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Development of a simulation program for the forward osmosis and reverse osmosis process

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ABSTRACT

Forward osmosis (FO) is an osmotic process that uses a semi-permeable membrane to effect separation of water from dissolved solutes by an osmotic pressure gradient. Unlike RO, FO does not require high pressure for separation, allowing low energy consumption to produce water. Therefore FO, a potential alternative to conventional membrane process, has been considered a novel technology for seawater desalination. There is no forward osmosis (FO) process simulation program yet, though. Therefore, the main objective of this paper is to develop such computer program based on the solution-diffusion model modified with the film theory for simulating and optimizing the FO, RO, and FO-RO hybrid process. The effect of concentration polarization on FO and RO process efficiency was also considered in the model. A MATLAB-based graphical user interface (GUI) program was used to develop the simulation program. Using the program, the effects of various factors, including the draw solution concentration, feed concentration, and feed pressure and temperature, on the FO and RO process performance were examined. The simulation results showed that the FO-RO hybrid process has higher recovery (66.8%) with reasonable flux (13.1 L/m²-h) and permeate concentration (382 mg/L) than the FO and RO process. Thus, the advantages of the FO-RO hybrid process over the FO and RO process are its low permeate concentration and high recovery, which are difficult to attain in the FO and RO process, respectively.

Keywords: Forward osmosis; Program; Model; Hybrid process; Simulation

1. Introduction

As the global water shortage become serious by rapid population growth, desalination of seawater and brackish water is becoming more important [1,2]. Recently, the reverse osmosis (RO) membrane process has been considered a promising technology for desalination. The performance of the RO membrane process is very sensitive to the quality of the feed water and the plant operating conditions, though. This means that the availability of reliable RO models is very important for process design and operation [3,4]. Thus, RO membrane makers have developed several computer programs such as ROSA, IMSDesign, and TorayRO to help possible customers simulate an RO process. RO membrane processes are expensive and energy-intensive yet, though.

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Their limited recovery of seawater, typically 35–50%, is another drawback [5]. Forward osmosis (FO) is an osmotic process that uses a semi-permeable membrane to effect separation of water from dissolved solutes by an osmotic pressure gradient. Unlike RO, FO does not require high pressure for separation, allowing low energy consumption to produce water [6]. Therefore FO, a potential alternative to conventional membrane process, has been considered a novel technology for seawater desalination [6]. There is no FO process simulation program yet, though. Therefore, the main objective of this paper is to develop such computer program based on the solution-diffusion model modified with the film theory for simulating and optimizing the FO, RO, and FO-RO hybrid process. The effect of concentration polarization on FO and RO efficiency was also considered in the program. A MATLAB-based graphical user interface (GUI) program was used to develop the program. Using the program, the effects of various factors, including the recovery, flux, draw solution concentration, feed concentration, and feed pressure and temperature, on the FO, RO, and FO-RO hybrid process performance were examined.

2. Mathematical model

The solution–diffusion model modified with the film theory was used to simulate the FO, RO, and FO-RO hybrid process. According to the solution-diffusion model, the water flux (J_w) and solute flux (J_s) equations for FO process can be defined as follows:

$$J_w = L_v \left(\pi_{D,b} - \pi_{F,b} \right) \tag{1}$$

and

$$J_s = L_s \left(C_b - C_p \right) \tag{2}$$

wherein L_v is the water transport parameter, L_s is the solute transport parameter, $\pi_{D,b}$ is the osmotic pressure on the draw solution side, $\pi_{E,b}$ is the osmotic pressure on the feed side, and C_D and C_F are the concentrations of the draw solution and the feed solution, respectively. The external concentration polarization (ECP) and the internal concentration polarization (ICP), which take place in the FO membrane process, reduce the permeate water flux due to the decrease in the effective osmotic pressure. The general water and solute flux equations were modified as follows, considering ECP and ICP to make accurate predictions [7]:

$$J_{w} = L_{v} \left(\pi_{D,b} \exp\left(-\frac{J_{w}}{k_{D}}\right) - \pi_{F,b} \exp\left(\frac{J_{w}}{k_{F}}\right) \right)$$
(3)

and

$$J_s = J_w C_p = L_s \left(C_b \exp\left(\frac{J_w}{k_F}\right) - C_p \right)$$
(4)

wherein k_F is the mass transfer coefficient for the external concentration polarization, and k_D is the mass transfer coefficient for the internal concentration polarization. Based on the mass transfer correlations, k_F and k_D are given as follows [8]:

$$k_F = 1.85 \frac{D}{d_h^{0.65} L^{0.33}} (\text{ReSc})^{0.33}$$
(5)

and

$$k_D = \frac{D\varepsilon}{\tau l} \tag{6}$$

wherein *D* is the diffusion coefficient, d_h is the hydraulic diameter, Re is the Reynolds number, Sc is the Schmidt number, ϵ is the porosity of the support layer, *l* is the thickness of the support layer, and τ is the tortuosity of the support layer.

For an RO system, the water flux (J_w) and solute flux (J_v) equations can be defined as follows:

$$J_w = L_v \left(\Delta P - \Delta \pi_{C_h} \right) \tag{7}$$

and

$$J_s = L_s \left(C_b - C_p \right) \tag{8}$$

wherein L_v is the solvent transport parameter, L_s is the solute transport parameter, C_b is the solute concentration in the bulk feed solution, C_p is the solute concentration at the permeate side, $\Delta \pi_{C_b}$ is the osmotic pressure at the solute concentration of C_b , and ΔP is the transmembrane pressure. As the filtering proceeded, however, the concentration polarization occurred. Using C_m (the solute concentrations on the membrane surface) instead of C_b , the aforementioned equations can be modified as follows:

$$J_w = L_v \left(\Delta P - \Delta \pi_{C_m} \right) \tag{9}$$

and

$$J_s = L_s \left(C_m - C_p \right) \tag{10}$$

 C_m is calculated according to the film theory to interpret the concentration polarization, and the solvent concentration profile on the surface can be calculated according to the following equation:

$$\frac{C_m - C_p}{C_b - C_p} = e^{\frac{J_w}{k}} \tag{11}$$

wherein k is the mass transfer coefficient for the back diffusion of the solute from the membrane to the bulk solution on the high-pressure side of the membrane [9], as follows:

$$k = 0.5510 \left(\frac{ud_h}{v}\right)^{0.4} \left(\frac{v}{D}\right)^{0.17} \left(\frac{C_b}{\rho}\right)^{-0.77} \left(\frac{D}{d_h}\right)^{-0.77}$$
(12)

wherein *u* is the crossflow velocity, d_h is the hydraulic diameter, v is the kinematic viscosity, and ρ is the solution density.

3. Solution methods

The procedure for solving the model equations are shown in Fig. 1. The models were developed in one dimension on the basis of the flux equations, while considering the ECP and ICP. The developed mathematical models should be solved iteratively because the equations in the model are highly nonlinear since the model considers the ECP and ICP. To solve the model, the membrane was divided into small segments, and their sizes were chosen to be small enough until the change in the calculated results was tolerable.

4. Program structure

The GUI data processing program allows a user to simulate the FO and FO-RO hybrid system immediately after data acquisition. The components of the program are shown in Fig. 2. The program is a set of m-files and has six major parts (an m-file is a user-defined function or script file composed of existing MATLAB commands and functions): Main window, FO optimization, RO optimization, FO process simulation, RO process simulation, and FO-RO hybrid process simulation.

In the Main window, the project information, user information, and design condition were inputted, and the simulation sub-module was selected. The optimization module used the permeate water flow rate, feed water qualities, and membrane properties as the input parameters. The simulation results for the optimum operating conditions of the FO and RO process were explored to minimize the energy consumption and sufficient boron rejection (less than 1.0 mg/L) for seawater desalination. The FO and RO process simulation module used the results of the optimization sub-module as input data. Using the FO and RO process simulation sub-module, the flux and recovery from each element was calculated to compare the local characteristics with the overall performance. In this program, only one kind of combined FO and RO system was considered. FO was used to treat



b) RO process



Fig. 1. Flowchart for the solution method of the model.

275

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File Edit Help	
Project Information	
- Project Information	Design Condition
Project	Sea Water
Notes	Draw Solution NH4HCO3
	Unit settings
	Calculation unit Metric
User Information	Temperature unit Celsius (oC)
Designer	Mathematical Model
Company	FO Optimization FO Opt.
Date Project Target	RO Optimization RO Opt.
	Forward Osmosis FO Simulation
Notes	Reverse Osmosis RO Simulation
	HyTOP(RO+FO) Desalination
	Statistical Model
	Artificial Neural Network ANN Simulation

Y.-J. Choi et al. / Desalination and Water Treatment 33 (2011) 273–282



Kd m/sec D MPIII 0.2 Simulation RESET 0.1 0 0.2 0.4 0.6 0.8	Max(Boron Rejection) & Min(Specific Energy Permeate water Permeate m3/day Temperature oC Membrane Membrane Transport Parameter Lv m2sec.kg Ls m/sec Ls_b m/sec Cl 0 Port Port	(v) 0. 0. 0. 0. 0. 0.	1 - 9 - 8 - 7 - 6 - 5 - 4 - 3 -					
	Simulation RESET	0.	1 0 0	0.2	0.4	0.6	0.8	
	Recovery 0 % Totle Vessel Number	0		Permeste Borop	0 0000	Specific Eperav	0	kiðih ím

b) FO optimizaiton

Fig. 2. Components of the simulation program.





c) RO optimization



d) FO process simulation

Fig. 2. Components of the simulation program.



e) RO process simulation



f) FO-RO hybrid simulation

Fig. 2. Components of the simulation program.

278

the concentrate from RO for high recovery. A recovery system for the drawn salt was assumed to have been used. The simulation program can predict any operating and performance parameter of the FO and RO process. Using the program, the effects of various factors, including the recovery ratio, permeate flux, temperature, and concentration polarization, on the FO and RO process performance were examined. Moreover, the optimum operating conditions were explored to minimize the energy consumption.

5. Results and discussion

The FO and RO process parameters and operating conditions that were used in this study are presented in Table 1. They were obtained from literature [9,10]. $L_{s_{-b}}$ of the FO membrane was assumed to have been the same as that of the RO membrane and the geometry of the FO membrane element was assumed to have been the same as that of the RO element.

Fig. 3 shows the simulation results for the optimum operating conditions of the FO and RO process, which were explored to minimize energy consumption and sufficient boron rejection (less than 1.0 mg/L) for seawater desalination. The FO process has the same permeate flow rate, feed water temperature, and feed water TDS conditions as the RO process. In this simulation, the required feed pressure was 61.0 bars in the RO process, and the concentration of the draw solution was 6 M in the FO process. Due to internal concentration polarization, though having the Lv that is similar to RO, FO process required high concentration draw solution. The recovery (40% vs. 55%) and water flux (11.2 L/m²-h vs. 16.2 L/m²-h) of the FO process were higher than those of the RO process. Moreover, the specific energy of the RO system was significantly higher than that of the FO system (3.25 kWh/m³ vs. 1.16 kWh/m³). The energy efficiency of the FO process that was used in this program was obtained from literature [11]. But the FO process has much larger permeability to NaCl than RO process (487 mg/L vs. 292 mg/L). This implies that the FO process may require another process to sufficiently reject salt.

Fig. 4 shows the simulation results for the FO and RO process in a spiral wound module. Under similar operating conditions, the recovery (39.1% vs. 54.8%) and water flux (11.4 L/m²-h vs. 16.2 L/m²-h) in the FO process were much higher than those in the RO process. The permeate TDS of the RO process was significantly lower than in the FO process (218 mg/L vs. 478 mg/L), though. The first element showed the highest flux (34.0 L/m²-h), but the flux was significantly reduced in the elements near the outlet. This is attributed to the increased feed solution concentration and the decreased draw solution concentrations, which resulted in the decrease in the effective osmotic pressure. A significant decrease in flux from each element was also observed in the RO process.

Table 1

Process parameters and operating conditions

Parameter	FO	RO
$L_{v'}$ m ² -s/kg	4.2×10 ⁻¹² [10]	3.6×10 ⁻¹² [9]
$L_{s'}$ m/s	4.5×10 ⁻⁸ [10]	1.96×10 ⁻⁸ [9]
$L_{s,b'}$ s/m	5.3×10 ⁻⁷ [9]	5.3×10 ⁻ 7 [9]
$k_{\rm F'} {\rm s/m}$	1.25×10 ⁵ [10]	_
Geometry	The same as an 8040 element	The same as an 8040 element
Feed NaCl concentration, mg/L	35,000	35,000
Draw solution	Ammonium carbon dioxide (2–6 M)	_
Temperature, °C	25	25

Fig. 5 shows the simulation results for the FO-RO hybrid process of seawater desalination. It was calculated that the FO-RO hybrid process has higher recovery (66.7%) with reasonable flux (13.1 L/m²-h) and permeate concentration (389 mg/L) than the FO and RO process. Thus, the advantages of the FO-RO hybrid process over the FO and RO system are its low permeate concentration and high recovery, which are difficult to attain in the FO and RO process, respectively.

6. Conclusions

In this study, a computer program for simulating and optimizing the FO, RO, and FO-RO hybrid process was developed using the MATLAB-GUI program. The program can make predictions of any operating and performance parameter of the FO, RO and FO-RO hybrid process. Under similar operating conditions, it was calculated that the FO process has higher flux and recovery than the RO process. But the permeate TDS of the FO process was significantly higher than in the RO process and FO process required high concentration draw solution due to internal concentration polarization. The FO-RO hybrid process performed better than the FO and RO process. This program is useful to test the developed FO membranes and design of the FO and FO hybrid process. Further studies are required to find the optimum configurations of FO and RO for various applications.

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a) FO optimization



b) RO optimization

Fig. 3. Simulation results for the optimum operating conditions of the FO and RO process.



a) FO process



b) RO process

Fig. 4. Simulation results for the FO and RO process in the spiral wound module.



Fig. 5. Simulation results for the FO-RO hybrid process of seawater desalination.

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