NEURAL NETWORK APPROACH FOR MODELING THE PERFORMANCE OF REVERSE OSMOSIS MEMBRANE PROCESSES

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1. Introduction

The lack of drinking water in many regions of the world has led to new development in desalination processes. There are different methods for desalinating water, such as distillation, electrodialysis, nanofiltration, and reverse osmosis. The efficiency of a reverse osmosis membrane desalination plants, which are most commonly used in water desalination technology, is often limited by membrane fouling. Both membrane life-time and separation performance (water flux and salt rejection) are adversely affected by several flux inhibiting boundary layer effects, especially concentration polarization, fouling and scaling. To advance the efficient operation of modern RO membrane desalination plants it is necessary to establish an effective approach to model plant operation and to identify deviations (as well as upsets) in process conditions due to fouling and mineral salt scaling.[1] Unfortunately, there are no first principle models available for predicting the development of fouling in full-scale RO plants. The major obstacles to developing such predictive models are the complexity of feed composition, the inability to realistically quantify the real-time variability of feed fouling propensity, lack of understanding of both the interplay of various fouling mechanism and the precise role of membrane surface properties and membrane interactions with various foulants and fouling precursors.[2] Using real-time measurements for various process variables, it should be possible to develop RO experimental models via Artificial Neural Networks (ANN) to describe the dynamics of full-plant performance. Such models should help understand and establish the relationships between process conditions and the onset of fouling and scaling. Moreover, the ANN approach should enable one to develop soft sensors for early identification of membrane fouling. The above information would in turn enable the development of effective process control strategies.

In the current study a neural network (NN) based RO model was developed for predicting the time evolution of permeate flux decline due to the occurrence of membrane fouling. Using real-time measurements of process variables as well as feed water quality from full-scale RO plants, a framework has been designed and NN models developed to evaluate in advance the onset of fouling with soft sensors.

2. Experimental data and methodology

2.1. Full-scale RO data

The experimental data used for building predictive models, was provided by WaterEye Corporation for a two-stage brackish water desalination plant located at Port Hueneme, California, schematically presented in Figure 1. The data consisted of the real-time evolution of several process variables, recorded every 10 minutes for about 3 months of operation, i.e., 9000 experimental data points. The monitored parameters included feed flow rate, conductivity, pressure, pH and temperature of the raw water feed; inter-stage pressure; flow rate, conductivity and pressure of the permeate; and flow rate, conductivity and pressure of the concentrate. The basic premise of the present approach was to utilize readily available process parameters in order to predict process upsets.[3]

System conditions such as flow rates, pressures, temperature, and concentrations can vary during the operation of a full-scale RO plant and cause changes in permeate flow rate and salt passage. A diagnosis of such changes is cumbersome, due to the fact that they can also be attributed to the occurrence of fouling or can just be the result of changes in operating conditions. To effectively evaluate system performance, it is necessary to compare permeate flow and salt passage rates at the same conditions, converting the actual RO data to a set of reference (standard) conditions. In the present work, the utilized standardization procedure was the ASTM 4516-00 [4] method which is based on normalizing the permeate flow rate with respect to temperature, pressure and concentration (included in the osmotic pressure factor). The reference temperature was selected as 25 ºC, while the reference pressure factor was calculated using the measurements corresponding to the first process monitoring point.

The standardization of permeate flow rate can be expressed as,

$$Q_{ps} = \frac{\left[P_{fs} - \frac{P_{fs} - P_{cs}}{2} - P_{ps} - \Pi_{fbs} + \Pi_{ps}\right] \cdot \left(TCF_s\right)}{\left[P_{fa} - \frac{P_{fa} - P_{ca}}{2} - P_{pa} - \Pi_{fba} + \Pi_{pa}\right] \cdot \left(TCF_a\right)} \cdot Q_{pa} \tag{1}$$

where Q_p is the permeate flow rate, P_f, P_c and P_p are the feed, concentrate and permeate pressures, respectively, Π_{fb}, Π_p are the feed-brine and permeate osmotic pressures, and TCF is the temperature correction factor, calculated as follows:

$$TCF = e^{3020 \cdot \left(\frac{1}{298,15} - \frac{1}{T}\right)} \tag{2}$$

in which T is the absolute temperature in degrees K.

The salt passage, defined as the ratio between the permeate and the feed-brine concentrations, was standardized as follows

$$\%SP_s = \frac{\left[EPF_a\right]}{\left[EPF_s\right]} \cdot \frac{\left[TCF_a\right]}{\left[TCF_s\right]} \cdot \frac{\left[C_{fbs}\right]}{\left[C_{fba}\right]} \cdot \frac{\left[C_{fa}\right]}{\left[C_{fs}\right]} \cdot \%SP_a \tag{3}$$

where EPF is the average RO element permeate flow rate, and C_{fb}, C_f, C_p are the feed-brine, feed and permeate concentrations, respectively. The feed-brine concentration was expressed as a log mean average, and calculated in terms of the recovery Y (the ratio between the permeate and the feed flows) according to

$$C_{fb} = C_f \cdot \ln\left[\frac{1/(1-Y)}{Y}\right] \tag{4}$$

In equations (1) and (3), the sub index *s* refers to standard (reference) conditions, while sub index *a* refers to actual conditions. The osmotic pressure (kPa) was estimated from

$$\Pi_{fb} = 0,2654 \cdot C_{fb} \cdot \frac{T}{1000 - \frac{C_{fb}}{1000}}; \ \Pi_p = 0,05 \cdot \Pi_{fb} \tag{5}$$

where the concentrations are expressed as “equivalent of sodium chloride”, in mg/l.

The compositions of the feed, permeate and concentrate streams are not measured in real-time in commercial RO plants. Therefore, one has to resort to conductivity measurements as surrogate for salt concentration. The common approach is to correlate conductivity with the total dissolved solids concentration (TDS) using sodium chloride as the correlating salt. Conductivity (μS/cm) - TDS (usually in units of mg/L) correlations can be obtained either from experimental measurements for the actual range of salt compositions of interest or based on thermodynamic multi-electrolyte calculations. In the present study the OLI Analyzer software [5], a multi-electrolyte thermodynamic process simulator was used to develop a range of conductivity – TDS correlations (using NaCl as the reference salt) for each of the process flows, resulting in the following TDS correlations. Thus, the equations used to calculate the equivalent NaCl concentrations are presented below:

Permeate: $TDS_{NaCl} = 0.3455 \cdot (\mu S/cm)^{1.0169}$; Feed-brine: $TDS_{NaCl} = 0.1409 \cdot (\mu S/cm)^{1.1567}$ (6)

Operational problems can be identified by plotting the time evolution of the normalized permeate flux and salt passage (see Figure 2), along with the evolution of pressure drop along the membrane channel (see Figure 3). When a significant change occurs in flux this is typically an indication of a deviation from the prescribed operational target. Process interruptions (e.g., membrane cleaning and/or replacement) can also be identified by discontinuities in the time evolution of the represented variables, especially when accompanied by large periods of missing data (e.g., no measurements are performed during the cleaning procedure) and from personal communication with either the plant operators or monitoring staff. For the present data set these occurred at operation times of 328 hr, 832 hr, 976 hr, 1671 hr and 1928 hr, as indicated by the vertical dotted lines in Figures 2 and 3.

2.2. Data preprocessing and analysis

Model output was expressed as permeate flux, normalized with respect to the standardized flux taken immediately after a cleaning procedure (or membrane replacement) to facilitate the identification of critical operation conditions. In selecting the input of experimental data to the ANN model, it is important to select variables that are physically meaningful, independent, easy and inexpensive to measure and capable of being monitored in real-time. Accordingly, flow rate, conductivity, pressure, pH, temperature of the feed and the measurement time were chosen as inputs. The process time was divided into equal intervals, from 25 hr to 125 hr, to set-up the span for the forecasting operation period. In addition, the normalized flux at the beginning of each time period was selected as an input variable in order to capture large time-scale events, i.e., to enable capturing the long-term memory of the RO system.

Neural network models were built using the back-propagation algorithm to establish the relationships between the selected inputs and the target variable (critical process event, e.g., fouling). The data set was divided into three subsets. The first 4600 points, corresponding to the first three periods of operation, were selected to train the NN algorithm. The remaining points, corresponding to the last three periods of operation, were chosen for testing the models. Validation was carried out with 20% of the data in the training set, selected randomly. Validation results were used as a stopping criterion of the learning algorithm. As a result, approximately 40% of the entire data set was used for training the network, 10% for validation purposes and 50% for testing the experimental model.

Various statistical approaches were applied for each time interval to determine the most suitable network architecture. The quality of the model was assessed with the application of the quality indicator defined by equation (7) over the training, validation, and test data sets.[6]

$$Q^2 = 1 - \frac{\sum\left(y_i - \hat{y}_i\right)^2}{\sum\left(y_i - \bar{y}\right)^2} \qquad (7)$$

In equation (7) y_i, $\hat{y}_i$, $\bar{y}$ are the experimental, predicted, and average values, respectively. For the ideal case of a perfect model, plotting the predicted points versus the experimental ones should result in a straight line with the slope equal to unity which would also result in the Q^2 index being unity. It is noted that Q^2 varies between 0 and 1, with prediction's quality increasing as Q^2 approaches 1.

3. Results

Figure 4 summarizes the results of the statistical analysis followed to select the optimal network architecture relative to the model's input variables configuration. Here the length of the time interval was varied from 25 hr to 125 hr and the number of neurons in the hidden layer ranged from 2 to 11. The results were combined into groups according to the network architecture. Each group contains five cases, the difference between them being the size of the periods used for dividing the time space. The dimension of each bar represents the Q^2 index calculated for the testing set.

As illustrated in Figure 4 the models ability to capture the changes in RO process performance generally increased as the time period decreased. Comparing different network architecture, it can be seen that in almost all the cases, the highest Q^2 value is obtained when dividing the time space into 25 hr periods, while the lowest Q^2 values are generally obtained when using the 125 hr time interval. Exceptions to this rule are the cases when using 2 or 7 neurons in the hidden layer. In general, when upon increasing the time interval the correlation index for the testing set decreased. The maximum absolute values for the Q^2 correlation index were obtained for 5, 9 and 11 neurons in the hidden layer and for time interval of 25 hr.

In order to find the optimal architecture of the NN, the data were analyzed using particular time intervals. When comparing the results for time intervals of 25 hr and 100 hr, the correlation index increased for 2 to 6 neurons in the hidden layer; subsequently, it decreased slowly with increasing number of hidden neurons. In these cases a bimodal graph was obtained with the maximum values of Q^2 at 5 and 9 hidden neurons, respectively. For the time intervals of 50 hr and 75 hr, the performance of the correlation followed a similar behavior of increasing correlation (i.e., Q^2) as the number of intermediate neurons increased from 2 to 6 but then remained nearly constant for higher values of hidden neurons. On the other hand, when the time space was divided into 125 hr periods, the maximum Q^2 values were obtained when using 2 or 7 neurons in the hidden layer.

Based on the above analysis, the optimal ANN model which yielded the highest quality index and simplest NN architecture was a 7:5:1 back-propagation neural network with a time interval of 25 hr. This model was selected for evaluating the RO process performance as illustrated in Figure 5. The experimental data points are represented with crosses and light color, while the predicted points are depicted as black full-dots. The vertical black lines denote the times of process shut down (e.g., for cleaning or changing the membrane modules). Figure 5a, presents the experimental training data points used for building the models, and the NN predictions for this operation period. Figure 5b, presents the forecast values of permeate flux by the ANN model and also the experimental values used for testing. As evident from both Figures 5a and 5b, the experimental results show a wide dispersion of permeate flux over the course of operation, whereas the predicted values of the ANN model presenting a slightly lower scatter, indicating that there is noticeable smoothing of the model forecasts. In all cases, the predicted values are in good agreement with the experimental values, not only for the first three periods of operation, that were utilized for the learning phase (Figure 5a), but also for the last three periods of operation, that were used solely for testing the prediction capability of the model (Figure 5b). It is noted, however, that there are prediction outliers in both Figures 5a and 5b; but this is attributed to the major scatter of the monitored variables at the above times.

4. Conclusions

A neural network model was developed to describe the dynamics of a brackish water RO desalination system, using real experimental data from a full-scale RO pilot plant in Port Hueneme, California. Model training was accomplished using normalized data following the ASTM 4516-00 method. The spectrum of possible network architectures was scanned to arrive at the optimal model, using a number of numerical algorithms that considering the selection of model variables and resulting model performance. Long-term memory was incorporated into the model by dividing the time space into equals intervals and selecting the initial normalized permeate flux (i.e., at the beginning of each time period) as additional model input. The best results were obtained using a 25 hr time interval and a network architecture with 5 neurons in the hidden layer. Using this approach, reasonable permeate flow forecasting can be attained and thus provide the capability of inferring the occurrence of membrane fouling.

The study revealed that the NN-RO models are able to successfully describe the RO process performance. Preliminary results are encouraging in demonstrating that the NN based RO models can be successfully used for interpolation, as well as for reasonable forecasting. Current work is ongoing to include the normalized salt passage in the overall model and extending the model to longer time range of process performance modeling.

5. References

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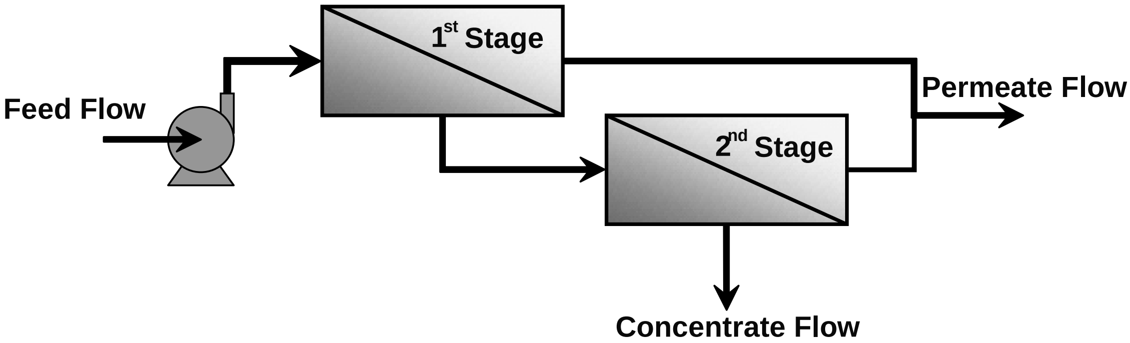

Figure 1. Schematic of a two-stage RO process

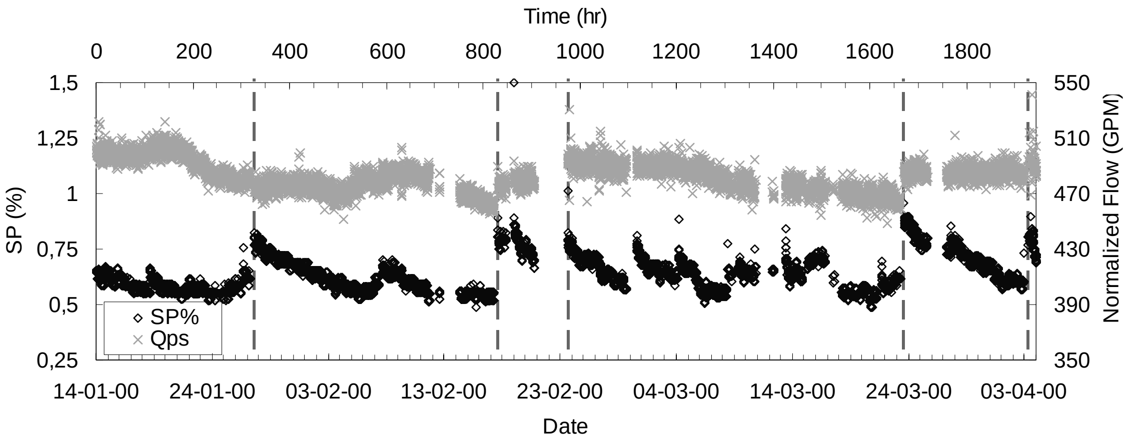

Figure 2. Time evolution of the normalized salt passage and normalized permeate flow

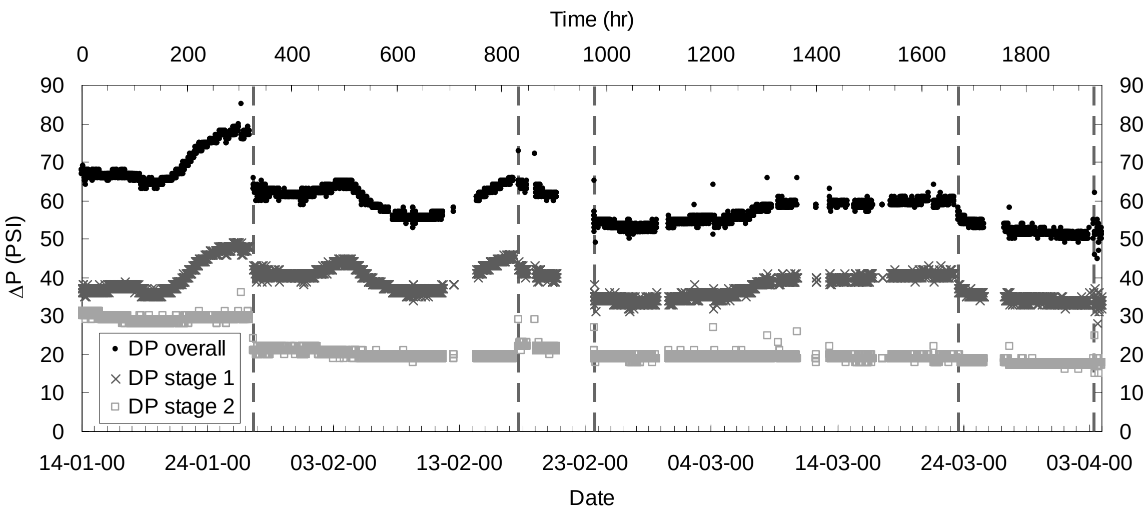

Figure 3. Time evolution of the pressure drop along the membrane channel, for each one of the two stages and also for the overall process

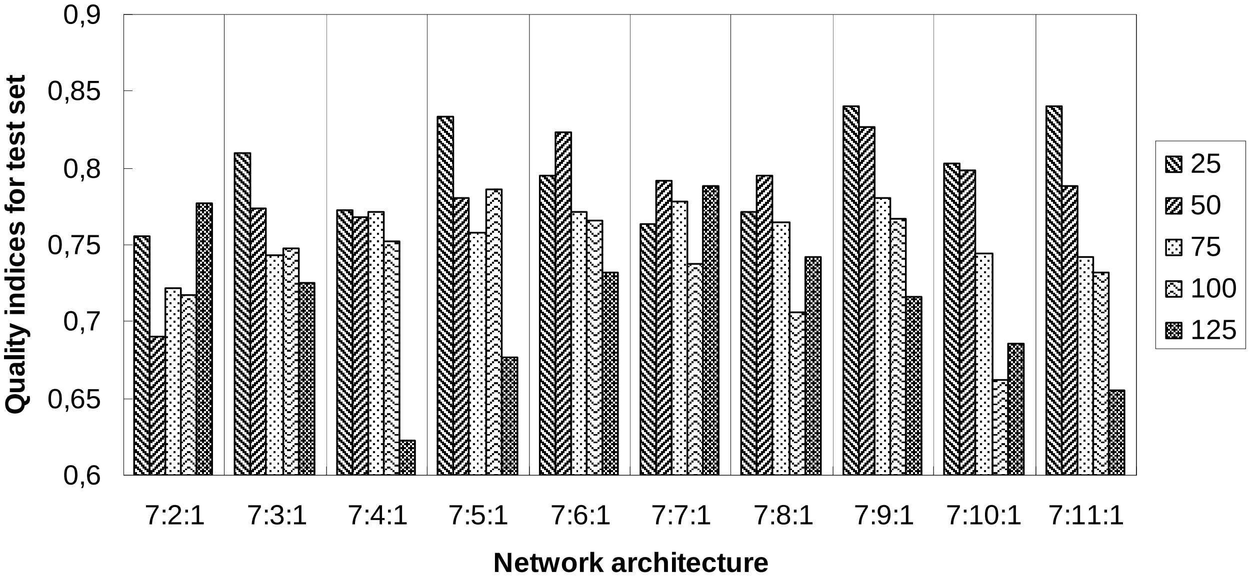

Figure 4. Network structure and optimal time span analysis

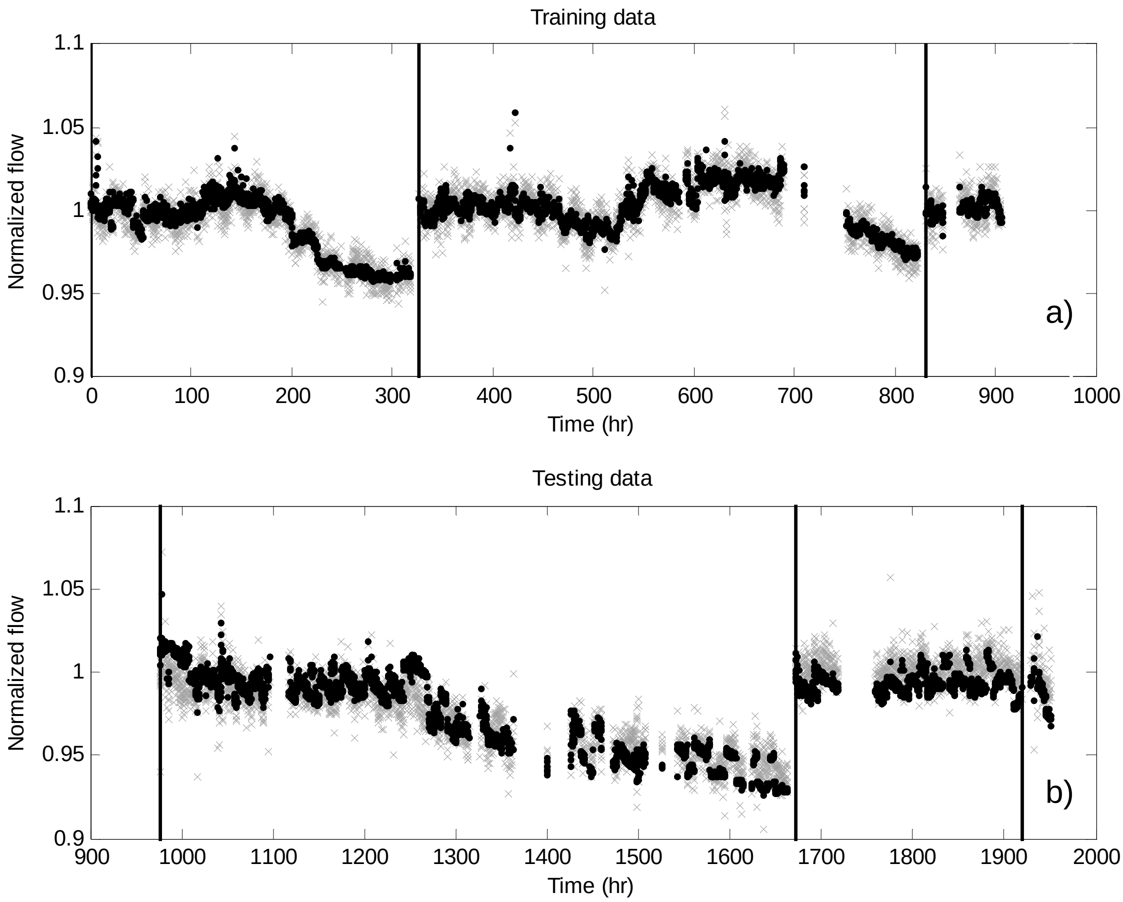

Figure 5. Training and testing data predictions for the model built using a 25 hr time span, and the neural network architecture 7:5:1