Article

Comprehensive Mathematical Modeling of Membrane Fouling Kinetics and Energy Consumption in Full-Scale Reverse Osmosis Processes

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Abstract: Membrane fouling is one of the primary obstacles to the energy efficacy and sustainability of reverse osmosis (RO) processes. The objective of this research is to develop a dynamic mathematical model that is integrated and predicts the impact of pollution accumulation on the performance of full-scale membranes. The Carman-Kozeny equation and cake layer growth kinetics based on Hermia's laws were combined with the fundamental transport models developed by Hoek et al. to describe hydraulic resistivity. Fouling-enhanced concentrating polarization was also represented using the advanced film theory developed by Sutzkover et al. The model predicts a significant correlation between fouling-induced resist growth (R_f) and flux decline. A steady increase in specific energy consumption (SEC) is a result of the necessary high operating pressure. This model provides a precise predictive tool that promotes the sustainability of desalination plants by optimizing chemical cleaning (CIP) schedules and reducing operating costs.

Keywords: Reverse Osmosis; Membrane Fouling; Mathematical Modeling; Concentration Polarization; Specific Energy Consumption; Fouling Kinetics

1. Introduction

A finite and distressing resource, clean water is only a small portion (approximately 2.5%) of the total water on Earth that is suitable for direct human use and ingestion [1,2]. Presently, the economic constraints that arise from a substantial imbalance between the supply and demand for water resources are having a detrimental impact on approximately 25% of the global population [3].

According to statistical projections [4], water stress may impact nearly half of the global population by 2030.

This is exacerbated by numerous factors such as the present industrialization, population growth, water pollution and climate change [5,6,7].

To meet this challenge, desalination has become an important alternative to produce purified water [9,10]. Thermal technologies such as multi-stage flash distillation (MSF) and multi-effect distillation (MED) have been used in the past. However, they are energy consuming and capital and operating costs are high [11,12,13[. Considering the great progress in the membrane science [14,15,16] the most optimistic feasible alternative is membrane based processes. Their features include small size, simplicity of operation and high energy efficiency. At present, reverse osmosis (RO) accounts for about 50% of the world's desalinated water [17].

Feed water characteristics, operational parameters and type of membrane used are some of the factors that affect the performance of a RO system [17]. However, the most important technological problem is contamination of the membrane, which results in an increase in the local osmotic pressure and hydraulic resistance due to concentration polarization.

2. Materials and Methods

3. Although there are many studies of contamination in the laboratory, the simulation of contamination in full-scale industrial systems is still a major challenge because of the variation of the water properties and flow distribution between the system inlet and egress. The reduction in the permeability of the membrane and the increase in the hydraulic resistance and osmotic resistance of the membrane affect the quality of the produced water and the salt removal effect.Hence, these factors should be considered to make accurate modeling[[18].

4. To develop effective corrosion control methodologies, it is crucial to understand the fundamentals, theory and modeling of desalination [17].

Dynamic modeling is a basic method for comprehending the complicated interactions between the flow of fluids, the transport of solutes and the accumulation of contaminants over time. Simulations based on Navier-Stokes and Advection-Diffusion equations can be used to visualize the contaminant layer and its direct effect on energy consumption, unlike static models.

5. Results and Discussion

Mathematical modelling of fouling phenomena in membranes

The theoretical foundation of this investigation is the development of a complete mathematical model which is able to describe the evolution of the stable state to the degradation state due to pollution. The osmotic pressure is determined from the Van't Hoff equation, $\pi = \phi \; i \; C \; R \; T$ (ϕ is the osmotic coefficient).

Other factors such as the current industrialization, population growth, water pollution and climate change further exacerbate the problem [5,6,7].

The strategic solution to overcome this problem and obtain purified water is desalination [9,10]. In the past, thermal technologies, like multi-stage flash distillation (MSF) and multi-effect distillation (MED) have been applied. They are however energy consuming and capital and operating costs are high [11,12,13[. With the tremendous advances in membrane science [14,15,16] membrane based processes are the most promising alternative that is feasible. The processes are small size, simple operation and high energy efficiency. Nowadays, about half of the desalinated water is generated by reverse osmosis (RO) [17].

The performance of a RO system is influenced by a number of factors such as feed water characteristics, operational parameters and type of membrane used [17]. The most critical technological issue is however the contamination of the membrane, which leads to an increase in the local osmotic pressure and an increase in the hydraulic resistance caused by concentration polarization.

Although there have been many laboratory studies, the simulation of contamination in full-scale industrial systems is still a challenge due to the different water properties and flow distribution from the system inlet to the egress. The decrease in the permeability of the membrane and the increase in hydraulic and osmotic resistance along the membrane directly affects the quality of the produced water and salt removal efficiency.Therefore, these factors should be taken into account to perform an accurate modelling[[18].

To design effective corrosion control methodologies, it is necessary to have a detailed understanding of the fundamentals, theory and modeling of desalination [17].

Dynamic modeling is a simple tool to understand the complex relationships of fluid flow, solute transport and contaminant buildup over time. The simulations based on Navier-Stokes and Advection-Diffusion equations can be used to visualize the contaminant layer and its direct effect on the energy use, unlike static models.

Modelling of membrane fouling phenomena

The theoretical foundation of this investigation is the development of a complete mathematical model which is able to describe the evolution of the stable state to the degradation state due to pollution. The osmotic pressure is determined from the Van't Hoff equation, π = ϕ i C R T (ϕ is the osmotic coefficient).

This is because of several factors such as the current industrialization, population growth, water pollution and climate change [5,6,7].

To meet this challenge, desalination has become a strategic alternative to produce purified water [9,10]. Thermal technologies such as multi-stage flash distillation (MSF) and multi-effect distillation (MED) have been used in the past. On the other hand, they require a lot of energy and have high capital and operational costs [11,12,13[. Given the great progress in membrane science [14,15,16] the most promising potential alternative is membrane based processes. These processes are characterized by their small size, ease of operation and energy efficiency. Currently, approximately half of the desalinated water produced is by reverse osmosis (RO) [17].

The effectiveness of a RO system is dependent on the characteristics of the feedwater, operating conditions and type of membrane used [17]. The major technological issue, however, is contamination of the membrane, which leads to an increase in the local osmotic pressure and an increase in the hydraulic resistance caused by concentration polarization.

While there are numerous laboratory studies of contamination, it is difficult to simulate contamination in full-scale industrial systems because the properties of the water and the distribution of the flow varies from the system inlet to the egress. The decrease in permeability of the membrane and the increase in the hydraulic and osmotic resistance of the membrane has an impact on the quality of the produced water and the effectiveness of salt removal.Hence, these factors should be considered to do the accurate modelling[[18].

To develop effective corrosion control methodologies, it is necessary to have a good understanding of the fundamentals, theory and modelling of desalination[17].

Dynamic modelling is a valuable tool to understand the complex interactions between fluid flow, solute transport and contaminant accumulation over time. But, simulations based on the Navier-Stokes and Advection-Diffusion equations can be helpful to visualize the spreading of the contaminant layer and its direct impact on energy use[19].

Mathematical Modeling Framework for Membrane Fouling Dynamics

The theoretical background of the present investigation is the construction of a full mathematical model which describes well the evolution from the stable state to the degradation state due to the pollution. The osmotic pressure is determined from the Van't Hoff equation, π = ϕ i C R T (ϕ is the osmotic coefficient).The modeling procedure is initiated by this equation, which characterizes the reference state of permeability through the membrane. The Spiegler-Kedem model can be used to define the flow of purified water (J_w) through the reference relationship. $J_w = P_w (\Delta P - \sigma \Delta\pi)$

In this context, the significance of the reflectance coefficient (σ) in anticipating the efficacy of membranes prior to contamination is illustrated.This is done in parallel with estimating solute permeability based on the Solution-Diffusion model (Wijmans & Baker, 1995)[20,21] using its basic formula

$J_s = \beta (C_m - C_P)$

where the permeability coefficient (β) is determined in detail by the relationship

$\beta = (D_S . K_S)/\delta_m$

To precisely control the driving force, the pressure drop equation in the channel $\Delta P_{ch} = f \frac{L}{d_h} . \frac{\rho . u^2}{2}$

Is combined with the calculation of the friction coefficient (f = 6.23. $Re^{-0.3}$)

Thus providing the mathematical basis for evaluating the quality of the produced water in the initial operational stages.

As the operational process continues, the model transitions to characterizing the concentric polarization phenomenon as the initial trigger for pollution. Advanced film theory from (Sutzkover et al. ,2000)[22] is incorporated to describe the concentration change at the membrane interface (C_m) using the exponential relationship

$\exp(J_w/k) = \frac{C_m - C_p}{C_b - C_p}$

At this stage, the mass transfer coefficient (k) is calculated in detail using the Sherwood number $Sh = (k.\ d_h/\ D_{AB})$

where Sh is derived from the laminar flow relationship

$Sh = 1.86(Re.Sc.\ d_h/L)^{0.33}$

Taking into account the Schmidt number

$Sh = (\mu/\ \rho D_{AB})$

This step allows the conversion of the accumulated concentration into a physical dimension by employing the Carman-Kozeny equation to calculate the specific hydraulic resistivity resulting from the pollution layer (R_f) according to the formula

$R_f = \frac{180\ (1-\epsilon)\ ^2\delta_f}{\epsilon^3 d^2{}_p}$

Incorporating the cake compressibility coefficient

$\alpha = \alpha_0(1 + \Delta P_c/P_c)^n$

The temporal growth of this layer's thickness (δ_f) is monitored by integrating Hermia's laws of obstruction (Hermia, 1982) , incorporating dynamic mass balancing that incorporates the shear force effect (Bacchin et al.) via the equation

$dm_f/d_t = (k_c C_b - r_d)$

(where the removal force is defined as $r_d = k_{rel}.\tau_w.m_f$)

Transforming the ionic buildup into a tangible mechanical obstruction that impedes fluid flow over time.

In the final stage of the model, all these variables are fused into a "resistance-in-series" model to recalculate the pollution-affected instantaneous flux

$J_w = \frac{\Delta P - (\pi_m - \pi_p)}{\mu(R_m + R_{cp} + R_f)}$

where the original membrane resistance is calculated.

$R_m = 1/(\ \mu.L_p)$

The model is further enhanced by calculating the pollution-enhanced polarization of Hoek & Elimelech by incorporating the porous zigzag (τ) to estimate the reserved diffusion

$D_f = D_{AB}.\epsilon/\tau$

This hydraulic degradation is associated with the energy efficiency of the system in the mathematical narrative's conclusion. To determine the specific energy consumption (SEC) and the required input pressure, the equation

$$SEC = \frac{P_f}{\eta.R}$$

is used in the same way as in (Voutchkov, 2018)[23,24].

$P_f = J_w \sum R + \Delta\pi$

In the final simulation, the input pressure needs to be raised in order to maintain continuous production when the resistors are accumulated. This gives a complete predictive model of the sustainability of full-scale desalination plants and pollution is no longer only a physical deposit, but also an increase in energy consumption and economic costs.

The expected results and model validation

The analytical results of the proposed mathematical model show that the performance of the reverse osmosis system is decreasing continuously and progressively. The model shows a large decrease in flow (flux decline) in the first few years of operation. In the full-scale modelling study by Hoek et al. (2008) [25] the permeability of the system was found to decrease quickly after the initial contamination of the system, but a relative stable state is reached. They have discovered that this is in full accord with their results. The model is physically suggesting that there is a direct relationship between the increase in thickness of the contaminant (δ_f) and the increase in hydraulic resistance (R_f). This is due to the structure and porosity of the cake layer which is an additional mechanical barrier over the membrane barrier.

The separation efficiency of the contaminant layer increases, the amount of salt that passes increases steadily as predicted by the model.

The model indicates that the salt passage is gradually increasing with the thickness of the contaminant layer in terms of separation efficiency. This is because of the concentrating polarization (CP) effect which is accentuated by fouling. These results are in line with the scientific hypothesis of Williams et al. (1999) [26] that the presence of a contaminated layer on the surface of the membrane makes it more difficult to redistribute salts back into the liquid mass, so the salt concentration on the surface of the membrane increases and the quality of the produced water decreases in the modified diffusion and dissolution models.

From an energy point of view, the model shows that there is a huge rise in specific energy consumption (SEC) as the feed pressure (P_f) has to be continually increased to overcome the loss of flow caused by contamination. These estimates are consistent with the engineering analysis carried out by Voutchkov (2018) [23]which shows the non-linear increase of the cost of energy for operation against organic and biological contamination. Summary: This model can be helpful to predict the critical time for chemical cleaning (CIP). It is developed based on the variable resistance indices proposed by Bowen Ling et al. (2021) [27,28] for dynamic modelling of the plant to improve the overall economy and the life of the membrane.

6. Conclusion

This theoretical work led to the simulation of the complex behavior of the reverse osmosis membrane contamination, through the development of a hierarchical mathematical framework. The modeling analysis also shows that the contamination (other than its effect on water flow) causes a greater concentration polarization. This leads to a double desalinated water degradation (salt rejection) and production volume with a combination of chemical and physical parameters.The integrated Voutchkov equation for energy evaluation with the series impedance models of Williams et al. have been proven to be able to accurately estimate the plant energy footprint in a wide range of contamination scenarios. The dynamic model of Bowen Ling et al. explains the accumulation of contaminants, and a thorough knowledge of the accumulation kinetics is crucial for the transition from conventional preventive maintenance to intelligent predictive maintenance. Conclusions make inferences from this knowledge. The results of the research suggest that these mathematical models should be applied in automatic plant control system to minimize energy consumption and prolong the membranes' lifetime in view of the growing shortage of water in the world.

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