Full Paper

SOLUTION-DIFFUSION MODEL FOR A SMALL SCALE REVERSE OSMOSIS SYSTEM

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Graphical abstract
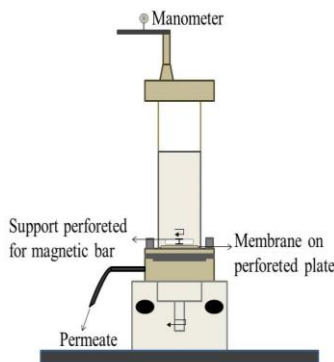
Abstract

Reverse osmosis (RO) often used for desalination, in producing the ultrapure water for electronics, pharmaceuticals and power generation industries and also it was used in small niche process such as food processing and pollution control. Analysis of membrane performance required multiple of experimental run. Experimental work can be time consuming and costly. Hence, this work aims to model a small scale RO system by using a solution-diffusion model to minimize the experimental work. The model was verified by comparing the data obtained from the model and experimental data. Other studies, which include, the influence of solute feed concentration on the RO system was also been investigated. A commercial RO Trisep flat sheet membrane was used. The solute permeate concentrations, solvent permeate flux, final solute feed concentrations and rejection rate of sodium chloride (NaCl) was analyzed to observe the membrane performance. Result shows that some experimental data has almost similar trend with the simulated data. Both solute feed concentration and rejection rate of NaCl over time show almost similar trends with percentage errors are 8.89% and 0.76% respectively. As solute feed concentration increased, the solute permeate concentration increased. In contrast to the solute permeate concentration, when the solute feed increases the solvent permeate flux decreases and rejection rate will also decrease.

Keywords: Reverse osmosis, solution-diffusion model, mathematical modeling, membrane, sodium chloride

1.0 INTRODUCTION

Reverse osmosis (RO) is a membrane separation technology that uses a semi-permeable membrane. RO separates solvents by retaining the solutes on the high solute concentrations side while allowing the pure solvents to pass through the membrane to the side with low solute concentrations [1]. RO system is mostly used for seawater and brackish desalination. Besides, RO has been demonstrated to have lower energy requirements compared to multistage flash evaporation [2]. In the last two decades, hundreds of RO seawater desalination plants have been built worldwide [3]. Besides desalination, RO is also used to produce ultrapure water for the electronics, pharmaceuticals, and power generation industries

and used in small niche process such as food processing and pollution control [4].

The mechanism of permeations can best be described by two models: (1) pore flow model, and (2) solution-diffusion model. In pore flow model, separation is done according to the size of the permeates in which the permeates that are smaller than the pore of the membranes will pass through the membrane and vice versa. In 2002, Idris and his co-researchers apply the surface force-pore flow model in order to determine the pore size of a membrane [5]. In solution-diffusion model (Figure 1), permeates dissolve in the membrane material and then diffuse through the membrane. In this model, permeates are separated according to their solubility in the membrane and the difference in diffusion rate. This model often used to describe the transport

mechanism in RO system [6]. The permeation in RO is determined by the polarity and solubility in the membrane polymer. The polarity of organic solutes can be influenced by (1)the hydrogen bonding ability, (2) the dissociation constant pKa and (3) the Taft of Hammett number [7]. The driving force for the solubility is often connected to the hydrogen bonds as well as the Debye and dispersing interaction [8].
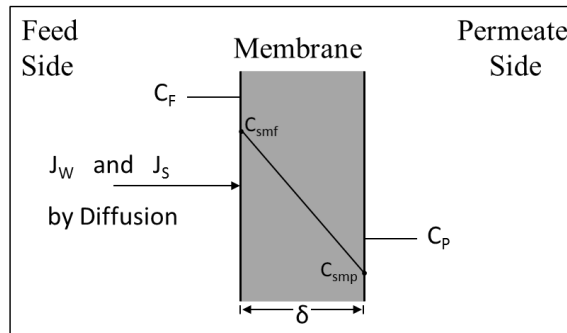
Figure 1 Schematic diagram of a solution-diffusion type membrane [7]

The solution-diffusion model assumes that [9]: (1) the RO membrane has a homogenous, nonporous surface layer, (2) both the solute and the solvent dissolve in this layer and then each diffuse across it, (3) the solute and solvent diffusion is uncoupled and due to its own chemical potential gradient across the membrane, and (4) these gradients are the result of concentration and pressure differences across the membrane. The advantage of solution-diffusion model is that only two parameters are needed to characterize the membrane. Because of this, the solution-diffusion model has been applied widely to both inorganic salt and organic solute system.

Analysis of membrane performance requires multiple experimental runs. Every run of experiments requires chemicals, membranes, and also time consuming. Chemicals and membranes are often expensive. Hence, a mathematical modelling is proposed to eliminate these limitations. From previous research, many mathematical models were developed. This mathematical model was used to describe the behavior of RO process [1, 10, 11]. By using this model also, the performance of the RO system can be predicted. The verification of the model is done by comparing the data obtained from the model and experimental data.

Thus this study aims is to investigate the effects of concentrations of feed on the RO system, to verify the solution-diffusion model by comparing the model with the experimental data and to predict the performance of the membrane as a function of time.

2.0 METHODOLOGY

A model is proposed in order to predict the performance of a RO system. The proposed model is combined with material balances on the feed tank, membrane module and product tank with membrane mass transfer models. The solution-diffusion model is used in this case representing membrane mass transfer models because only two parameters are needed in order to characterize the membrane system. Non-linear differential equations representing the feed concentration as a function of operating time is obtained. The non-linear equations are then solved using the fourth order Runge-Kutta method because of its advantages of self-starting and stability [3]. To verify the model, an experimental data is used to compare the data obtained from the model. Using the verified model, the effects of the feed concentration can easily be analyzed.
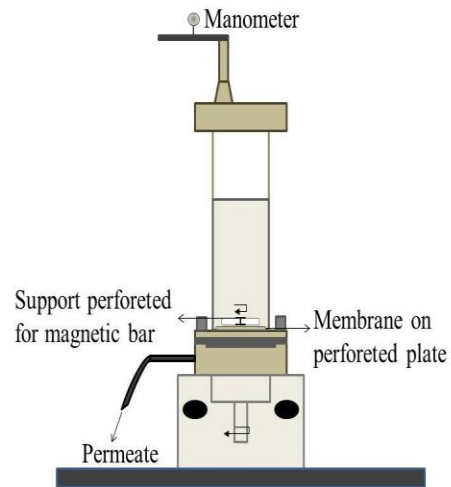
Figure 2 Experimental setup of dead-end filtration

Figure 2 shows a dead-end filtration unit that will be used in this analysis. The RO membrane will be located on the perforated plate for stirring purposed. The permeate concentration, C_p will be measured from the sample collected from the permeate stream. From experiment, some data can be calculated.

Solvent Flux,
$$J_w = (Q_p/S_a)\ C_{wp} \qquad \text{(Equation 1)}$$

where, J_w is solvent flux (kg/m^{2}hr), Q_p is volumetric production rate of permeate (m^3/hr), S_a is membrane surface area (m^2) and C_{wp} is concentration of solvent (water) in permeate (kg/m^3).

Solute concentration in permeate,

$$C_p = (J_s C_{wp})\ /\ J_w \qquad \text{(Equation 2)}$$

where, C_p is permeate concentration (kg/m^3) and J_s is solute flux, it depends on concentration gradient (kg/m^{2}hr)

Membrane rejection,

$$R = (1 + ((B_s C_{wp})/A_w + (\Delta P - \Delta\pi)))^{-1} \quad \text{(Equation 3)}$$

where, B_s is solute permeability constant (m/hr), A_w is solvent (water) permeability constant, it depends on membrane structure (h/m), ΔP = Hydraulic pressure applied across the membrane (kg/m h^2) and $\Delta\pi$ = Osmotic pressure difference of the solution on the feed and permeate side (kg/m h^2). Since it is a batch system, eventually the feed volume will be run to exhaustion and feed concentration can only be measured in the beginning and at the end of the experiment. Raw data from the experiment are given in appendix.

3.0 RESULTS AND DISCUSSION

Figure 3(a) shows graph of solute permeate concentrations versus time. The solute permeates concentrations increases over time. This is due to the increases in concentration of solute at upstream [2] and the increases of osmotic pressure, which ultimately decreases the driving force for mass transfer and product flux [11]. Hence, as the solute feed concentration increases, the driving force will also increases with time and leads to the increases in solute permeate concentration. In Figure 3(b) it can be seen that the solvent permeate flux decreases as the time increases. This is because of the permeate concentration polarization phenomenon. The concentration polarization occurs when the solute concentration in feed is higher compared to concentration of solvent. So, large amount of solute will form at the surface of a membrane than in the bulk solution and block the solvent from pass through the membrane [12]. Higher solute feed concentration also will increase the solute osmotic pressure. Hence, the solvent flux will decrease as well as decreasing of driving force for mass transfer of solvent [13]. This trend is similar with a journal [14] that using same feed solution on thin-film composite (TFC) membrane. It reported that as the NaCl concentration increases, the water flux decreases because of the increases of osmotic pressure. The increases of osmotic pressure cause the driving force for the mass transfer decreases and lower the water flux [15].

Figure 3(c) shows graph of rejection rate of sodium chloride (NaCl) over time. From the graph, it shows that feed with solute concentrations of 1.0 kg/m^3 has the highest rejection rate. This is because feed with low solute concentration has low solute driving force in feed side. Hence, only small amount of solute will pass through the membrane and result in higher rejection rate of solute. This trend of data can be found in a journal [10] where when feed concentration of NaCl increases, the rejection rate decreases slightly due to the increasing of osmotic pressure.
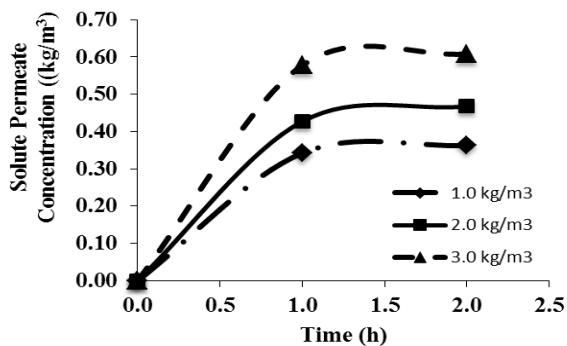
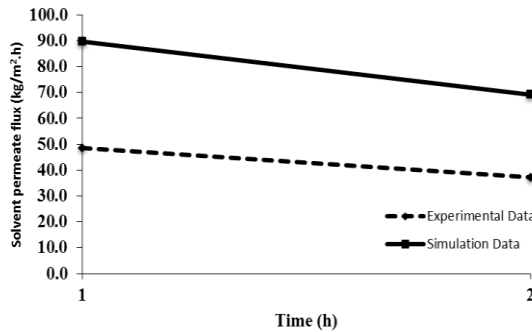(a) Solute permeates concentration
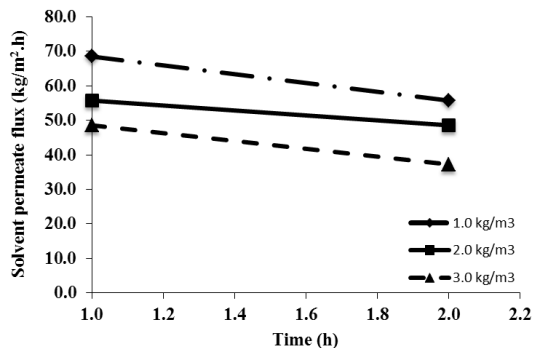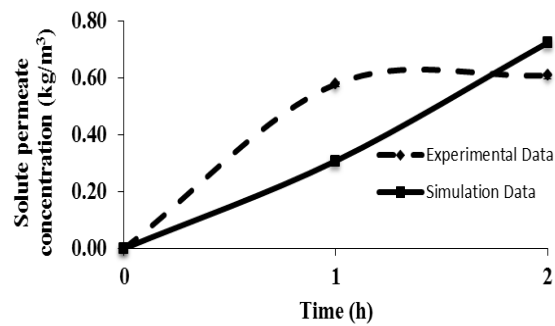

(b) Solvent permeates flux
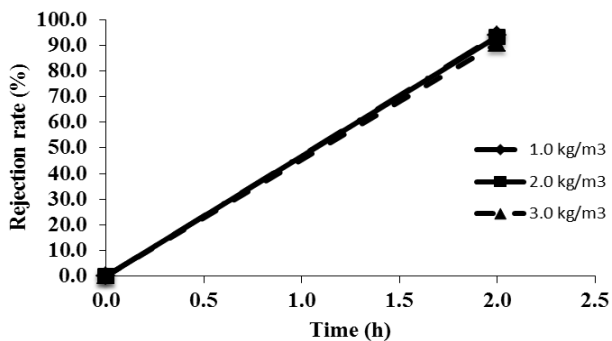
(c) Rejection Rate

**Figure 3** Effect of different concentration on membrane performance

Figure 4(a) shows that as time increased, the solvent permeate flux decreased. The simulation data also suggest similar trend. Even though both plots showed the same behaviour, the experimental value has a lower value compared to the simulation data. Figure 4(b) shows a graph of experimental data and simulation data of solute permeate concentration over time. Both experimental data and simulation data shows that as time increased the solute permeate concentrations increased. The experimental results are in closed match with the simulation data with average percentage error of 13.92%.

Figure 4(c) shows a graph of experimental data and simulation data of solute feed concentration over time. The experimental data for the solute feed concentration is in a good agreement with the model with average percentage error of 8.89%. Figure 4(d) shows a graph of experimental data and simulation data of rejection rate of sodium chloride (NaCl) over time. The experimental data and simulation data fitted almost with average percentage error of 0.76%.
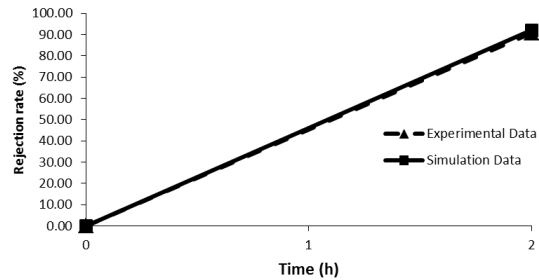

(a) Solvent permeates flux

(b) Solute permeates concentration
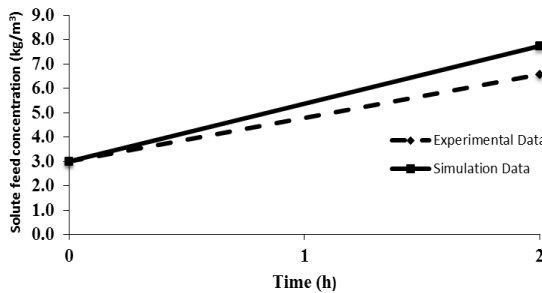
(c) Solute feed concentration

(d) Rejection rate of NaCl

Figure 4 The comparison of membrane performance between experimental data and simulation data

4.0 CONCLUSION

The solution diffusion model has been successfully employed to investigate the effect of various feed concentration and also to predict the membrane performance. In this study, it indicates that some experimental data has almost similar trend with simulation data while the others need more improvement. The verification of similarity between those data can be identified by calculating the percentage error. Both solute feed concentration and rejection rate of NaCl over time give almost similar trends with percentage errors are 8.89% and 0.76% respectively. As solute feed concentration increased, the solute permeate concentration increased. In contrast to the solute permeate concentration, when the solute feed increases the solvent permeate flux decreases and rejection rate will also decrease. Experimental data was use to verify the model and was then used to predict the membrane performance as a function of time. The RO system performance was modelled using the solution-diffusion model.

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APPENDIX

Raw Data from Experiment

Table 1 Solute permeate conductivity and concentrations at solute feed concentrations of 1.0 kg/m^3

Time (h)	Conductivity (mS)			Concentration (kg/m^3)			
	1	2	3	1	2	3	Average
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	0.8300	0.8200	0.8100	0.3466	0.3424	0.3382	0.3424
2	0.8600	0.8700	0.8800	0.3591	0.3633	0.3674	0.3633

Table 2 Solute permeate conductivity and concentrations at solute feed concentrations of 2.0 kg/m^3

Time (h)	Conductivity (mS)			Concentration (kg/m^3)			
	1	2	3	1	2	3	Average
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	1.0400	1.0200	1.0100	0.4342	0.4259	0.4217	0.4273
2	1.1200	1.1000	1.1400	0.4676	0.4593	0.4760	0.4676

Table 3 Solute permeate conductivity and concentrations at solute feed concentrations of 3.0 kg/m^3

Time (h)	Conductivity (mS)			Concentration (kg/m^3)			
	1	2	3	1	2	3	Average
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	1.4000	1.3600	1.3900	0.5846	0.5678	0.5804	0.5776
2	1.4800	1.4300	1.4600	0.6180	0.5971	0.6096	0.6082

Table 4 Solute feed conductivity and concentrations in the beginning and the end of experiments at solute feed concentrations of 1.0 kg/m^3

Time (h)	Conductivity (mS)			Concentration (kg/m^3)			
	1	2	3	1	2	3	Average
0	2.44	2.49	2.45	1.0188	1.0397	1.0230	1.0000
2	14.37	14.33	14.22	6.0000	5.9833	5.9374	5.9736

Table 5 Solute feed conductivity and concentrations in the beginning and the end of experiments at solute feed concentrations of 2.0 kg/m³

Time (h)	Conductivity (mS)			Concentration (kg/m³)			
	1	2	3	1	2	3	Average
0	5.00	5.03	4.98	2.0877	2.1002	2.0793	2.0000
2	15.48	15.50	15.45	6.4635	6.4718	6.4509	6.4621

Table 6 Solute feed conductivity and concentrations in the beginning and the end of experiments at solute feed concentrations of 3.0 kg/m³

Time (h)	Conductivity (mS)			Concentration (kg/m³)			
	1	2	3	1	2	3	Average
0	7.35	7.30	7.25	3.0689	3.0480	3.0271	3.0000
2	15.80	15.75	15.69	6.5971	6.5762	6.5511	6.5748