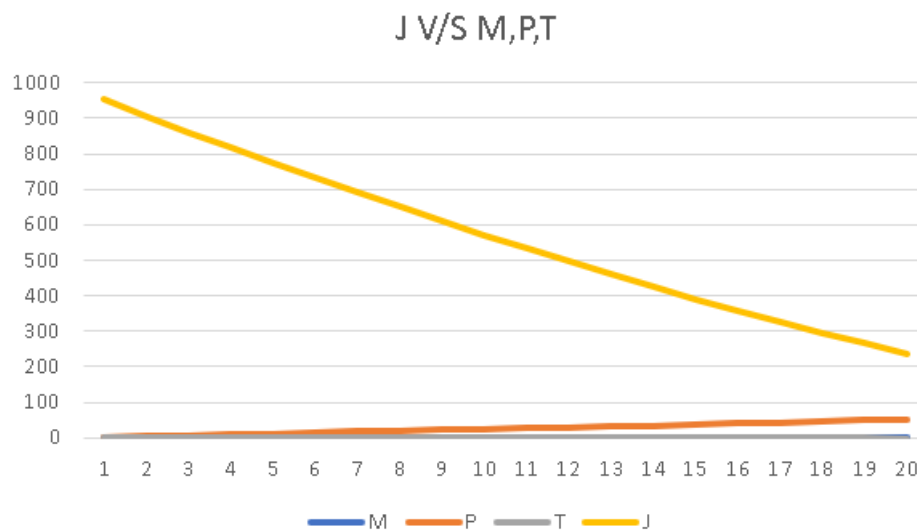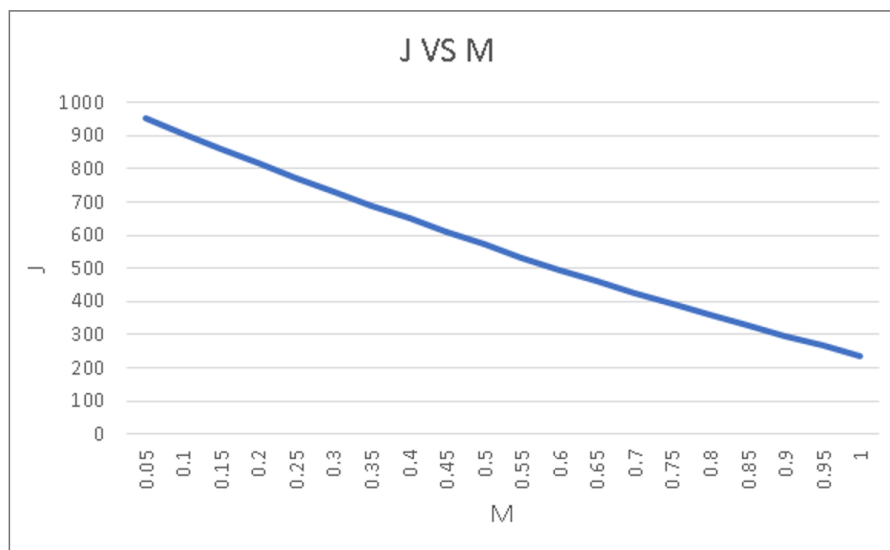
$$A = \frac{(100 - \pi)}{10}$$
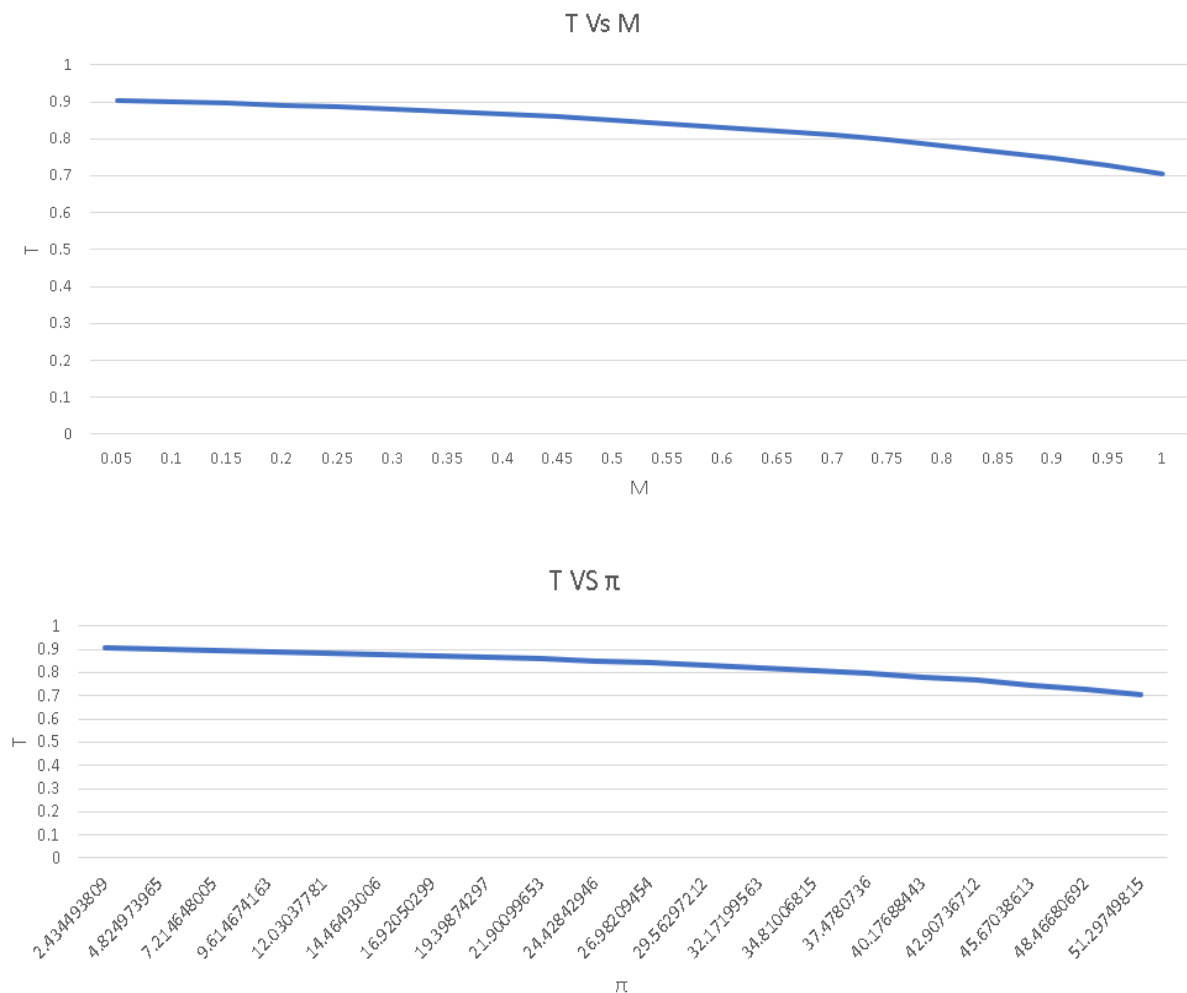
Here we can observe that Membrane rejection decreases as the feed side concentration increases, this may happen due to concertation polarization at the membrane surface. It is the accumulation of solutes near the membrane surface, resulting in a concentration gradient that negatively affects the performance and efficiency of the separation process.

Flux

$$J_w = A_w \left(\Delta P - \Delta \pi \right)$$

Water flux decreases as the feed side concentration increases, this may happen due to concertation polarization at the membrane surface or fouling phenomena such as adsorption, pore-blocking and deposition of solidified solutes, but in our case, this decrease in flux is mostly due to concentration polarization as the concentration gradient form near the membrane surface.

Conclusion

By introducing Virial equations accuracy in predicting flux and rejection ratio is increased. Electrolytic interactions of the solutes in the solution are incorporated using virial equations in the calculation of Osmotic pressure. Assumption of keeping the activity coefficient constant is relaxed.

By introducing the virial equations in the analysis, we have also taken into consideration the electrolytic effect of the charged particles in the solution. The effect of the nearby charged particle in the osmotic pressure and the flux is taken care of by using the virial equations.