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Modeling of an RO water desalination unit using neural networks

Abderrahim Abbas *, Nader Al-Bastaki

Department of Chemical Engineering, College of Engineering, University Of Bahrain, P.O. Box 32038, Bahrain

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Abstract

In this paper, a feedforward neural network (NN) model is developed to predict the performance of a reverse osmosis (RO) experimental setup, which uses a FilmTec SW30 membrane. Sixty-three experimental data were generated for training and testing the network. The considered ranges of operating conditions were chosen so as to include those encountered in a large number of the worldwide brackish water and seawater RO plants. The NN was fed with three inputs: the feed pressure, temperature and salt concentration to predict the water permeate rate. The fast Levenberg–Marquardt (LM) optimization technique was employed for training the NN. The network learned the input–output mappings with accuracy for interpolation cases, but not for extrapolation.

Keywords: Reverse osmosis; Water desalination; Neural networks; Process modeling

1. Introduction

Desalination of sea and brackish waters is the main source for supplying fresh water in many Middle Eastern countries, which suffer from the scarcity of rainwater and absence of lakes and rivers. About half of the worldwide desalination capacity is installed in the Gulf Co-operation Council (GCC) countries alone [1].

The major technologies used for water desalination are reverse osmosis (RO) and multistage flash distillation (MSF). Recently, the former has gained more dominance particularly for brackish water desalination. The rapid growth of RO is attributed to a number of techno-economic factors, including low energy requirements, low operating temperature, modular design and low water production costs [2]. In a study conducted in 2001, Wade [3] has shown the water production costs for an RO process with an energy recovery system to be much lower than that corresponding to MSF and multi-effect desalination (MED). Using plants with capacity of 31,822 m^3/d and a fuel cost of US$ 1.5/GJ as a basis of comparison, Wade estimated the water production costs for MSF, MED and RO with brine booster to be (in US$/$m^3$), 1.04, 0.95 and 0.75, respectively. With today's high costs of energy, the difference in water production costs between the energy intensive thermal systems and RO is expected to be much more pronounced in favor of RO. Among the other attractive features of RO is its modular nature. This feature has made it possible to design desalination processes of various sizes using RO ranging from small scale to large scale. Also, it makes the maintenance of RO systems flexible. A large-scale RO plant consists of a large number of modules (membrane elements). Specific membrane modules that deteriorate or malfunction due to aging, or excessive fouling can be easily replaced. A wide range of RO membrane types have been developed by the membrane manufacturers to suit various purposes, such as high flux membranes (suitable for brackish water), high rejection membranes (suitable for seawater) and fouling resistant membranes (suitable for feed waters leading to excessive fouling). Still another advantage of the RO process is that it is operated by pressurizing the feed water using high-pressure pumps to pressures well above the osmotic pressure, which is proportional to the concentration of the solutes in the feed water. This makes the design less complicated, as there is no requirement for boilers or for coupling with a power plant to make use of its waste heat, which is required by the thermal desalination processes.

In terms of modeling, one of the disadvantages of RO is the difficulty of obtaining a rigorous mechanistic model of the process, which accounts for several important operating factors such as the feed temperature, concentration polarization and fouling [4]. One reason is the fact that the mass transfer and fouling mechanisms are not well understood. The availability of reliable

* Corresponding author. Tel.: +973 17876880; fax: +973 17680935.
E-mail addresses: arabbus@eng.uob.bh (A. Abbas), naderbsk@eng.uob.bh (N. Al-Bastaki).

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RO models is of paramount importance for process analysis and design as well as forecasting long-term performance. For example, the decision-makers can use such models to predict when to change membrane elements.

During the last 15 years, neural networks (NNs) have been the focus of much attention, largely because of their wide range of applicability and ease with which they handle complex and highly nonlinear problems. NNs were successfully applied to problems from various areas including the business, medical and industrial fields [5]. Process modeling is an area where NNs of varying configurations and structures have been considered as alternative modeling techniques, particularly in cases where reliable mechanistic models cannot be obtained [6–11].

Recently, a few studies have considered the application of NNs to the modeling and control of desalination plants [12–17]. MSF desalination was the main focus of these studies. Al-Shayji and Liu [12,13] employed feedforward neural networks trained by the back-propagation algorithm to model the performances of two industrial plants: an MSF and an RO plants located in Kuwait and Saudi Arabia, respectively. The limited information given for the RO case showed the considered NN to outperform the model based on regression analysis. Jafar and Zilouchian [14] used a radial basis function network (RBFN) to model the performances of two RO plants with different feed water intakes. The performance of this network was compared to that of a feedforward network trained by the back-propagation algorithm. They found the RBFN to learn much faster than the feedforward network, but requires additional computational burden. However, it is not clear what operating conditions were used as the inputs to the considered models nor the amount of data used for training and testing the NNs.

Several investigations have considered the use of NNs for modeling other membrane separation processes [18,19]. Cabassud et al. [18] used NN for the modeling of ultrafiltration processes for drinking water applications. The model consisted of two interconnected recurrent neural networks coupled with Darcy's law. They compared the results of the model with data obtained from an experimental pilot plant and found the model predictions to be satisfactory for different water quality and changing operating conditions. Razavi et al. [19,20] used two NN models with a single hidden layer each to predict the dynamic performance of a milk ultrafiltration process. They studied the effects of changing the operating temperature and transmembrane pressure and obtained very good agreement between the experimental and model results. Shetty and Chellam [21] used NN, with one hidden layer of eight neurons, to predict the fouling of membranes for nanofiltration of ground and surface waters. The inputs to the NN model included the flow rate, permeate flux and feed water quality parameters, such as pH, UV and total dissolved solids concentration. With only about 10% of experimental data employed for training, the networks used were found to accurately predict the fouling of the nanofiltration membrane. Bowen et al. [22] used a NN to predict the rejections of four single salts (NaCl, Na_2SO_4, $MgCl_2$ and $MgSO_4$) and mixtures of these salts at a nanofiltration membrane. The optimized NN was tested with rejection data obtained from a pilot plant based on a spiral-wound membrane. The overall agreement between the NN predictions and the experimental results was found to be very good for both single salts and mixtures.

As stated earlier, the amount of published work that is available in the literature on the application of NNs to desalination processes in general and RO desalination in particular remains to be limited. The usefulness of this modeling technique and the confidence to which it can be implemented to RO desalination plants still requires further verification using different types of membranes and experimental conditions. The main objective of this paper is to develop a NN for predicting the performance of an RO unit, which is based on a FilmTec SW30 membrane. Three key operating parameters, namely the feed temperature, pressure and salt concentration are fed to the network to predict the water production rate. The considered ranges of operating conditions were chosen so as to include those encountered in a large number of the worldwide brackish water and seawater RO plants. One additional important aspect of this work is to test the ability of NNs to interpolate and extrapolate actual RO data.

2. Neural network modeling

Neural networks are mathematical models designed to mimic certain aspects of neurological functioning of the brain. A NN is a parallel structure consisting of nonlinear processing elements (neurons or nodes) interconnected by fixed or variable weights. The nodes are grouped into layers. A typical network consists of an input layer, at least one hidden layer and an output layer. The most widely employed networks have one hidden layer only [7]. For a feedforward NN the information propagates in one direction only—the forward direction. An example of a three-layer feedforward NN is shown in Fig. 1. In this case, each node within a given layer is connected to all the nodes of the previous layer. The node sums up the weighted inputs and a bias, and passes the result through a linear or nonlinear function. For more information on the topology of NNs, the interested reader may consult the excellent book by Hertz et al. [23].

A NN is trained by presenting it with a set of known inputs and outputs. It learns the patterns of these inputs and outputs by manipulating the weights of the nodes' connections. The

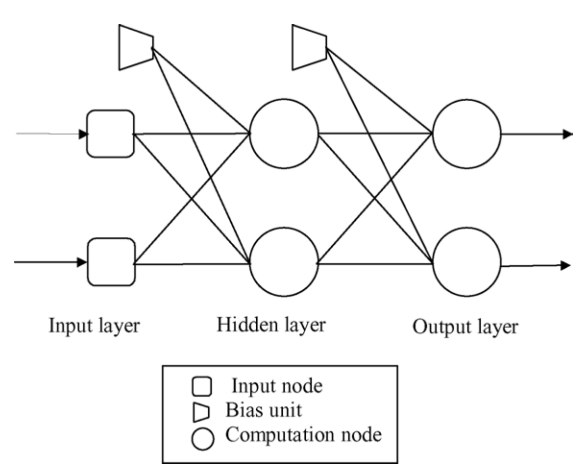

Fig. 1. Structure of a feedforward network with two input nodes, one hidden layer with two nodes and two output nodes.

weights are adjusted until the optimization criterion is minimized. The most widely used criterion is the root-mean-square error (RMSE):

$$\mathrm{RMSE} = \left\{ \frac{1}{N} \sum_{i=1}^{N} (P_{i,\mathrm{actual}} - P_{i,\mathrm{predicted}})^2 \right\}^{1/2} \quad (1)$$

where N is the total number of output values used for training and P refers to the output values.

Currently, the most widely employed algorithm for training NNs is the back propagation approach [6,23]. It uses the steepest descent traditional optimization technique to adjust the network weights to minimize the RMSE between the actual values and the values predicted by the network for a set of training data, sequentially on an input–output pair basis. However, the back-propagation techniques are known to converge slowly. In this paper, the fast Levenberg–Marquardt (LM) optimization technique [24] is used for training the network.

3. Experimental

3.1. Data generation

The experimental data employed for modeling was obtained from an RO rig based on a spiral wound FilmTec SW30 membrane, Fig. 2. A feed salt/water solution is fed to the membrane by a high-pressure pump. Two streams leave the membrane unit: a permeate stream and a concentrate solution. Each of these two streams passes through a rotameter to measure its flow rate. A full description of the rig is given in the paper by Al-Bastaki and Abbas [25]. In this study, the permeate rate is used as the performance measure of the membrane.

The feed solution used was prepared by mixing sodium chloride, which is, by far, the major solute present in seawater, with tap water. To investigate the performance of the membrane over a wide range of operating conditions, three key feed parameters were varied from run to run, namely the feed pressure, temperature and sodium chloride concentration. In all experiments, the feed flow rate and permeate side pressure were maintained constant at 0.5 m^3/h and atmospheric pressure, respectively. The water recovery was allowed to vary. Note that in industrial RO plants the recovery is generally maintained close to a desired value by gradually increasing the feed pressure over time so as to overcome the reduction of the permeation flux caused by membrane fouling and compaction.

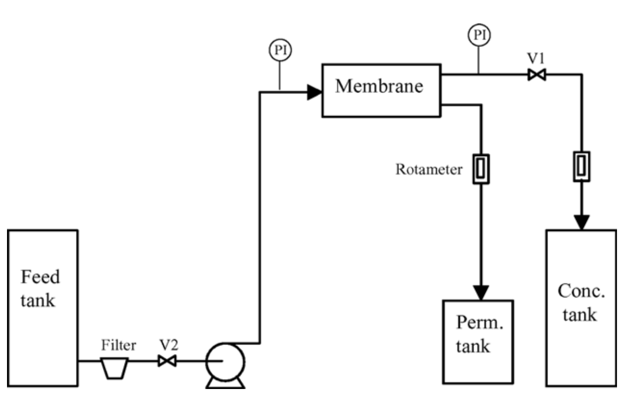

Fig. 2. Experimental setup.

Table 1
Permeate rate as a function of feed pressure, concentration and temperature

Feed pressure (bar)	Feed concentration (g/l)	Permeate rate (l/h)		
		10 °C	20 °C	30 °C
20	0.0	12.9	23.0	26.9
20	0.5	13.2	22.9	26.5
20	2.0	12.5	22.4	26.0
20	5.0	10.7	20.2	23.1
20	10.0	8.8	15.5	17.1
20	20.0	4.9	7.9	10.5
20	30.0	1.7	4.5	9.2
40	0.0	22.4	41.8	51.0
40	0.5	22.3	41.4	49.5
40	2.0	22.0	39.6	46.0
40	5.0	20.5	35.5	44.1
40	10.0	17.3	32.3	36.3
40	20.0	13.0	23.2	25.5
40	30.0	9.9	15.2	20.9
60	0.0	34.0	59.0	72.0
60	0.5	33.2	57.9	70.6
60	2.0	32.7	55.2	65.5
60	5.0	31.0	51.4	63.2
60	10.0	28.2	49.0	55.6
60	20.0	22.6	37.5	43.2
60	30.0	19.5	28.8	30.6

The duration of each experimental run was 30 min. The process was allowed to reach steady state during the first 10 min followed by collection of the permeate for the next 20 min. The permeate production rate was then obtained manually through division of the amount of the product collected by the run duration (20 min). The readings obtained from the rotameters were in close agreement with these more accurate manually calculated values. The results of the experiments performed are given in Table 1. Each of these 63 experimental values was obtained by averaging the results of two repeated runs. In addition, all repeated runs lead to permeate fluxes, which were in close agreement. As expected, Table 1 shows that the permeate rate increases with increasing pressure and temperature and decreases with increasing feed concentration.

3.2. Network structure

As mentioned earlier, the NN used in this study has a feedforward structure trained using the LM optimization method. The inputs to the network were the operating pressure, temperature and feed concentration, and the output was the permeate rate. The optimum number of hidden layers and nodes within each layer are problem specific, and there is no procedure available to know this a priori. For this reason, a trial and error approach (multiple runs) was followed to arrive at the best network architecture. These included one and two hidden layers, and 3, 5, 10 and 15 nodes per each hidden layer. The activation function used in the hidden nodes is the sigmoidal function:

$$f(x) = \frac{1}{1 + e^{-x}} \tag{2}$$

where x is the sum of the weighted inputs to the neuron and $f(x)$ represents the output of the node. As for the output layer nodes, a simple linear activation function was employed, $f(x) = x$.

The simplest network that yielded good results (small RMSE values) without over-fitting the data had one 5-node hidden layer. Several values of the learning rate and number of epochs (iterations) have also been tested while training the network. Two hundred epochs and a learning rate of 0.05 were found to be adequate. An additional stopping criterion employed was a change of <10^{-6} in the RMSE value from epoch to epoch. These parameters' values were used in all computations in this work.

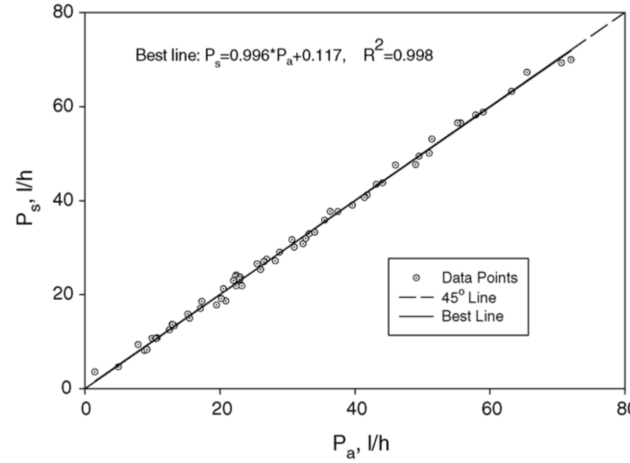

Fig. 4. Simulated (P_s) vs. actual (P_a) permeate rates (Case 1).

4. Results

Initially, the network was trained using all 63 data points. This is referred to as Case 1. A plot of the RMSE and the number of iterations is shown in Fig. 3. This figure shows a sharp drop in the RMSE in the first few iterations (fast training). This is a well-known characteristic of the LM optimization method. The training stopped after 150 iterations with an RMSE value of 1.04.

The trained network was then simulated by feeding it with all of the data used for training. Fig. 4 presents a plot of the network outputs (predicted permeate rates) versus the targets (actual permeate rates). All points are close to the 45° line, which means that the network has learnt the input–output mappings with a good degree of accuracy. To quantify the agreement between the actual and predicted permeate flow rates, linear regression was used to fit a line to the predicted target data set. As shown in Fig. 4, the obtained best line has a slope of 0.996 and an intercept of 0.117. It is very close to the perfect prediction, or 45° line, which has a slope of 1 and an intercept of 0. The value of the correlation coefficient $R^2 = 0.998$.

In a second case, the experimental data was split into two sets: a set of 42 points, composed of the data corresponding to the operating temperatures of 10 and 30 °C (see Table 1), were used for training the network. The rest of the data (21 points corresponding to an operating temperature of 20 °C) were employed for testing or validating the trained network. The results of this second case are presented in Fig. 5 where the permeate rates predicted by the trained network, at an operating temperature of 20 °C are plotted versus their corresponding experimental values. The best line fit indicates the good quality of the network predictions. A slope of 1.08 and an intercept of −2.54 represent a reasonably good agreement between the predicted and experimental values of the permeate rate. The coefficient of correlation R^2 has a value of 0.989. This example, has demonstrated the well-known fact that NNs exhibit very good interpolation capabilities.

To check the reliability of the NN for extrapolation, a third case was considered. In this case, the experimental data were again divided into two sets. The set first set (training set) was composed of the data corresponding to the 10 and 20 °C operating temperatures. The second set, which contained the data corresponding to an operating temperature of 30 °C was used for testing the network. The network was trained and then simulated using the test data set. A linear regression between the actual and predicted permeate rates was then performed. A line, having a

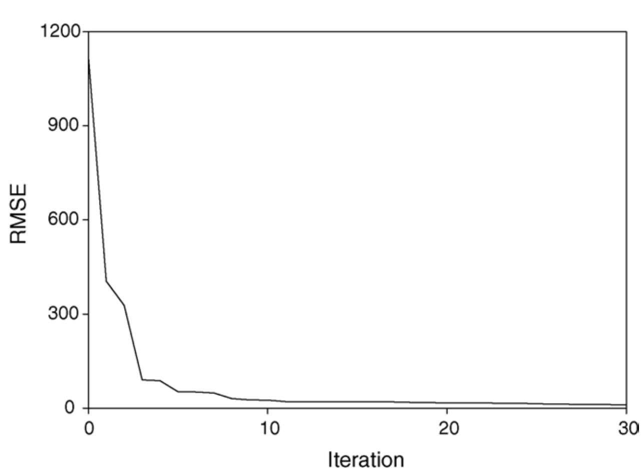

Fig. 3. RMSE as a function of the number of iterations (epochs).

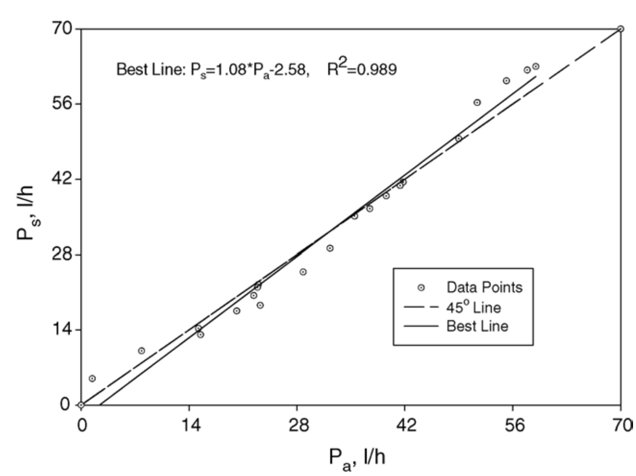

Fig. 5. Predicted vs. actual permeate rates at 20 °C (Case 2).

slope of 0.381 and an intercept of 84.8, was obtained. These two values indicate that the network did not yield reasonable predictions of the experimental permeate rates. This performance of the network is attributed to the limited number of training data used and the fact that, generally, NNs do not yield reliable results when used to extrapolate actual data [23,24].

5. Conclusion

A feedforward neural network was built to model the performance of an RO experimental setup, which was subjected to a series of different operating conditions. The network inputs were the operating pressure, operating temperature and feed concentration, and the output was the permeate rate. The use of the Levenberg–Marquardt optimization technique led to fast training of the network. Simulations of the trained network yielded permeate rates, which are very close to the actual values. The NN was also found to interpolate the data with good accuracy. As expected, however, the network did not produce acceptable results when used for data extrapolation.

References

[1] K. Wangnick, IDA Worldwide Desalting Plants Inventory Report No. 17, Wangnick Consulting GmbH, Gnarrenburg, Germany, 2002.
[2] W.F.J.M. Nooijen, J.W. Wouters, Optimization and planning of seawater desalination, Desalination 89 (1) (1992) 1–19.
[3] N.M. Wade, Distillation plant development and cost update, Desalination 136 (1–3) (2001) 3–12.
[4] B.S. Parekh (Ed.), Reverse Osmosis Technology: Application for High-Purity Water Production, Marcel Dekker Inc., New York, 1988.
[5] H. Demuth, M. Beale, User's Guide: Neural Network Toolbox for Use with Matlab, The Mathworks Inc., 2000.
[6] C.A.O. Nascimento, R. Giudici, R. Guardani, Neural network based approach for optimization of industrial chemical processes, Comp. Chem. Eng. 24 (9–10) (2000) 2303–2314.
[7] N. Delegrange-Vincent, C. Cabassud, M. Cabassud, L. Durand-Bourlier, J.M. Laine, Neural networks for long term prediction of fouling and backwash efficiency in ultrafiltration for drinking water prediction, Desalination 131 (1–3) (2000) 353–362.
[8] M.J. Willis, G.A. Montague, C. Di Massimo, M.T. Tham, A.J. Morris, Artificial neural networks in process estimation and control, Automatica 28 (6) (1992) 1181–1187.
[9] G.M. Pigram, T.R. Macdonald, Use of neural network models to predict industrial bioreactor effluent quality, Environ. Sci. Technol. 35 (1) (2001) 157–162.
[10] A.R. Mirzai, J.R. Leigh, An overview of the applications of neural networks in process engineering, Comput. Control Eng. J. 3 (5) (1992) 105–112.
[11] T.W. Karjala, D.M. Himmelblau, Dynamic data rectification by recurrent neural networks vs. traditional methods, AIChE J. 40 (11) (1994) 1865–1875.
[12] K. Al-Shayji, Y.A. Liu, Neural networks for predictive modeling and optimization of large-scale commercial water desalination plants, Proc. IDA World Congr. Desalination Water Sci. 1 (1997) 1–15.
[13] K. Al-Shayji, Y.A. Liu, Predictive modeling of large-scale commercial water desalination plants: data-based neural network and model-based process simulation, Ind. Eng. Chem. Res. 41 (25) (2002) 6460–6474.
[14] M.M. Jafar, A. Zilouchian, Adaptive receptive fields for radial basis functions, Desalination 135 (2001) 83–91.
[15] A.F. Abdulbary, L.L. Lai, K.V. Reddy, S.M. Al-Gobaisi, Artificial neural networks as efficient tools of simulation, Proc. IDA World Congr. Desalination Water Sci. 4 (1995) 361–374.
[16] S. Parenti, S. Bogi, A. Massarani, Industrial application of real time neural networks in multistage desalination plant, Proc. IDA World Congr. Desalination Water Sci. 1 (1995) 457–467.
[17] S. Ramasamy, P.B. Deshpande, S.S. Tambe, B.D. Kulkarni, Identification and advanced controls of MSF desalination plants with neural networks, Proc. IDA World Congr. Desalination Water Sci. 1 (1995) 36–51.
[18] M. Cabassud, N. Delgrange-Vincent, C. Cabassud, L. Durand-Bourlier, J.M. Lainé, Neural networks: a tool to improve UF plant productivity, Desalination 145 (1–3) (2002) 223–231.
[19] S.M.A. Razavi, S.M. Mousavi, S.A. Mortazavi, Dynamic modeling of milk ultrafiltration by artificial neural network, J. Membr. Sci. 220 (18) (2003) 47–58.
[20] S.M.A. Razavi, S.M. Mousavi, S.A. Mortazavi, Dynamic prediction of milk ultrafiltration performance: a neural network approach, Chem. Eng. Sci. 58 (18) (2003) 4185–4195.
[21] G.R. Shetty, S. Chellam, Predicting membrane fouling during municipal drinking water nanofiltration using artificial neural networks, J. Membr. Sci. 217 (1–2) (2003) 69–86.
[22] W.R. Bowen, M.G. Jones, J.S. Welfoot, H.N.S. Yousef, Predicting salt rejections at nanofiltration membranes using artificial neural networks, Desalination 129 (2) (2000) 147–162.
[23] J.A. Hertz, A.S. Krogh, R.G. Palmor, Introduction to the Theory of Neural Computation, Addison Wesley, New York, 1991.
[24] M.T. Hagan, M. Menhaj, Training feedforward networks with the marquardt algorithm, IEEE Trans. Neural Netw. 5 (1994) 989–993.
[25] N. Al-Bastaki, A. Abbas, Periodic operation of a reverse osmosis water desalination unit, Sep. Sci. Tech. 33 (1998) 2531–2540.