Controlling Water Quality using Reverse Osmosis: The Development of Simplified Dynamic Model

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Abstract: Reverse osmosis (RO) is a compact process for the removal of ionic and organic pollutants from contaminated water. This study deals with the development of dynamic model for tubular reverse osmosis unit. The proposed model describes the unit as a series of single tubes, each tube is described by two ordinary differential equations (ODE) and the whole module is to be described by sets of differential algebraic equations. The tubes are modeled and solved sequentially where the output of any tube becomes the input for the next one. The predictions of steady state and dynamic models are in good agreement with the experimental results of a lab scale RO unit. This model is simpler than the currently used distributed models; besides it gives more insight than black box models. This model can be used to improve the understanding of RO processes as well as to develop different model-based control algorithms for this process.

1. INTRODUCTION

Many mathematical and mechanistic models have been developed to describe reverse osmosis membranes (RO). Some of these models rely on relatively simple concepts while the others are more complex and require sophisticated solution techniques. Models that adequately describe the performance of the reverse osmosis membranes both dynamically and at steady state are required in designing RO processes and developing different model-based control algorithms as well. Models that predict separation characteristics also minimize the number of experiments that must be executed to describe a particular system.

While the results of the steady state analysis are of significant value, knowledge of the unsteady state behaviour becomes important in starting up the system and in controlling the quality of the concentrated stream leaving the system. Generally, in the literature, there are two approaches to develop dynamic models for RO processes. In the first approach, input-output transfer functions are developed by introducing either a step or an impulse changes in pre-specified inputs and monitoring process outputs (Alexiadis et al., 2006, Burden et al., 2001, Assef et al., 1997, Alatiqi et al., 1989). While the input-output (black-box) modeling approach is practical for many control applications, the developed transfer functions do not reflect the physical structure of the process; instead they reflect only the input-output relationship of the process.

The second approach to the dynamic modeling of RO processes consists in the development of theoretical models that are based on first law principles. Membrane processes are distributed parameter systems for which the state variables (e.g concentration) would vary with both axial and radial directions besides its variations with time. The resulted models are partial differential equations (PDEs) in time, and in one or two space positions. The complexity of these models depends on the nature of assumptions used and the level of rigor in the modelling. Unlike the input-output models, the theoretical models give physical insight into the process. However, there are few studies in the literature on the development of theoretical dynamic models for RO processes. Most of these recent studies rely on the use of computational fluid dynamics (CFD) (Fletcher and Wiley, 2004, Wiley and Fletcher, 2002). While CFD models predict well the responses as functions of both time and spatial location, they require significant computational time and thus would be too slow to use for on-line control.

The objective of this contribution is to propose a simple dynamic model for a tubular RO process. This model is based on the idea developed by Harris and coworkers (Harris et al., 1976) who used well-known physical laws of conservation to develop a steady state model. This model is modified, in this work, so that it can be used to study the dynamic behaviour of the tubular modules. Moreover, model predictions are verified experimentally. The developed model is rigorous enough to give detailed insight into the reverse osmosis process. But, the model is simple enough so that it can be implemented in designing different control algorithms.

2. MODEL DEVELOPMENT

Here the process consists of a membrane module where a number of RO tubes are connected in series. To model the dynamic behaviour of the module, it is divided into axial increments, Δx, as shown in Fig. 1. Each increment is treated as separate membrane tube with constant permeate flux, tube-side pressure and velocity. The increments are modeled and solved sequentially, e.g. the output of increment j becomes the input for the next increment, j+1. The following

assumptions have been made in the development of our model:

1. The solution contains only one solute and one solvent (binary solution).

2. The water permeability, L_p, is constant and is independent of pressure.

3. The flow inside the tubes is turbulent.

4. The polarization at the surface of the membrane is described by Nernst film model.

5. The osmotic pressure can be represented by the van't Hoff equation.

6. On permeate side; mixing is prefect in the radial direction.

7. Axial diffusion and angular effects (e.g. due to natural convection) are ignored.

8. Radial pressure drop is negligible.

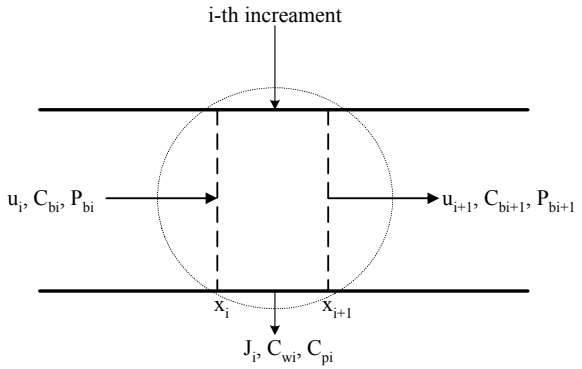

Fig.1. Sketch of reverse osmosis module.

2.1 Governing Equations

The permeate flux (J_{vi}) is described by the three parameter nonlinear Spiegler-Kedem (SK) model, at the i-th increment it is given by (1)

$$J_{v,i} = L_p\left[(p_{b,i} - p_{p,i}) - (R_j^{'})^2 \nu RTc_{w,i}\right] \tag{1}$$

The wall brine concentration at the i-th increment can be calculated using the following equation

$$c_{w,i} = c_{b,i} \cdot \frac{\exp\left(\frac{J_{v,i}\cdot Sc^{2/3}}{j_i \cdot u_i}\right)}{R_j^{'} + (1-R_j^{'})\cdot \exp\left(\frac{J_{v,i}\cdot Sc^{1/3}}{j_i \cdot u_i}\right)} \tag{2}$$

where j_i is Chilton-Colburn factor. For turbulent flow in smooth circular tubes it is given by Bird et al. (2002)

$$j_i \cong 0.0395\,Re_i^{-1/4} \tag{3}$$

Note that the calculation of J_{vi} is not possible unless the wall concentration is known. At the same time, c_{wi} requires j_{vi} in order to be calculated. Thus, an iterative calculation procedure is required to estimate J_{vi}.

To obtain salt concentration in the brine leaving increment i, a dynamic salt balance about this increment is carried out. The resultant concentration is given by the following equation

$$\frac{dc_{b,i+1}}{dt} = \left(\frac{u_i \cdot c_{b,i}}{\Delta x}\right) - \left(\frac{u_{i+1}\cdot c_{b,i+1}}{\Delta x}\right) - \left((1-R_j^{'})\cdot \frac{4J_{v,i}}{d}\right)\cdot c_{w,i} \tag{4}$$

The velocity of the brine leaving increment i, u_{i+1}, can be obtained from a volumetric balance about the i-th increment which gives

$$u_{i+1} = u_i - 4J_{v,i}\Delta x / d \tag{5}$$

Pressure dynamics in the brine side, for increment i, can be calculated by using the energy balance about that increment. Assuming that the tubes are horizontal and the RO module is isothermally operated, it can be proved that pressure dynamics in the brine side is given by (6).

$$\frac{dp_{b,i+1}}{dt} = \frac{u_i}{\Delta x}\cdot\left(p_{b,i} + 0.5\cdot 10^{-7}\cdot \rho_{b,i}\cdot u_i^2 - 2\cdot 10^{-7}\cdot f_F \cdot \Delta x \cdot u_i^2 \cdot \frac{\rho_{b,i}}{d}\right) - \frac{u_{i+1}}{\Delta x}\cdot\left(p_{b,i+1} + 0.5\cdot 10^{-7}\cdot \rho_{b,i+1}\cdot u_{i+1}^2\right) - \left(\frac{4\cdot J_{v,i}}{d}\right)\cdot\left(p_{b,i} + 0.5\cdot 10^{-7}\cdot \rho_{p,i}\cdot J_{v,i}^2\right) \tag{6}$$

with f_F is Fanning friction factor, given by

$$f_F \cong 2\cdot j \tag{7}$$

The permeate production rate for the i-th increment is given by

$$q_i = J_{v,i}\cdot \pi \cdot d \cdot \Delta x \tag{8}$$

Summing up the permeate production rate from all increments gives the cumulative permeate production rate which is defined by

$$q = \sum_{i=1}^{n} J_{vi}\cdot \pi \cdot d \cdot \Delta x \tag{9}$$

The cumulative average salt concentration of the product water can be obtained by multiplying the quantity of water produced in certain increment by the salt concentration in that increment. Rearranging the resulted equation gives

$$c_{p,i} = c_{p,i-1}\cdot \frac{\sum_{i=1}^{n-1} q_i}{q} + \frac{(1-R_j^{'})\cdot c_{w,i}\cdot J_{v,i}\cdot \pi \cdot d \cdot \Delta x}{q} \tag{10}$$

3. PILOT-SCALE EXPERIMENTAL SET-UP

A schematic of the RO unit (SOLTEQ) is shown in Figure 2. The unit comes with a pair of tubular polyamide membrane film (Micro 240 module) with a cross flow configuration. In addition to the module, the RO unit consists of feed tank, product tank and a hot water tank. The feed tank is connected

to a high pressure plunger pump while the hot water tank has a centrifugal pump. The maximum design pressure is 64 bar

Membrane characteristics and operating conditions are listed in Table 1.

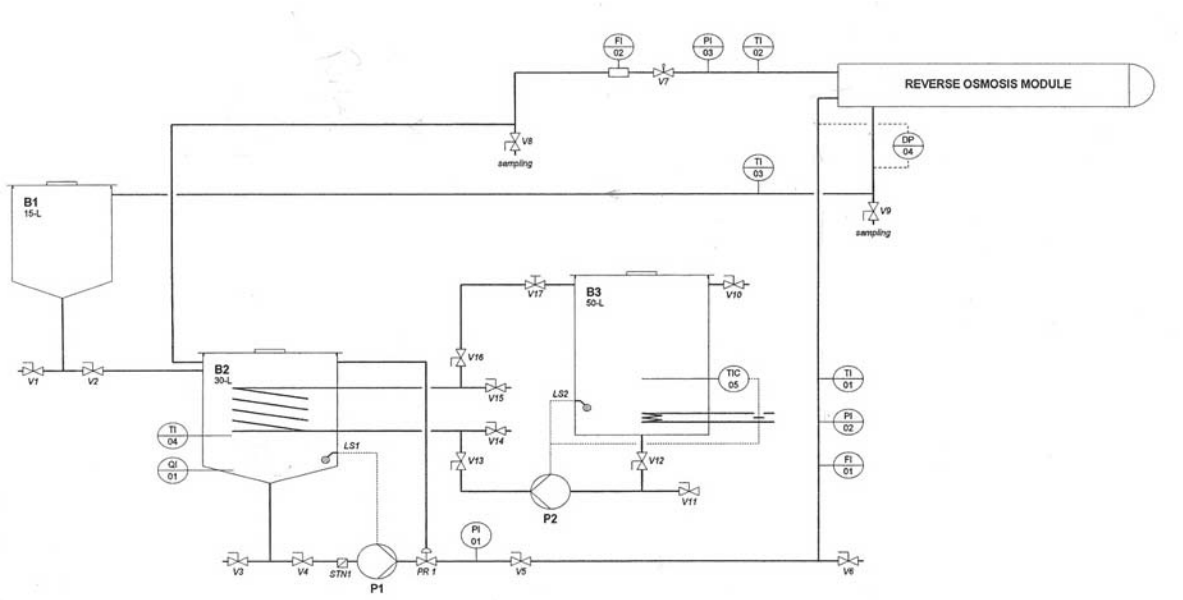

Fig.2. Process schematic.

and temperature is 80 ^{o}C. The data were collected in intervals of 5 seconds. Temperature was measured using on-line probe and the inlet and outlet operating pressures were measured using on-line pressure gauges. Feed and brine concentrations were measured employing conductivity meter.

The feed tank has the capacity for one run. After each run it is drained of excess feed and filled with tap water. Then the unit is flushed with tap water to remove brine from the membrane chambers. After flushing, all lines are closed until the next run.

The start up procedure for each run is as follows. First, the NaCl solution is prepared by mixing a known quantity of NaCl with tap water. Next, the control valves are opened to predetermined positions to set the flow pressure, and trans-membrane pressure. Then, the feed pump is started and the control valves are adjusted to obtain the desired flow pressure, and trans-membrane pressure. Generally, it takes around a minute until the flow rate is stable. The unit is maintained at the steady state conditions for about five minutes, and then readings can be taken. Note that transient measurements are taken directly after starting up the pump.

3. RESULTS AND DISCUSSION

The dynamic model developed in the previous section is first validated at steady state against experimental data. For given experimental conditions, steady measurements were taken after approximately 5 min. The permeate and the brine were recycled to the feed tank in order to keep the feed concentration constant. Then at a given feed velocity and an initial concentration, the permeate flux of the solutions, J_v, was measured under various trans-membrane pressures.

Table 1. Input conditions

Parameter	
Membrane characteristics	
Membrane diameter (cm)	1.25
Membrane length (cm)	60
Operating conditions	
Ambient temperature (°C)	30
Feed pressure (bar)	35
Feed solute concentration (ppm)	2000
Inlet velocity (cm/s)	6.8

Fig. 3 shows the variations of the permeate flux with the trans-membrane pressure. This pressure was varied up to a value of 20 bars. The figure shows reasonable agreement between the experimental values and the models predictions. The values of flux are in the order of 10^{-5} m/s. The figure also shows that the higher the trans-membrane pressure, the higher the flux. This is due to the increase in the driving force (difference between feed pressure and osmotic pressure) with the feed pressure. Operating at high pressures for the feed stream also yields better product quality (lower salt concentration of the permeate). The disadvantage of using high values of feed pressure is the additional pumping cost. It can be noted that the experimental values could be fit by a straight line with a correlation coefficient R^2=0.96. It is worth mentioning that this linear dependency clearly indicates that the resistance due to the concentration polarization was too small in these experiments.

Fig. 4 shows the time variations of the brine concentrations at the feed rate of 6.8 cm/s for different positions inside the module. The figure shows that the RO process approaches steady state rather quickly after permeation begins. In this work, nominal residence time based on inlet velocity ranged from 4.4 to 26.1 sec. It should be noted that only the variations of the brine concentrations at the exit of the membrane module could be compared against the experimental data. The brine concentration at the end length of the membrane is seen to increase from 2000 to 2180 and reaches a steady state value at around 20 seconds. The figure shows reasonable agreement with the experimental results.

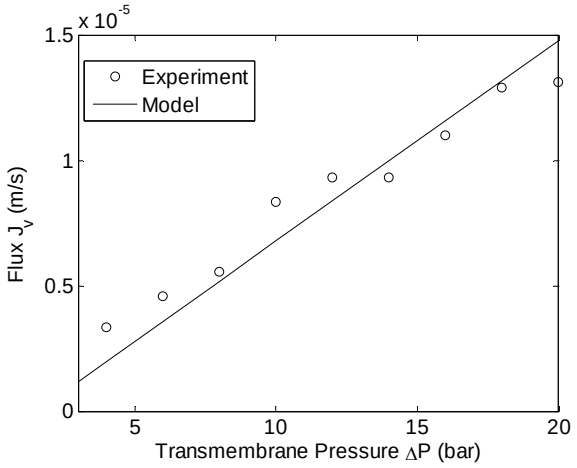

Fig.3. Steady state model validation.

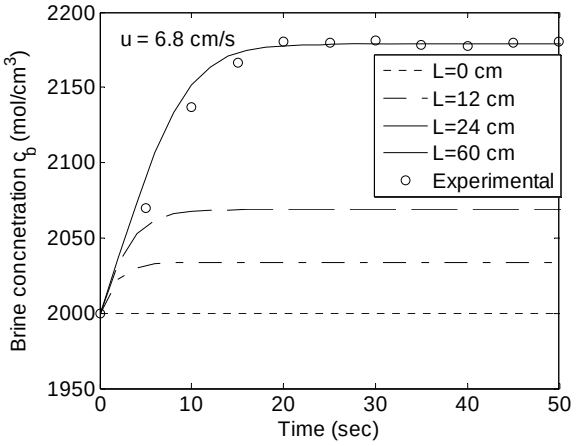

Fig.4. Dynamics of brine concentration at different axial locations inside membrane tube.

Fig. 5 shows the effect of a 10% step response in the feed flow rate (i.e. inlet velocity), which is stepped at t = 50 second, from 0.5 to 0.55 m^3/s. It can be seen that the brine concentration at the different positions decreases and reaches a new steady state in around 20 seconds. The increase in the inlet velocity reduces the amount of accumulated salt on the membrane surface. If the concentration at the membrane surface is reduced, the osmotic pressure will decrease, which results in an increment in the flux. However, as more fluid is brought to the membrane surface with the increased flux and more salt is rejected, the concentration of salt at the surface re-accumulates until the new steady-state flux is reached. This work will be extended to implement this model in developing nonlinear model predictive controller (NLMPC) to regulate both permeate quality and quantity through manipulating feed pressure and brine flow rate.

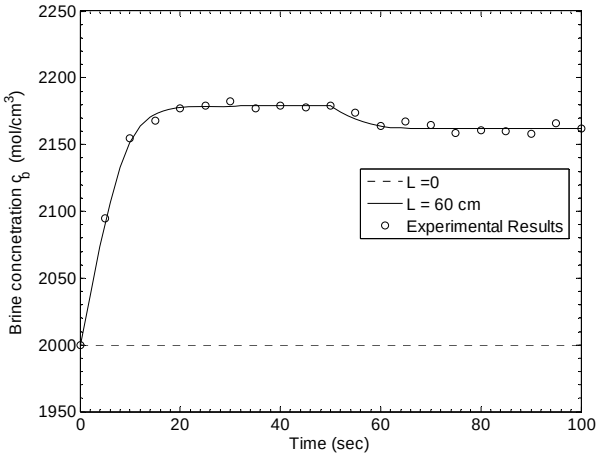

Fig.5. Dynamic response for 10 % positive step change in the feed rate.

4. CONCLUSIONS

A dynamic model for tubular membranes was developed in this study. The proposed model considers the unit as a series of single tubes with appropriate minor pressure losses introduced between them. Each tube is described by coupled algebraic-ordinary differential equations. The tubes are modeled and solved sequentially where the output of any tube becomes the input for next tube. Both steady state and dynamic behaviors were validated against a lab scale experimental unit. The developed model can be used to study the effect of various operating parameters such as the feed flow rate, feed concentration and feed pressure. Besides, this model can be used to design different model-based control algorithms to control the RO process. This model is developed for pilot-plant scale set-up. To use the model to describe industrial RO processes, the model has to be modified to describe the effect of fouling on different process variables. This will be the next step in this research.

ACKNOLWDGEMENT

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NOMENCLATURE

c_b	Salt concentration in brine	mol/cm^3
c_p	Salt concentration in permeate	mol/cm^3
c_w	Salt concentration at the wall	mol/cm^3
f_F	Fanning friction factor	-
J_v	Volume flux density through membrane	cm/s
j	Chilton-Colburn factor	-
L	Membrane length	cm
L_p	Hydraulic permeability	cm/s atm
P_B	Brine pressure	MN/m^2
P_F	Feed pressure	MN/m^2
P_P	Permeate pressure	MN/m^2
q	Permeate production rate	cm^3 /s
R	Universal gas constant	cm^{3}atm/K.mol
R'_j	Intrinsic salt rejection coefficient	-
Re	Reynolds number	-
Sc	Schmidt number	-
T	Operating temperature	ºK
u	Brine average velocity	cm/s
Δx	Tube length	cm
Greek		
η	Viscosity	Pa.s
ν	Number of ions produced on complete dissociation of one molecule of electrolyte	-
ρ_b	Brine density	g/cm^3
ρ_p	Permeate density	g/cm^3
Subscripts		
i	Segment number	-

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