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# Development of a mathematical model for the prediction of concentration polarization in reverse osmosis desalination processes

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## ABSTRACT

Concentration polarization is referred to the buildup of salts on the high-pressure side of the reverse osmosis membrane surface. It is created due to the rejection of the dissolved salts by reverse osmosis membrane while convective flow carries salt up to the membrane surface. Therefore, the salt concentration at the membrane surface increases to a value exceeding the bulk salt concentration producing a salt boundary layer at the membrane surface. Concentration polarization affects the performance of the reverse osmosis process significantly. It increases the osmotic pressure at the membrane surface leading to a reduction in water flux and an increase in salt leakage. Also, the membrane lifetime is susceptible to decrease by high salt concentration, and concentration polarization will aggravate this effect. The present work focuses on the utilization of a combined film theory and diffusion transport through the membrane. In this work, the solution diffusion transport model and film theory will be combined to obtain an explicit expression for the water flux through the reverse osmosis process. This formula will help in the formulation of concentration polarization using limited data on water, salt and membrane properties as well as the mass transfer coefficients. By this approach, a predictive mathematical model for concentration polarization in reverse osmosis desalination processes was developed. The developed model depends on two dimensionless parameters that can be evaluated by providing water and solute permeability coefficients, operating conditions and mass transfer coefficient. The model was verified against published data, and a good agreement was found.

*Keywords:* Mathematical modeling; Concentration polarization; Membrane processes; Reverse osmosis; Permeate flux

## 1. Introduction

In the last few years, there are significant advances in membrane technologies that used for desalination in improving the cost effectiveness and performance of the processes. The major membrane technology used for water desalination is reverse osmosis (RO). RO is a pressure-driven membrane separation process in which a dense membrane allows diffusion of the water and salts. Diffusion of salts is much lower compared with water, which results in a rejection of the salts. This process leads to accumulation of the rejected salts at the front of the membrane surface, and concentration gradient is formed with highest concentrations directly at the membrane surface. Concentration polarization is the unwanted and inevitable effect of the increased salt concentration in the boundary layer, close to the membrane surface [1]. RO suffers from concentration polarization, since it leads to increased salt leakage through the membrane, increased the probability of scale/fouling development and decreased in the production of water.

The effect of concentration polarization on RO membrane performance was studied intensively. Matthiasson and Sivik [2] and Bhattacharyya et al. [3] have reported that due to the development of concentration polarization, the following phenomena were observed:

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- There is an increase in the salts flux through the membrane because of an increased concentration gradient across the membrane.
- The deposition of salts on the surface can change the separation characteristic of the membrane.
- There is an exhibition of changes in membrane separation properties.
- There is an increase in water flux with less osmotic pressure causing an increase in concentration polarization.
- Formation of gel on the membrane surface increases the hydrostatic resistance.

Zhou et al. [4] studied the effect of concentration polarization on the performance of the spiral-wound membrane modules. While Lyster and Cohen [5] studied the effect of concentration polarization in a rectangular RO membrane channel. Also, Strathmann [6] studied the control of concentration polarization in RO in a thin-channel RO test device under laminar flow conditions. They found that the thin-channel laminar flow concept is also applicable to high-flux membranes.

Modeling of concentration polarization for RO process can be performed either numerically or analytically. Kim and Hoek [7] developed a numerical concentration polarization model to enable a local description of permeate flux and salts rejection in cross-flow RO separations. They predicted that the channel averaged water flux and salt rejection by the developed numerical model. The model did not reflect real membrane separations in spiral-wound elements where complex hydrodynamics takes place due to feed spacers.

Denisov [8] analyzed and discussed two different models of concentration polarization, which have been used in the literature for interpretation of experimental data on ultrafiltration using the gel layer model and the osmotic pressure model. This analysis allows obtaining an expression for the limiting flux which not involve as the unstirred layer thickness. In deriving expression for the limiting flux, the concentration dependence of the viscosity was neglected, and the possibility of membrane fouling was ignored.

Zaidi et al. [9] studied salt and water transport in RO thin-film composite seawater desalination membranes. Two different approaches, irreversible thermodynamics model and solution-diffusion model (SDM), have been thoroughly presented. They found that in the SDM, the salt transport is mainly determined by salt permeability and salt concentration while salt permeability itself is strongly affected by salt diffusivity, solubility, and membrane thickness. They presented a review of the transport models for salt and water through reverse for better prediction of RO membrane performance.

Srinivasan et al. [10] developed a numerical model that could simulate the simultaneous development of velocity and concentration profiles in two-dimensional and axisymmetric empty RO channels. In this model, the quadratic expression for the concentration profile in the concentration polarization layer was assumed. This assumption may underestimate the wall concentration because the concentration profile in the concentration boundary layer is exponential-like rather than quadratic.

Song and Liu [11] analyzed and studied the model for concentration polarization in cross-flow RO channels with the shear flow. They found that the capacity to move the accumulated salt downstream in the shear flow is smaller than that in the plug flow because the highest salt concentration occurs with the lowest cross-flow velocity in the vicinity of the membrane surface. Comparison of the developed model with the analytical model shows that analytical model could be used to predict permeate velocity under certain conditions.

Therefore, there are different models for the prediction of concentration polarization and flux behavior of RO membrane systems. Most of these models were developed using implicit or explicit assumptions, which limited their validity. The objective of this work is to develop a mathematical model for the concentration polarization in RO using film theory in conjunction with diffusion transport through the membrane with realistic assumptions.

Film theory model provides an evaluation of the membrane wall concentration. On the other hand, the SDM, which based on diffusion of the salt and water through the membrane, offers a good view of the passage of salt through a RO membrane. Concentration polarization then can be predicted by combining film theory model and diffusion transport.

Combined film theory model and diffusion transport through RO membrane were used to formulate a mathematical model to estimate the permeate velocity. The obtained model was validated against published data, and it was in good agreement with these data.

## 2. Modeling of concentration polarization

To obtain an explicit formula for evaluating of permeate flux in RO, a mathematical model for the prediction of concentration polarization was developed. The estimation of the concentration polarization is essential to predict the water flux. Film theory and diffusion transport through the membrane can be combined to arrive at equations that predict the permeate flux and wall concentration. The film theory is simple, analytical and somewhat accurate for most RO processes. The film theory is often used to simplify the transport problem to a one-dimensional mass-transfer problem by assuming that axial solute convection near the membrane surface is negligible.

SDM is commonly used to provide a prediction of the flow of water and salt through the membrane. This model incorporates three steps: sorption, diffusion and desorption. In SDM, solvent and solute molecules dissolve into the membrane on the high-pressure side, diffuse through the homogeneous nonporous surface layer of the membrane independently and emerge on the low-pressure side.

### *2.1. Development of concentration polarization model*

The salt concentration near the membrane surface increases due to the rejection of the salt at the membrane surface. This leads to an accumulation of salts in a mass transfer boundary layer adjacent to the membrane surface across which salt concentration changes. Therefore, concentration gradient is created, then salt will diffuse away from the membrane surface. At steady state, the convection of salt molecules toward the membrane equals to the diffusion of salt molecules back to the feed side. This phenomenon is illustrated in Fig. 1 and represented by the material balance expressed by Eq. (1):

$$J_S = C_i J_v - Ds\frac{dc}{dx} \tag{1}$$

$$Cp = \frac{Js}{J_v} \tag{2}$$

where $J_s$ and $J_v$ are the molar salt and water fluxes across the membrane, respectively; $C_i$ is salt concentration; $D_S$ is the salt diffusion coefficient; and $C_p$ is product water concentration.

Defining $C_b$ as the bulk salt concentration, $C_s$ as the membrane surface (wall) concentration and δ is the thickness of the boundary layer, then by integration of Eq. (1) taking the following film boundary conditions into account:

$$\{x = 0, \quad C_i = C_S \quad \text{and} \quad x = \delta, \quad C = C_b\}$$

$$\frac{C_S - C_p}{C_b - C_p} = e^{\frac{J_v}{K_b}} \tag{3}$$

where $K_b = \dfrac{Ds}{\delta}$ and is defined as the mass transfer coefficient, m/s.

Eq. (3) is known as concentration polarization factor (CPF).

From CPF, the concentration boundary layer (δ) can be calculated after finding the mass transfer coefficient, $K_b$, since the mass transfer coefficient is equal the diffusion coefficient divided by the concentration boundary layer.

To calculate the wall concentration, the steady-state condition is assumed. At steady state, the concentration of retained salt in the concentration polarization layer satisfies the following equation [12]:

$$v(x)C + D\frac{dc}{dy} = 0 \tag{4}$$

where $x$ and $y$ are the longitudinal and transverse coordinates (m). $v(x)$ is the permeate flux at $x$, and $C$ indicates the concentration of retained salt (mol/m$^3$), and $D$ is the salt diffusion coefficient (m$^2$/s).

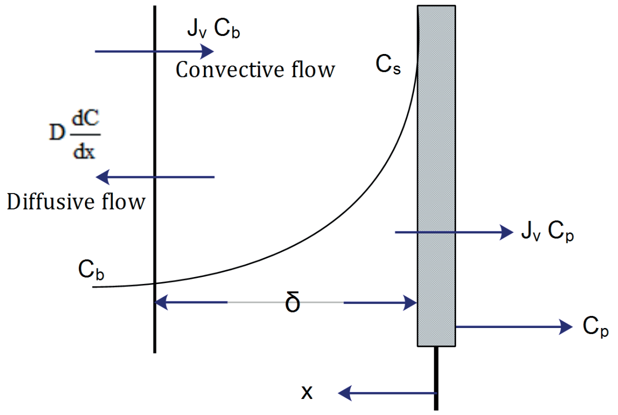

Fig. 1. Schematic of the boundary layer adjacent to the membrane surface.

Eq. (4) states that the longitudinal salt flux at any point ($x$) along the channel is equal to the total amount of salt rejected by the membrane from the inlet to the location $x$.

The solution of Eq. (4) can be written as follows:

$$\begin{aligned} \int -\frac{v(x)}{D}dy &= \int \frac{1}{c}dC \\ -\frac{v(x)y}{D} &= \ln C \\ \therefore C = Ae^{-\frac{v(x)y}{D}} \end{aligned} \tag{5}$$

where $A$ is an integration constant to be determined.

The concentration profile due to the diffusion–convection phenomena can be described by a Navier–Stokes equation as follows:

$$\frac{dc}{dt} + u\frac{dc}{dx} + v\frac{dc}{dy} - D\left[\frac{d^2c}{dx^2} + \frac{d^2c}{dy^2}\right] = 0 \tag{6}$$

where $u$ is the fluid velocity in the longitudinal ($x$) direction, and $v$ is the fluid velocity in the transverse ($y$) direction.

At steady state, transverse diffusion is greater than axial diffusion, then combine Eq. (6) with Eq. (1) to become:

$$\int_0^\infty \gamma y \, C \, dy = \int_0^x R \, v(\acute{x}) \; C_b \; dx \tag{7}$$

where $C_b$ is a salt concentration in the bulk (mol/m$^3$); $R$ is salt rejection; $\gamma$ is wall share rate (s$^{-1}$); and $\acute{x}$ is dummy integration variable.

Substituting value of $C$ from Eq. (5) into Eq. (7) in order to find value of $A$.

$$\int_0^\infty \gamma y \, Ae^{-\frac{v(x)y}{D}} dy = RC_b \int_0^x v(\acute{x})dx \tag{8}$$

After integrating the left-hand side:

$$A = R\frac{C_b}{\gamma D^2} v(x)^2 \int_0^x v(x) \quad dx \tag{9}$$

Substituting Eq. (9) in Eq. (5):

$$C = \left[R\frac{C_b}{\gamma D^2} v(x)^2 \int_0^x v(x) \; dx\right] e^{\frac{v(x)y}{D}} \tag{10}$$

At $y = 0$, wall concentration can be found from Eq. (10):

$$Cw = \left[R\frac{C_b}{\gamma D^2} v(x)^2 \int_0^x v(x) \; dx\right]$$

The osmotic pressure can be found by the following equation:

$$\Delta\pi = n \varnothing RTc$$

where $\Delta\pi$ is the osmotic pressure in Pa; $n$ is the number of ions in the electrolyte; $c$ is the concentration of the electrolyte; and $\varnothing$ is the osmotic coefficient for single- and multi-component electrolyte solutions.

Osmotic pressure can be rewritten due to concentration polarization as follows:

$$\Delta\pi = n \varnothing RTCw = n\varnothing RT\left[R\frac{C_b}{\gamma D^2}v(x)^2\int_0^x v(x)\ dx\right] \tag{11}$$

The transport equation for permeate flux with the existence of concentration polarization is given by

$$v(x) = \frac{\Delta P - \Delta\pi}{R_m} \tag{12}$$

$$\Delta P = v(x)R_m + \Delta\pi \tag{13}$$

where $\Delta P$ is the transmembrane pressure (applied pressure), Pa, and $R_m$ is membrane resistance, Pa s/m.

Substituting Eq. (11) in Eq. (13):

$$\Delta P = v(x)R_m + n\varnothing RT\left[R\frac{C_b}{\gamma D^2}v(x)^2\int_0^x v(x)\ dx\right] \tag{14}$$

Eq. (14) can be substantially simplified by rewriting it into a dimensionless form.

$$\Delta F = \frac{\Delta P}{\Delta\pi}$$

$$V = v\left(\frac{L}{\gamma D^2}\right)^{\frac{1}{3}}$$

$$X = \frac{x}{L}$$

where $L$ is the length (m) of the filtration channel; $X$ dimensionless longitude distance and $x$ is distance axial. Therefore, Eq. (14) becomes:

$$\Delta F = \left(\frac{R_m}{\Delta\pi}\right)[\gamma D^2\ /L]^{\frac{1}{3}}V + V^2\int_0^x V \quad dx \tag{15}$$

The term in the square bracket is a dimensionless parameter that fully characterizes the cross-flow RO process. This dimensionless parameter $N_s$ can be defined as follows:

$$NS = \left(\frac{R_m}{\Delta\pi}\right)(\gamma D^2\ /L)^{\frac{1}{3}} \tag{16}$$

At $X \neq 0$, it can be shown that the permeate flux satisfies the following differentiating of Eq. (15).

$$\left(NsV^{-3} - 2\Delta FV^{-4}\right)dv = dx \tag{17}$$

Integrating Eq. (17) with boundary condition, $x = 0, V = \frac{\Delta F}{Ns}$, the following expression is obtained:

$$4 - \frac{3Ns}{\Delta F}V = \left[\frac{6x}{\Delta F} + \left(\frac{Ns^3}{\Delta F}\right)\right]V^3 \tag{18}$$

The local permeate velocity, $V_{(x)}$, in the cross-flow RO channel can be found from Eq. (18) as follows:

$$V^3Ns^3 + 6V^3\Delta F^3x + 3\Delta F^2Ns\ V - 4\Delta F^3 = 0 \tag{19}$$

Upon solving this cubic equation, the local permeate velocity is then equal to:

$$\mathrm{V}(\mathrm{x}) = \sqrt[3]{\left[\left(\Delta\mathrm{F}^3\frac{\sqrt{\dfrac{24\Delta\mathrm{F}^2\mathrm{x} + 5\mathrm{Ns}^3}{\left(6\Delta\mathrm{F}^2\mathrm{x} + \mathrm{Ns}^3\right)}}}{6\Delta\mathrm{F}^2\mathrm{x} + \mathrm{Ns}^3}\right) + \frac{2\Delta\mathrm{F}^3}{6\Delta\mathrm{F}^2\mathrm{x} + \mathrm{Ns}^3}\right]} - \left[\Delta\mathrm{F}\frac{\mathrm{Ns}}{6\Delta\mathrm{F}^2\mathrm{x} + \mathrm{Ns}^3\sqrt[3]{\left[\left(\dfrac{\sqrt{\dfrac{24\Delta\mathrm{F}^2\mathrm{x} + 5\mathrm{Ns}^3}{\left(6\Delta\mathrm{F}^2\mathrm{x} + \mathrm{Ns}^3\right)}}}{6\Delta\mathrm{F}^2\mathrm{x} + \mathrm{Ns}^3}\right) + \dfrac{2\Delta\mathrm{F}^3}{6\Delta\mathrm{F}^2\mathrm{x} + \mathrm{Ns}^3}\right]}}\right] \tag{20}$$

### 2.2. Local velocity parameters

The developed equation for the local permeate velocity, Eq. (20), contains two dimensionless parameters ($\Delta F$ and $N_s$) that need to be determined in order to predict permeate flux using the model:

$$\Delta F = \frac{\Delta P - \Delta\pi}{\Delta\pi} \tag{21}$$

$$Ns = R_m\left(\frac{1}{\Delta\pi}\right)\left(\frac{D^2\gamma}{L}\right)^{1/3} \tag{22}$$

These parameters depend on solution properties and system parameters as well as the mass transfer coefficient. The mass transfer coefficient can be estimated from the correlation between Sherwood, Reynolds and Schmidt numbers as follows [13]:

$$Sh = \frac{K_b d}{D_s} = \gamma.\mathrm{Re}^a.S_{ci}^b.\left(\frac{d_h}{W}\right)^c, \quad \mathrm{Re} = \frac{du\rho}{\mu}, \quad S_{ci} = \frac{\mu}{\rho D_s}$$

where $d$ is the height of feed channel; $u$ is the cross-flow velocity; and $\mu$ and $\varrho$ are the viscosity and density of water, respectively.

The constants $\lambda$, $a$, $b$ and $c$ are mass transfer coefficient constants, and their values are: $\lambda = 0.065$, $a = 0.875$, $b = 0.25$ and $c = 0.00$ [13].

Table 1
Comparison between predicted and published values of permeate water velocity

| Parameter | Zhou et al. [4] | Kim and Hoek [7] | Song and Yu [14] |
|---|---|---|---|
| Membrane properties and physical data: | | | |
| Applied pressure, $\Delta p$ (Pa) | $6 \times 10^{6}$ | $7 \times 10^{5}$ | $1.0 \times 10^{7}$ |
| Bulk concentration, $C_b$ (mol/m$^3$) | 1.7 | 50 | 2,000 |
| Temperature, $T$ (K) | 298 | 298 | 298 |
| Osmotic pressure, $\Delta\pi$ (Pa) | $8.432 \times 10^{3}$ | $248 \times 10^{3}$ | $5.4 \times 10^{6}$ |
| Membrane Water permeability, $A$ (m/Pa s) | $4.5 \times 10^{-10}$ | $2.15 \times 10^{-11}$ | $4.5 \times 10^{-12}$ |
| Diffusion coefficient, $D$ (m$^2$/s) | $9.6 \times 10^{-9}$ | $1.6 \times 10^{-9}$ | $9.6 \times 10^{-9}$ |
| Channel length, $L$, m | 6.0 | – | 1.0 |
| Membrane resistance, $R_m$ (Pa s/m) | $1.0 \times 10^{11}$ | $1.0 \times 10^{9}$ | $5.0 \times 10^{11}$ |
| Wall shear rate, $\gamma$ (s$^{-1}$) | 1,000 | 1,000 | 1,000 |
| Membrane salt rejection, $R_o$ | 1 | 1 | 0.55 |
| Evaluation of model parameters ($\Delta F$ and $N_s$): | | | |
| $N_s$ | 2.95 | $5.5 \times 10^{-2}$ | 4.14 |
| $\Delta F$ | 711 | 1.8 | 0.84 |
| Prediction of the permeate water velocity by the developed model: | | | |
| Permeate water velocity, $V$ (m/s) | $1.42 \times 10^{-5}$ | $5.7 \times 10^{-6}$ | $4.96 \times 10^{-6}$ |
| Published data on permeate water velocity: | | | |
| Permeate water velocity, $V$ (m/s) | $1.47 \times 10^{-5}$ | $6.00 \times 10^{-6}$ | $5.00 \times 10^{-6}$ |
| $\lvert$Error %$\rvert$ | 3.5% | 5.2% | 0.81% |

## 3. Model validation

The obtained model for estimating the permeate velocity was verified against published data of Zhou et al. [4], Kim and Hoek [7] and Song and Yu [14]. The published value of permeate water velocity of Zhou et al. [4], Kim and Hoek [7] and Song and Yu [14] were $1.47 \times 10^{-5}$, $6.00 \times 10^{-6}$ and $5.00 \times 10^{-6}$ (m/s), respectively. In order to check the validity of the developed expression, all necessary membrane properties and physical data of Zhou et al. [4], Kim and Hoek [7] and Song and Yu [14] were obtained and substituted into the local permeate velocity formula (Eq. (20)). Therefore, the corresponding values of the predicted permeate water velocity by the developed model were $1.42 \times 10^{-5}$, $5.7 \times 10^{-6}$ and $4.96 \times 10^{-6}$. Table 1 shows membrane properties and physical data as well as both published and predicted values of the permeate water velocity. Estimated errors are between 8.1% and 5.2%.

## 4. Conclusions

RO desalination plants have become widely used for providing potable water. It is also utilized in industrial and municipal applications. RO suffers from various operational problems. Concentration polarization is considered one of the most phenomena that reduce water productivity and limit the membrane life. Therefore, concentration polarization may significantly affect the membrane performance in RO. Concentration polarization is developed during the prolong operation of the RO plant. It can be avoided or at least delayed if better maintenance is attained. This can be achieved by modeling of the concentration polarization and predicted the tendency of its formation.

The prediction of concentration polarization is very important phenomena in keeping a steady productivity of the RO process. In this work, a steady-state formulation of concentration polarization was carried. A mathematical model was developed analytically to predict the concentration polarization in the RO desalination processes. In future work, permeate velocity will be used to study the concentration polarization phenomena to estimate the wall concentration using the concentration polarization factor. A detailed parametric study will be conducted to illustrate the variation of the production flux, wall concentration and membrane water permeability with different operating parameters such as the applied pressure, feed concentration and membrane water permeability.

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