Simulations of Full-Scale Reverse Osmosis Membrane Process

Lianfa Song¹; Seungkwan Hong²; J. Y. Hu³; S. L. Ong⁴; and W. J. Ng⁵

Abstract: Performance of a two-stage full-scale reverse osmosis (RO) process for a desalination plant in Florida was simulated with a mathematical model based on the principles of membrane transport and mass conservation. In this model, water flux at any point along the filtration channel is calculated locally according to the basic transport theory of RO membranes. The changes in cross-flow velocity and salt concentration along the filtration channel were determined using mass balance principles of water and salt. Simulations of the plant performance were compared with the in-plant observation data over a period of more than 300 days. The results showed that the model could adequately describe the performance of the full-scale RO process based on a few module and operating parameters. The study also revealed that salt rejection of a RO membrane changed with feed salt concentration. The osmotic pressure coefficient that fits best with performance of this plant was substantially lower than the value determined with the “rule of thumb” (i.e., osmotic pressure in psi=0.01×total dissolved solids in mg/L) and had to be determined specifically for the particular feed water being processed.

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Introduction

Water reclamation and desalination with a reverse osmosis (RO) membrane have gained increasing popularity in many regions over the world as traditional resources of drinking water are diminishing in quantity and/or deteriorating in quality (Beverly et al. 2000; Taylor and Hong 2000). It is estimated that about 80% of the installed capacity of water desalination in North America comes from RO processes (Morin 1994). Although both spiral-wound (SW) and hollow fine-fiber (HFF) RO membranes are commonly used in drinking water production, spiral-wound elements are by far the predominant configurations of RO membranes for drinking water production (AWWA 1999). Spiral-wound modules are less susceptible to membrane fouling and are easier to clean when they are severely fouled (Taylor and Jacobs 1996).

Several spiral-wound elements in series, held in a cylindrical pressure vessel, are usually used in water reclamation and desalination applications. The purpose of such arrangement is to achieve a high recovery in a single stage configuration (≥50%) (Wilbert et al. 1998). Due to the high recovery, cross-flow velocity, and salt concentration vary substantially along a long filtration channel. Furthermore, owing to the increase in osmotic pressure, permeate velocity can be much smaller in the last few elements than those in the beginning of a pressure vessel. This phenomenon is termed as a “hydraulic unbalanced problem” and is an important feature of the RO membrane processes used for low salinity feed waters (Wilf 1997). The variations of these variables should be considered for accurate prediction of RO treatment plant performance (Van der Meer et al. 1998).

The RO process in water reclamation and desalination are usually treated as a homogeneous system that can be adequately simulated with simple membrane transport theories (Slater and Brooks 1992; Wilf and Klinko 1994). In a homogeneous system, all process parameters, such as cross-flow velocity and salt concentration, are treated as constant throughout the filtration channel (see Fig. 1). Permeate velocity of the whole RO process is simply determined by the net driving pressure divided by the membrane resistance. As a result, this simulation method is only applicable to small flat membrane cells within which the variations of salt concentration and other parameters are negligible. The intrinsic limitation of the method makes it impossible to accurately simulate a full-scale RO process in water reclamation and desalination, where salt concentration and other parameters vary substantially along the filtration channel. Marinas and Urania (1996) noted the importance of the localized system parameters of a RO process in a study on solute transport through RO membranes. Further efforts are needed to incorporate the localized parameters for a more accurate simulation of the RO process in water reclamation and desalination.

The objective of this study is to present a new simulation method for the performance of a full-scale RO process based on the localized variables. Observation data of a full-scale RO membrane system in the Jupiter Water Treatment Plant in Florida are used to demonstrate the superiority of the new method. For this
purpose, an overview of Jupiter Water Treatment Plant is first provided. Then, the performance of a full-scale RO process is simulated and compared with the in-plant observations. Finally, the significance of a few key parameters of the full-scale RO process is discussed.

Jupiter Water Treatment Plant

The City of Jupiter, located in southeastern Florida, operates a 9 MGD RO water treatment facility. The source water for this facility is drawn from the Floridan Aquifer, 1,200–1,600 ft below the ground surface. Ten wells, with a full capacity of 21.1 MGD, provide this facility with a consistent supply of source water throughout the year. The raw water drawn from all wells flows into a common pipe and is transported to the treatment facility.

Upon arrival, the water is split between two independent membrane systems, bank 1 at 6.0 MGD and bank 2 at 3.0 MGD. Both banks provide similar physical and chemical pretreatment to the raw water prior to membrane filtration. Unlike other typical membrane treatment facilities, the chemical pretreatment for the Jupiter water system consists solely of the continuous dosing of 3.0 mg/L Flocon 100, a commercially available polyacrylic antiscalant. Following antiscalant addition, the water is passed through ten banks of prefilters, equally divided between banks 1 and 2. Each prefilter bank houses a total of 425 commercial filters-polypropylene wound polycore microfilters, with a nominal pore size of 5.0 μm. To avoid excessive head loss and to ensure proper pretreatment, these microfilters are replaced regularly once every three months.

After the source water has been pretreated, it is pressurized by a total of six (four for bank 1 and two for bank 2) vertical turbine pumps. The pressurized water is then transported to the membrane systems of banks 1 and 2. Bank 1 consists of four identical two-stage trains, each producing 1.5 MGD. Each train contains 37 pressure vessels in the first stage, and 14 pressure vessels in the second stage. The pressure vessel contains six Hydranautics CPA2 membrane elements connected in series. Bank 2 consists of two identical two-stage trains, also producing 1.5 MGD each. These trains each contain 31 pressure vessels in stage one, 13 pressure vessels in the second stage, and six Hydranautics ESPA1 membrane elements per pressure vessel. In addition to the feed water pumps, feed pressure to the second stage is increased by an interstage turbine booster pump, which is powered by the concentrate flow of the second stage.

Both banks 1 and 2 of Jupiter Water Treatment Plant are operated at a constant feed flow rate. Feed pressure is automatically adjusted to maintain a constant recovery at 75%. Operational parameters of bank 1 were recorded for 160 days in the period from 2 January to 10 December, 1998. Part of the observations is summarized in Table 1. Flow velocity and salt concentration in the feed are plotted in Fig. 2. From Fig. 2, it can be seen that feed flow velocity was constant at 0.140 m/s but there were significant variations in feed salt concentration (approximately 17% to 23.4%) from the mean value of 4,850 mg/L total dissolved solids. Feed pressures at both stages are shown in Fig. 3, which vary from −5.0% to +17% and from −7.6% to +23.4% from the mean values of 1.32 × 10^6 and 1.54 × 10^6 Pa, respectively.

### Table 1. Variation in Operational Conditions

<table>
<thead>
<tr>
<th>Date (mm/dd/yy)</th>
<th>Flow1 (m/s)</th>
<th>ΔP1 (Pa)</th>
<th>C1 (mg/L TDS)</th>
<th>Flow2 (m/s)</th>
<th>ΔP2 (Pa)</th>
<th>C2 (mg/L TDS)</th>
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<tr>
<td>01/02/98</td>
<td>0.140</td>
<td>1.30 × 10^6</td>
<td>4813</td>
<td>0.153</td>
<td>1.49 × 10^6</td>
<td>11520</td>
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<td>1.50 × 10^6</td>
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<tr>
<td>01/05/98</td>
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<td>1.30 × 10^6</td>
<td>4640</td>
<td>0.152</td>
<td>1.50 × 10^6</td>
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<td>01/07/98</td>
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<td>1.28 × 10^6</td>
<td>5114</td>
<td>0.152</td>
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<td>12/07/98</td>
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<td>0.155</td>
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<td>Average</td>
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<td>4849</td>
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<td>1.54 × 10^6</td>
<td>11151</td>
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<td>Minimum</td>
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<td>1.26 × 10^6</td>
<td>3891</td>
<td>0.145</td>
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<td>8890</td>
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<tr>
<td>Maximum</td>
<td>0.141</td>
<td>1.54 × 10^6</td>
<td>6189</td>
<td>0.160</td>
<td>1.90 × 10^6</td>
<td>15744</td>
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<tr>
<td>Variation (%)</td>
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<td>−5.0–17.0</td>
<td>−19.8–27.6</td>
<td>−5.4–3.7</td>
<td>−7.6–23.4</td>
<td>−20.3–41.2</td>
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</tbody>
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Model Development

Governing Equations

The RO membrane elements in each pressure vessel can be represented by a long filtration channel with a permeate wall on one side and an impermeate wall on the other side. The length, width, and height of the channel are indicated by $L$, $W$, and $H$, respectively, as shown in Fig. 1. The permeate velocity, cross-flow velocity, and salt concentration in the channel are denoted with $v(x)$, $u(x)$, and $c(x)$ with $x$ being the distance from the entrance.

To facilitate model development, complete mixing in the transversal direction of the channel is assumed. With this assumption, the governing equations in one spatial dimension are sufficient to define the problem.

Owing to the osmotic pressure difference, $\Delta \pi$, across the membrane, the net driving force for permeate through the membrane is

$$
\Delta p = \Delta p_0 - k \frac{12 u \eta dx}{H^2}
$$

where $\Delta p_0$ = initial transmembrane pressure; $k$ = friction coefficient due to the existence of spacers and other irregularities; and $\eta$ = viscosity of the solution.

Salt concentration along the filtration channel is controlled by both water and salt transfers across the membrane. Salt transfer across a RO membrane is strongly affected by intrinsic membrane properties, salt concentration, and operating conditions such as pressure. Fundamental theories of salt transfer are inadequate to simulate a full-scale RO process. In this study, a uniform salt rejection is assumed for all membrane elements in the same pressure vessel. According to mass balance of salt content, salt concentration at any point in the filtration channel can be calculated with

$$
c = \frac{1}{u} \left[ c_0 u_0 H (1 - r) \int_0^x v dx \right]
$$

where $c_0$ = feed concentration; and $r$ = membrane salt rejection.

A cross-flow RO filtration system is completely defined with a mathematical model consisting of Eqs. (1)–(4), i.e., there are four independent equations for four unknowns. One feature of the model is that all these equations are written for an arbitrary point in the filtration channel, rather than treating the system uniformly. Another characteristic of the model is that only fundamental principles, namely, membrane transport and mass balance, are involved. Mass balance is a universal principle and the membrane transport theory of water is verified with innumerable experiments. A more realistic description of the cross-flow filtration system can, therefore, be achieved in this way.

Process Parameters

Parameters of membrane elements and the operating conditions need to be determined before the governing equations can be solved. The parameters of membrane elements can be obtained or calculated directly from the data provided by the membrane manufacturer. Examples of these parameters include the height, width, and length of the membrane channel.

The feed flow rate is usually specified in the design of a RO system. The initial cross-flow velocity, $u_0$, can be calculated from the feed flow rate with

$$
u_0 = \frac{Q_{\text{feed}}}{WH}
$$

where $Q_{\text{feed}}$ = flow rate to a membrane element. When the pres-
sure drop along a pressure vessel is known, the friction coefficient, \( k \), can be determined by integration of Eq. (3):

\[
k = \frac{H^2}{12\eta} \frac{\Delta p_0 - \Delta p_n}{\int_0^1 u dx}
\]  

(6)

where \( \Delta p_n \) = transmembrane pressure at the end of the vessel. A simple experiment can be conducted to determine the friction coefficient. In the experiment, the outlet of the permeate flow is blocked so that the cross flow through the whole pressure vessel is a constant. Thus, Eq. (6) can be simplified to

\[
k = \frac{H^2}{12\eta} \frac{\Delta p_0 - \Delta p_n}{u_0 L}
\]  

(7)

Osmotic pressure of the feed water is an important factor in most reverse osmosis processes. Osmotic pressure resulting from the disperse force of salts in a solution is usually a monotonic function of salt concentration. It has been noted from practical observations that a linear relationship often exists between osmotic pressure and salt concentration.

For a nonionizing solute, the osmotic pressure can be determined with the Van’t Hoff formula,

\[\Delta \pi = \frac{R_s T \Delta c}{M_w}\]

(8)

where \( \Delta \pi \) = osmotic pressure; \( R_s \) = universal gas constant; \( T \) = absolute temperature; \( \Delta c \) = salt concentration difference between the feed and the permeate; and \( M_w \) = molar molecular weight of the solute. The unit for solute concentration in Eq. (8) is mg/L and a conversion coefficient might be required if other units of solute concentration are used. The Van’t Hoff formula can be modified to include ionization of solute in water by adding an ionization number, \( N_{ion} \), which is the number of ions that can be derived from one salt molecule:

\[\Delta \pi = \frac{N_{ion} R_s T \Delta c}{M_w}\]

(9)

When complete ionization is assumed, \( N_{ion} \) for a 1-1 salt (e.g., NaCl) is 2.

As salt constituents of raw waters can be very complex and vary substantially with location and time, it is impractical to use a fixed \( N_{ion} \) to calculate osmotic pressure in a reverse osmosis process. Therefore, empirical relationships are usually employed to determine the osmotic pressure based on a collective measurement of the total amount of salts in water, usually the total dissolved solids (TDS). The empirical equation of osmotic pressure usually takes the following form:

\[\Delta \pi = f_{os} \Delta c\]

(10)

where \( f_{os} \) = osmotic coefficient that converts salt concentration, \( \Delta c \), in term of mg/LTDS to osmotic pressure. When psi is used as the pressure unit, the coefficient needs to be divided by a conversion factor of 6.895 \times 10^3. It is worthy to note that the salt composition in the feed water varies from place to place. Therefore, the osmotic coefficient in principle is specific to a particular type of water and has to be determined exclusively for that type of water.

**Numerical Procedure**

A numerical procedure for solving Eqs. (1)–(4) is presented below. The filtration channel is first divided into \( n \) segments of equal intervals \( \Delta x \). The segments are numbered from the entrance (1) to the end of the filtration channel (\( n \)). Correspondingly, salt concentration, cross-flow velocity, transmembrane pressure, and permeate velocity in segment \( i \) are denoted as \( c_i \), \( u_i \), \( \Delta p_i \), and \( v_i \), respectively.

In the first segment, the variables are assigned with their initial values as

\[v_1 = \frac{\Delta p_0 - \Delta \pi(c_0)}{R_m}\]

(11)

\[u_1 = u_0\]

(12)

\[c_1 = c_0\]

(13)

\[\Delta p_1 = \Delta p_0\]

(14)

From segment 2 to segment \( n \), values of the variables are calculated with discrete forms of the governing equations,

\[v_i = \frac{\Delta p_{i-1} - \Delta \pi(c_{i-1})}{R_m}\]

(15)

\[u_i = u_{i-1} - v_{i-1}\Delta x/H\]

(16)

\[c_i = c_{i-1} - \frac{(1 - r)v_{i-1}\Delta x/H}{u_{i-1}}\]

(17)

\[\Delta p_i = \Delta p_{i-1} - \frac{12k\eta}{H^2}u_{i-1}\Delta x\]

(18)

With an iteration scheme, cross-flow velocity \( v_i \), salt concentration \( c_i \), transmembrane pressure \( \Delta p_i \), and permeate flux \( v_i \) along the entire filtration channel can be readily determined.

The recovery is defined as the ratio of the amount of permeate production to that of feed water supply and is an important parameter for the overall performance of a RO process. The recovery, \( R \), can be calculated from the numerical solution as follows:

\[R = \int_0^L u(x) dx = 1 - \frac{u_n}{u_0}\]

(19)

The average permeate flux \( V \), which is another overall parameter of a RO system, is determined from the numerical solution as

\[V = \frac{(u_0 - u_n)H}{L}\]

(20)

The average salt concentration in the permeate can also be determined numerically as

\[c_p = \frac{\int_0^L u(x) c dx}{\int_0^L u(x) dx} = \frac{u_0 c_0 - u_n c_n}{u_0 - u_n}\]

(21)

Although the model is capable of determining the values of all localized parameters of a RO system at any point of the filtration channel, the overall parameters are more relevant or convenient to be used to indicate the performance of a RO system.

**Results and Discussions**

**Parameters of Membrane Process**

The parameters used in the simulations are listed in Table 2. Some of the parameters were determined with trial simulations. It was found that satisfactory simulations could be obtained with \( R_m = 1.03 \times 10^{11} \) Pa/s. The membrane resistance calculated from the manufacturer’s standard testing data was \( 1.10 \times 10^{11} \) Pa/s. According to the manufacturer’s specification, the resistance of
CPA2 membrane can vary from $-35\%$ to $+15\%$ of its reported value. Therefore, the estimated membrane resistance for the Jupiter RO plant fell within the resistance range of the element specified by the manufacturer.

The simulated permeate fluxes in both stages agreed well with the operation data when the value of $f_{os}$ was set to 55.0 Pa l/mg. This osmotic coefficient is equivalent to $7.98 \times 10^{-2}$ psi l/mg, which is smaller than the commonly used “rule of thumb” value of 0.01 psi l/mg. The lower value of the osmotic coefficient suggested that there was a large portion of heavier ions in the salt composition of the ground water from the Floridan aquifer. This observation demonstrated that there is a need to determine the osmotic coefficient for each given type of feed water. The friction coefficient $k$ of CPA2 membrane element was identified to be 7.00. This means that pressure loss in a channel filled with a network of spacers was seven times greater than in a spacer-free channel.

Salt rejections used in the simulations were 98.0% in stage 1 and 96.7% in stage 2. The manufacturer certified that the membrane has a minimum rejection of 99.3% under standard test when the feed concentration was 1,500 mg/L of sodium chloride. The reduced salt rejections in the Jupiter RO plant are reasonable because salt rejection usually declines with increasing feed salt concentration (Soltanieh and Gill 1981; Song 2000).

### Model Simulations

With the parameter values mentioned above, the dependence of water recovery on the applied pressure was simulated for both stages. The operational conditions of the Jupiter RO plant were used in the simulations. The average feed flow velocities of 0.140 and 0.154 m/s were used in stages 1 and 2, respectively. Three salt concentrations were used for each stage, which were the mean, minimum, and maximum feed salt concentrations (See Table 1). The recoveries for the mean salt concentration are plotted in Fig. 4 (with the thick lines). The recoveries for the corresponding minimum and maximum feed salt concentrations are also plotted in the same figure (with the thin lines), which appear above and below the recoveries for the mean feed concentrations. The solid lines represent the recoveries in stage 1 while the broken lines are for those in stage 2.

The lines in Fig. 4 show that recoveries increase with increasing pressure, but the increasing rates decrease toward the high end of the pressure range. Nonlinearity between the recovery and the pressure becomes obvious when the pressure is greater than 1,500 kPa. The recoveries in both stages can be readily estimated from Fig. 4 for any given pressure. Conversely, the required working pressures to attain a specified recovery can also be easily determined from Fig. 4. For example, the recoveries in Jupiter RO plant are 60% and 40% for stages 1 and 2, respectively. The associated working pressures can be determined by the following procedure: (1) draw horizontal lines from 60 and 40% on the recovery axis; and (2) from the intersections of these two horizontal lines with the recovery lines, the mean working pressures were found to be around 1,350 and 1,550 kPa for stages 1 and 2, respectively.

### Comparison of Observations and Simulations

The monitored and predicted recoveries in both stages are plotted in Fig. 5. The monitored recoveries were at about 60 and 40% with little fluctuations for stages 1 and 2, respectively. The recovery was a performance parameter in the Jupiter RO plant that was controlled by automation. The feed pressures would be adjusted accordingly to maintain a relatively constant recovery. Figure 5 shows that the simulated recoveries have greater fluctuations than the monitored values. One reason for this discrepancy could come

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**Table 2. Parameter Values for Model Simulation**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tr>
<td>Temperature, °C</td>
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</tr>
<tr>
<td>Water viscosity (at 25 °C), Pa s</td>
<td>$0.890 \times 10^{-3}$</td>
</tr>
<tr>
<td>Feed channel height, m</td>
<td>$6 \times 10^{-4}$</td>
</tr>
<tr>
<td>Total length of membrane, m</td>
<td>6</td>
</tr>
<tr>
<td>Membrane resistance Pa s m$^{-1}$</td>
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</tr>
<tr>
<td>Friction coefficient due to spacers</td>
<td>7.0</td>
</tr>
<tr>
<td>Salt rejection</td>
<td>98.0% in 1st stage, 96.7% in 2nd stage</td>
</tr>
<tr>
<td>Number of steps in channel discretion</td>
<td>500</td>
</tr>
</tbody>
</table>

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**Fig. 4. Simulations of dependency of water recoveries on pressure in both stages**

**Fig. 5. Comparison of monitored and simulated recoveries in both stages**
from the feed pressure. A constant pressure was used in the simulations for a whole day that could not fully reflect the real-time controlled pressure used in operation. Aside from the greater fluctuations, which are within 10% for most of the time, the simulated recoveries in both stages agreed well with the monitored results.

The monitored and simulated TDS concentrations in the concentrate and permeate flows in both stages are compared in Figs. 6 and 7, respectively. The simulations basically predicted the magnitude of the TDS concentrations in both the concentrate and permeate flows. The trend of the TDS concentration in the concentrate flows was reproduced relatively well with the simulations. However, some peaks and valleys were observed in the monitored salt concentrations in the permeate flows that differed substantially from the simulated values. This might be partially caused by the automatic control of the recovery at a constant value. Seasonal variation of salt composition in feed water can be another reason for the deviation of the simulations from the observed salt concentrations in the permeate flows.

The simulated pressures of the concentrate flows out of stages 1 and 2 are plotted in Fig. 8. The concentrate pressures out of both stages were seen satisfactorily predicted with simulations. The results showed that the pressure loss in a channel filled with a network of spacers could be accurately described with Eq. (3) with a friction coefficient to account for the effect of the network of spacers present in the channel.

Conclusions

The performance of a full-scale desalination plant with a spiral-wound RO membrane can be adequately simulated with the proposed model [Eqs. (1)–(4)] based on local membrane transport and mass conservation relationships on water and salt. Due to the existence of the network of spacers in the filtration channel, it is acceptable to assume complete mixing in the transverse direction in the channel. This assumption greatly simplifies the governing equations for the performance of a RO process.

Simulations of the performance of the RO process at the Jupiter water plant demonstrated that the osmotic coefficient was strongly dependent on the composition of feed water. Since feed water composition can vary significantly from plant to plant, it is essential to determine the osmotic coefficient specifically for the feed water that is to be treated. The resistance of the CPA2 membrane element used in the Jupiter RO plant was verified to be $1.03 \times 10^{11}$ Pa s/m, which is within the specified range given by the manufacturer. This observation suggested that the resistance obtained from manufacturer test data under standard conditions could be used in the simulations of the full-scale water treatment plant. The network of spacers in the spiral-wound membrane element can significantly increase pressure loss through the element.

Salt rejection appeared smaller in stage 2 than in stage 1 of the Jupiter RO plant. It showed that salt rejection decreased with increasing salt concentration, as demonstrated in many previous experimental observations. However, such a dependency of salt...
rejection on salt concentration cannot be adequately predicted by any existing fundamental membrane transport theories. More sophisticated theories on salt transport across the RO membrane have to be developed for more advanced modeling and simulations of the RO membrane process in water reclamation and desalination.

Notation

The following symbols are used in this paper:

- $c$ = salt concentration (mg/L);
- $c_0$ = feed salt concentration (mg/L);
- $c_p$ = average permeate salt concentration (mg/L);
- $f_{os}$ = osmotic coefficient (Pa L/mg);
- $H$ = channel height (m);
- $k$ = friction coefficient due to existence of network of spacers in channel;
- $L$ = channel length (m);
- $M_w$ = molecular weight (g/mol);
- $N_{ion}$ = ionization number;
- $Q_{feed}$ = feed flow rate to membrane element (m$^3$/s);
- $R$ = water recovery;
- $R_g$ = universal gas constant (Pa L mol$^{-1}$ K$^{-1}$);
- $R_m$ = membrane resistance (Pa s/m);
- $r$ = membrane salt rejection;
- $T$ = absolute temperature (K);
- $u$ = cross-flow velocity (m/s);
- $u_p$ = feed flow velocity (m/s);
- $V$ = average permeate velocity (m/s);
- $v$ = permeate velocity (m/s);
- $W$ = channel width (m);
- $x$ = distance from the entrance (m);
- $\Delta c$ = difference of salt concentration (mg/L);
- $\Delta p$ = transmembrane pressure (Pa);
- $\Delta \pi$ = osmotic pressure (Pa); and
- $\eta$ = water viscosity (Pa s).

References


