Research Article

SEPARATING MgBr₂, KBr, and NaBr USING NANOFILTRATION MEMBRANE – THEORETICAL

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INTRODUCTION

Water need is increasing because of the decreasing sources of clean water. One of the processes used in obtaining clean water is Nanofiltration membrane. Nanofiltration membrane is a process that has properties lying between ultrafiltration membrane and reverse osmosis membrane properties. Nanofiltration membrane is used in different applications such as softening water, removing hardness, removing natural organic matter, removing heavy metals, removing viruses and bacteria, and concentrating organic dyes. Nanofiltration membrane is characterised by the Nernst-Planck equation, where it describes the solute concentration change inside the membrane and change in concentration between feed and permeate streams.

Theory

Transport of ions through Nanofiltration membrane is described by the Extended Nernst-Planck equation [1]; in terms of three concepts which are the concentration gradient, the electrical potential gradient and the pressure difference across the membrane. Ion diffusion across Nanofiltration membrane is caused by the concentration gradient and the electrical potential gradient, while the convection of ions across Nanofiltration membrane is caused by the pressure difference across the membrane. The extended Nernst-Planck equation is

\[
j_i = K_{ix} c_i j_v - D_{ix} \frac{d c_i}{dx} - \frac{z_i e D_{ix}}{RT} \frac{d \Psi}{dx}
\]

(1)

where \((j_i)\) is the flux of ion \((i)\) based on the membrane area \((\text{mol/m}^2\cdot\text{s}), (D_{ix})\) is the hindered diffusivity \((\text{m}^2/\text{s}), (c_i)\) is the concentration in the membrane active layer \((\text{mol/m}^3), (z_i)\) is the valence of ion \((i), (K_{ix})\) is the hindrance factor for convection inside the membrane, \((j_v)\) is the volume flux based on the membrane area \((\text{m/s}), (R)\) is the gas constant \((\text{J/mol.K}), (T)\) is the absolute temperature \((\text{K}), (F)\) is Faraday constant \((\text{C/mol})\) and \((\Psi)\) is the electrical potential \((\text{V})\). The ion flux \([2]\) is

\[
j_i = C_{ix} j_v
\]

(2)

where \((C_{ix})\) is the concentration of ion \((i)\) in permeate \((\text{mol/m}^3)\). By substituting equation (2) into equation (1) then the concentration gradient is obtained as follows [3]

\[
\frac{dc_i}{dx} = \frac{1}{D_{ix}} (K_{ix} c_i - C_{ix}) - \frac{z_i e D_{ix}}{RT} \frac{d \Psi}{dx}
\]

(3)

The membrane effective charge is assumed to be constant

\[
\sum_{i=1}^{3} z_i c_i = -X_d
\]

(4)

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where \( X_d \) is the effective membrane charge density (equivalent/m²). The electro-neutrality condition in the bulk solution is

\[
\sum_{i=1}^{n} z_i C_i = 0 \tag{5}
\]

The electrical potential gradient (\( d\Psi/dx \)) is obtained by integrating and rearranging equation (3) over the conditions given by equations (4) and (5)

\[
\frac{d\Psi}{dx} = \frac{\sum_{i=1}^{n} z_i D_i \Delta \Psi_0}{R T} \tag{6}
\]

The Donnan equilibrium was assumed to apply at the feed/membrane interface and at the membrane/permeate interface; which is

\[
\left( \frac{y_{i,p}}{y_{i,f}} \right) = \Phi \exp \left( -\frac{z_i F}{R T} \Delta \Psi \right) \tag{7}
\]

where \( y_{i} \) is the concentration of ion (i) in the membrane, \( y_{i,f} \) is the activity of ion (i) in the bulk solution, \( \Delta \Psi_0 \) is the Donnan potential (V) and \( \Phi \) is the steric partitioning term. Assuming dilute solution and the activity coefficient is equal to unity, and then the Donnan equilibrium would be

\[
\left( \frac{C_{i,p}}{C_{i,f}} \right) = \exp \left( -\frac{z_i F}{R T} \Delta \Psi \right) \tag{8}
\]

where \( C_{i,p} \) is the ion concentration in the solution (mol/m³). Solving equations (3) and (6) over the following boundary conditions

at \( x = 0 \rightarrow C_i = C_{i,f} \)

at \( x = \Delta x \rightarrow C_i = C_{i,p} \)

where \( C_{i,p} \) is the concentration of the ion in the permeate (mol/m³) and \( C_{i,f} \) is the concentration of the ion in the feed (mol/m³). The hindered diffusivity [1] [3] is

\[
D_{i,p} = K_{i,d} D_{i,\infty} \tag{9}
\]

where \( D_{i,\infty} \) is the bulk diffusivity (m²/s) and \( K_{i,d} \) is the hindrance factor for diffusion. The hindrance factor for diffusion is

\[
K_{i,d} = K^{-1}(\lambda_{i,o}) \tag{10}
\]

where \( K \) is the hydrodynamic drag coefficient. The hindrance factor for convection is

\[
K_{i,c} = (2 - \Phi_{i}) G_{i,o} \tag{11}
\]

where \( G \) is the hydrodynamic drag coefficient and \( \Phi \) is steric partitioning term. The hydrodynamic drag coefficients [3] (K) and (G) are

\[
K^{-1}(\lambda_{i,o}) = 1.0 - 2.3 \lambda_i + 1.15 \lambda_i^2 + 0.2 2 \lambda_i^3 \tag{12}
\]

\[
G(\lambda_{i,0}) = 1.0 + 0.0 5 \lambda_i - 0.98 8 \lambda_i^2 + 0.4 44 \lambda_i^3 \tag{13}
\]

The steric partitioning term is

\[
\Phi = (1 - \lambda)^2 \tag{14}
\]

where \( \lambda \) is the ratio of ion or solute radius/pore radius. The stokes radius of component (i) to pore radius ratio (\( \lambda \)) is given as follow

\[
\lambda = \frac{r_i}{r_p} \tag{15}
\]

where \( r_p \) is the effective pore radius and \( r_i \) is the radius of component (i). The rejection [4] is

\[
R = 1 - \frac{C_{i,p}}{C_{i,f}} \tag{16}
\]

Equation (3) was used to calculate the ion concentration inside the membrane in order to calculate the ion concentration at the permeate side, as a result the membrane rejection would be calculated by equation (16). Euler mathematical method was used to solve the extended Nernst-Planck equation using FORTRAN programming tool. The used salts were potassium bromine (KBr), magnesium bromine (MgBr₂), and sodium bromine (NaBr) [5]. The program was run for flow rates ranging between 1x10⁻⁷ to 1x10⁻⁵ m²/s/m, membrane pore radius ranging between 6x10⁻¹⁰ to 5x10⁻⁹ m, and the salts initial concentration was assumed to be 10 mol/m³ [6].

RESULTS

Two ions

The used salts where KBr, NaBr, and MgBr₂. For each salt solution, the module was run at different volumetric flow rates per membrane surface area ranging between 1x10⁻⁷ to 1x10⁻⁵ m³/m²/s [7]. For KBr solution; it was noticed that no rejection was obtained, where the K⁺ and Br⁻ passed through the membrane. But as the flux decreased the rejection increased. Br⁻ rejection was higher than K⁺ (figures 1 and 2). Also the rejection of K⁺ and Br⁻ increased as the membrane pore radius increased [6] [7].

![Figure 1](https://example.com/figure1.png)

**Figure 1** K⁺ rejection versus membrane pore radius (r_p).

For NaBr solution; it was noticed that no rejection was obtained, where the Na⁺ and Br⁻ passed through the
membrane. But as the flux decreased the rejection increased. \( \text{Br}^{1-} \) rejection was higher than \( \text{Na}^{1+} \) (figures 3 and 4) [2]. Also the rejection of \( \text{Na}^{1+} \) and \( \text{Br}^{1-} \) increased as the membrane pore radius increased.

For \( \text{KBr} \) and \( \text{MgBr}_2 \) the rejection of \( \text{K}^{1+} \) decreased as the flux increased and membrane pore radius increased. It was noticed that the rejection for both \( \text{Mg}^{2+} \) and \( \text{Br}^{1-} \) ions increased as the membrane pore radius increased and as the flux increased. Both \( \text{Mg}^{2+} \) and \( \text{Br}^{1-} \) ions had the lowest rejection values at the highest flux and lowest membrane pore radius (figures 5 and 6) [7].

It was noticed that \( \text{NaBr} \) and \( \text{KBr} \) had similar rejection behavior, while \( \text{MgBr}_2 \) rejection behavior differed.

### Three ions

The ions were obtained from mixing two salts, where the used salts were \( \text{KBr} \), \( \text{NaBr} \), and \( \text{MgBr}_2 \). The mixtures were \( \text{KBr} \) and \( \text{NaBr} \), \( \text{KBr} \) and \( \text{MgBr}_2 \), \( \text{NaBr} \) and \( \text{MgBr}_2 \). For \( \text{KBr} \) and \( \text{NaBr} \) solution, the rejection of \( \text{K}^{1+} \) decreased at the minimum membrane pore radius, but the rejection increased as the membrane radius increased and the flux increased (figure 7). The rejection of \( \text{Na}^{1+} \) increased and the flux increased and the membrane pore radius increased (figure 8). The rejection of \( \text{Br}^{1-} \) increased as the flux increased and membrane pore radius increased (figure 9) [2] [7].
For KBr and MgBr₂, the rejection of K⁺ decreased as the flux increased and membrane pore radius increased. But at the lowest and highest flux, the rejection increased as the membrane radius increased (figure 10) [8]. The rejection of Mg²⁺ decreased as the flux increased and membrane pore radius increased (figure 11). The rejection of Br⁻ increased as the flux increased and membrane pore radius increased (figure 12) [5].

For NaBr, and MgBr₂, the rejection of Mg²⁺ decreased as the flux increased and membrane pore radius increased (figure 11). The rejection of Na⁺ from NaBr and MgBr₂ solution was similar to the rejection from KBr and MgBr₂ solution. The rejection of Mg²⁺ from NaBr and MgBr₂ solution was similar to the rejection of Br⁻ from KBr and MgBr₂ solution [8].

The four ions were obtained from three salts mixture; the salt from KBr and MgBr₂ solution. The rejection of Na⁺ was higher than the rejection of Na⁺. The rejection of Mg²⁺ was lower than the rejection of Na⁺ and the rejection of K⁺. While the rejection of Mg²⁺ was lower than the rejection of Na⁺. The rejection of Br⁻ decreased as the membrane pore size increased, and increased as the flux increased (figure 17) [7].
The rejection of Br$^{1+}$ was lower than the rejections of Mg$^{2+}$ and K$^{1+}$ but higher than the rejection of Na$^{1+}$ [8].

![Figure 13](image) k$^{1+}$ rejection versus membrane pore radius (r$p$).

![Figure 14](image) Na$^{1+}$ rejection versus membrane pore radius (r$p$).

![Figure 15](image) Mg$^{2+}$ rejection versus membrane pore radius (r$p$).

![Figure 16](image) Br$^{1+}$ rejection versus membrane pore radius (r$p$).

**CONCLUSION**

Euler mathematical method was used to solve the extended Nernst-Planck equation, where FORTRAN programme was used to solve the model. The used model is known for its limitation and for being descriptive more than predictive and in-order to overcome these limitations experimental parameters were used; to be able to compare the theoretical results with the experimental results. The chosen ions were Na$^{1+}$, Mg$^{2+}$, K$^{1+}$ and Br$^{1+}$ ions [5]. The feed concentration was assumed to be equal to 10 mol/m$^3$. The membrane active layer thickness was assumed to be equal to 20.0E-6 m. The model was solved for different volume flux values that ranged between 1.0E-7 to 1.0E-5 m$^3$/m$^2$.s [4]. For each volume flux the membrane pore radius was changed in a range between 6.0E-10 to 5.0E-9 m [7]. It was noticed that the rejection of ions increased as the ion mixture increased; the rejection of two different ions had a negative value, while the rejection of ions from triple and quadratic mixture increased. The increase of the ions rejection is a result of the increase of the charge in bulk area at the membrane surface [1]. Besides that, the ions rejection increased as the flux increased which supports the increase of the ions charge in the bulk area. Also the rejection decreased as the membrane pore radius increased, were the ion would pass easily through the membrane [8].

More work need to be done in-order to improve this method such understanding the physics of solutions and the properties of ions because they have great effect on the nanofiltration separation process.

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**Work cited**

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