



Prediction of RO Membrane Performances by Use of Adaptive Network-Based Fuzzy Interference Systems

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Abstract

This study aims to develop an Adaptive Network-based Fuzzy Inference System technique (ANFIS) and using the parameters of a complex mathematical model in the RO membrane performances. The ANFIS was constructed by using a subtractive clustering method to generate initial fuzzy inference systems. The model trained by 70% of the data set and then its validity is examined by remained 30% data set. The result indicated that this method could predict the performance of the RO membrane faster and more accurately than previous numerical techniques. The squared correlation coefficient between real data and predicted data of this technique was 0.9973 for separation factor, 0.9916 for NP and 0.9975 NT, which are better in comparison with numerical methods, and previous Artificial Neural network used by the author to model these membranes. It was observed that the squash factor, reject ratio, and accept ratio has no significant effect on ANFIS performance. Results showed that for all cases better performances achieved when this parameter has a value of more than 0.5, as 0.86 for separation factor, 0.91 for net pre flux, and 0.83 for total flux. This technique just takes a few seconds to model RO membrane performance which is very faster than other numerical methods. So, this technique could be a powerful method to predict RO membranes.

Keywords:

ANFIS,
Membrane,
RO Performances,
Separation

Introduction

Membrane processes are attractive due to economic characteristics and lack of requirement for phase changing. Reverse osmosis (RO) used as a separation technique to remove a high amount of impurities from solutions in petrochemical and biochemical industries. RO is one of the most effective methods for the desalination process, treatment of oily wastewater in chemical process industries, and the production of ultra-pure water (UPW) in the electronic industry [1-8].

In the desalination process, seawater is compressed more than its osmotic pressure and only water molecules transmit through the membrane [4]. RO processes enable to produce purified water, even recycling of nutrients as a form of permeate from municipal wastewater stream potentially rich in solids, soluble salts, microorganisms, and dissolved organic compounds [7]. In recent years, RO separation technology has been used as the primary technology of UPW production operation for removing pollutants from source water [8].

By the advancement of different separation technologies as well as RO applications, the prediction of this method has a significant role in this scope. Therefore, extensive research has

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been conducted to provide a developed mathematical model for predicting membrane under different conditions [9-19].

Among the existing models, the Surface Force-Pore Flow (SF-PF), Modified Surface Force-Pore Flow (MD-SF-PF), and especially its extended model (Ex- MD-SF-PF) can properly model RO membrane functions. In contrast to the proposed complex models, accurate results can be obtained by using new algebraic techniques such as a neural network with fewer calculations [18-22]. Although these models verified experimental data accurately, due to complex differential equations, it needs heavy numerical calculations for obtaining some desirable results. For example, a study which was done in 2010 by CFD method that predicts RO membrane performances with the square coefficient error between 0.89 to 0.99, this technique takes about 40 minutes to model this phenomenon [23].

During the last 20 years, Artificial Intelligence methods such as Artificial Neural networks, Heuristic algorithms, and Fuzzy methods have been used in all engineering fields. This fact is due to their applicability and its simplicity to solve complex nonlinear equations in less time than conventional analytical and numerical methods. These methods have been used successfully in various problems including the chemical industry. So, these methods as an alternative approach could be applied for process modeling, particularly in cases where reliable other models cannot be considered.

Artificial Intelligence techniques were used previously in the RO membrane modeling field, most of these studies done with Artificial neural networks [24-36]. Adaptive network-based fuzzy Inference System is a new technique which combines Artificial neural network with fuzzy logic, so this method is a more powerful technique to model complex phenomena [37]. The author in a previous manuscript has an attempt to Predict the RO Model performance parameter, at that attempt, a feed-forward artificial neural network was used to construct the model. That attempt has good correlation coefficient between experimental data and predicted data, the result showed that separation factor (f) was predicted with a correlation square coefficient equal to 0.933, Pure solvent flux with a correlation coefficient square equal to 0.996, and total Flux with correlation coefficient square equal to 0.996. Also, neural networks could predict this parameter accurately, but because of the Adaptive network base, Artificial networks are a combination of fuzzy logic and Neural Networks and usually could be predicted complicated parameters more accurate than other soft computing models, in this study this technique is used to Model RO membrane.

The main purpose of this paper was to evaluate membrane performances such as separation factor (f), pure solvent flux (N_p), total flux passing through the membrane by use of adaptive network-based fuzzy inference system (ANFIS) and comparing the result with a method which is based on CFD method [23]. The results could be obtained through input parameters including average longitude concentration, operational condition, and MD-SF-PF model parameters. It could be expected that the ANFIS technique should estimate RO membrane performance with negligible errors. Therefore, this method can be used to evaluate the RO membranes in both industry and laboratory experiments.

Theory

Reverse Osmosis

The direct osmosis process is the spontaneous diffusion of fluid through a permeable membrane from the low solute concentration area to the high solute concentration area. The pressure difference (osmotic pressure) forces the liquid to diffuse through the membrane. If an external pressure applied to reverse more than the osmotic pressure, the pure solvent moves in the opposite direction which is called reverse osmosis. In the following step, the molecules of

solvent (water) move from dilute concentration (brackish water) to a higher concentration area. As a result, the RO process is the tendency of molecules to diffuse via a semi-permeable membrane by acting pressure on the solution. Usually, pure solvent flux (N_P) and total flux (N_T) are measured. The difference between the concentration of input and output solutes is the Separation factor (f) and it can be calculated from Eq. 1. Fig. 1 depicts a simplified general scheme of the RO membrane separation process [20-22].

$$f = \frac{C_{A1} - C_{A3}}{C_{A1}} \quad (1)$$

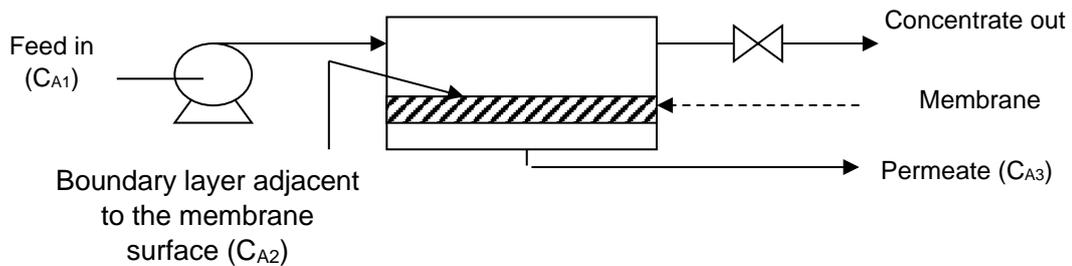


Fig. 1. General scheme of the RO membrane process.

The separation factor is defined in Eq. 2 based on the concentration polarization of solute near the membrane (C_{A2}) is greater than its bulk concentration (C_{A1}).

$$f' = \frac{C_{A2} - C_{A3}}{C_{A1}} \quad (2)$$

There are several driving forces involved in separation processes such as the difference in concentration, pressure, and electrical. In RO membranes, the main parameters are concentration and pressure gradients [20-22].

MD-SF-PF Model

In the MD-SF-PF mechanism base model, membrane structure is supposed to have circular cross micro-pores. Therefore, the concentration and velocity depend on axial and radial directions. The solute-membrane relation is determined by the Sutherland type potential function, which changes through the radial orientation of the micropores [19]. The coefficient of Friction indicates the hydrodynamic drag on the solute molecules and is measured by the proportion of the diffusivity coefficient of solute in solution to diffusivity coefficient within a micro-pore [19-22].

In the following section, the model parameters (θ_1, θ_2), and properties of Membrane τ / ε (Friction constants, R_w and X_{A1}, X_{A2}) have been used as input data set. The axial and radial coordination directions are presented as follows:

Where τ is pore length and R_w is wall pore radius.

$$\rho = \frac{r}{R_w} \quad (3)$$

$$\zeta = \frac{z}{\tau} \quad (4)$$

The differential equation indicating the velocity profile across through (α) the membrane porous media which is calculated by the following equation.

$$\left[\frac{d^2\alpha(\rho)}{d\rho^2} + \frac{1}{\rho} \frac{d\alpha(\rho)}{d\rho} \right] + \frac{1}{\beta_1} \left[\frac{\Delta P}{\pi_2} - \frac{\pi_2\sigma_2(\rho) - \pi_3\sigma_3(\rho)}{\pi_2} \right] - \frac{1}{\beta_1} \left(1 - \frac{1}{b(\rho)} \right) [\alpha(\rho) + \omega(\rho)] \left[1 + \frac{1 - \left(\frac{\pi_3}{\pi_2} \right) k^*(\rho)}{\exp[(\alpha(\rho) + \omega(\rho))] - 1} \right] \exp(-\Phi(\rho, 0)) = 0 \quad (5)$$

where:

$$\beta_1 = \frac{\eta D_{AB}}{R_w^2 \pi_2} \quad (6)$$

$$\sigma_2(\rho) = 1 - \exp(-\Phi(\rho, 0)) \quad (7)$$

$$\sigma_3(\rho) = 1 - \exp(-\Phi(\rho, 1)) \quad (8)$$

$$\omega(\rho) = \frac{V_A}{RT} [\Delta p - (\sigma_2(\rho)\pi_2 - \sigma_3(\rho)\pi_3)] \quad (9)$$

$$k^*(\rho) = \frac{\exp(-\Phi(\rho, 1))}{\exp(-\Phi(\rho, 0))} \quad (10)$$

$$\alpha(\rho) = \frac{U_B(\rho)\tau}{D_{AB}} \quad (11)$$

According to the Van't Hoff's equation, the osmotic pressure is:

$$\pi = (\nu^+ + \nu^-) C_A RT \quad (12)$$

In order to predict the separation coefficient and fluxes parameters in the membrane modeling, the presence of concentration is unavoidable and it is estimated from the concentration equation.

$$C_{A3} = C \left[1 + CRT \frac{l_1}{l_3} \right]^{-1} \quad (13)$$

In which:

$$l_1 = \int_0^1 \alpha(\rho) \rho d\rho \quad (14)$$

$$l_3 = \int_0^{1-\lambda} [\alpha(\rho) + \omega(\rho)] \left(\pi_2 + \frac{\pi_2 - k^*(\rho)\pi_3}{\exp[(\alpha(\rho) + \omega(\rho))] - 1} \right) \frac{\exp(-\Phi(\rho, 0))}{b(\rho)} \rho d\rho \quad (15)$$

The solute and solvent fluxes are given below:

$$N_A = \varepsilon J_A = \frac{2}{X_{AB}} (\varepsilon / \tau) \int_0^{1-\lambda} \frac{[\alpha(\rho) + \omega(\rho)]}{b(\rho)} \left(\pi_2 + \frac{\pi_2 - k^*(\rho)\pi_3}{\exp[(\alpha(\rho) + \omega(\rho))] - 1} \right) \exp(-\Phi(\rho, 0)) \rho d\rho \quad (16)$$

$$N_B = \varepsilon J_B = \frac{2}{X_{AB}} (\varepsilon / \tau) CRT \int_0^1 \alpha(\rho) \rho d\rho \quad (17)$$

And the total flux is express as:

$$N_T = (N_A + N_B) = \frac{2}{X_{AB}} \left(\frac{\varepsilon}{\tau} \right) (l_3 + CRT l_1) \quad (18)$$

And the pure solvent flux is described as:

$$N_p = A\Delta P, \quad A = \frac{CR_w^2}{8\eta(\tau/\varepsilon)} \quad (19)$$

The equation for friction parameter $b(\rho)$ is given below:

$$b = \frac{X_{AB} + X_{AM}}{X_{AB}} = \frac{D_{AB}}{D_{AM}} \quad (20)$$

$$b(\rho) = \begin{cases} b_{Faxen} \exp\left(\frac{E}{R_w(1-\rho)}\right) & \text{when } \rho < 1-\lambda \\ \infty & \text{when } \rho \geq 1-\lambda \end{cases} \quad (21)$$

The solute-membrane interactions are presented by a potential function (Φ) which is a diffusive phenomenon that indicates the applied force on the solute. In the “MD-SF-PF” mathematical model the equation can be defined as one dimensional.

$$\Phi(\rho, \zeta) = \begin{cases} \frac{\theta_1}{R_w} e^{\theta_2 \rho^2} & \text{when } \rho < 1-\lambda \\ \infty & \text{when } \rho \geq 1-\lambda \end{cases} \quad (22)$$

Fuzzy Systems

Fuzzy logic (FL) and fuzzy inference systems (FIS) have wide applicability and they are a promising approach for analyzing ambiguous, imprecise, or subjective data. A fuzzy inference process widely combines fuzzy rules, membership functions, fuzzification, and defuzzification. By using fuzzy inference in optimization problems, it is simple to be understood and interpreted ordinary crisp input-output data. Generally, there are two main classes of fuzzy inference processes, namely Mamdani and Sugeno FIS, a typical Mamdani FIS system. Sugeno type of fuzzy inference consists of fuzzy sets or membership functions in the premise part. A FIS has two inputs and two ST rules are usually as follows:

$$R^1: \text{ if } x_1 \text{ is } A_1^1 \text{ and } x_2 \text{ is } A_2^1 \text{ then } f_1 = p_1x_1 + q_1x_2 + c_1$$

$$R^2: \text{ if } x_1 \text{ is } A_1^2 \text{ and } x_2 \text{ is } A_2^2 \text{ then } f_2 = p_2x_1 + q_2x_2 + c_2$$

For modeling complex problems in this study, the first order ST FIS based model is primarily used to evaluate the relationships between inputs and outputs [38].

ANFIS

ANFIS is a multi-layer adaptive network-based fuzzy inference system suggested by Jang. An ANFIS construct of five layers to perform different node operations to learn and tune coefficients of FIS using a hybrid approach. Simply ANFIS combined neural network and fuzzy inference systems to do more accurate modeling [37]. Fig. 2 shows a schematic of ANFIS, in this system every input is valorized using membership functions, fuzzy inference systems are applied (just Sugeno type), some operations like neural networks will be done and then output is defuzzified [38].

There are several forms to make FIS in ANFIS like subtractive clustering method and grid partitioning, also in MATLAB there are four parameters that affect ANFIS including range of influence, reject ratio, accept ratio, and squashing factor [3].

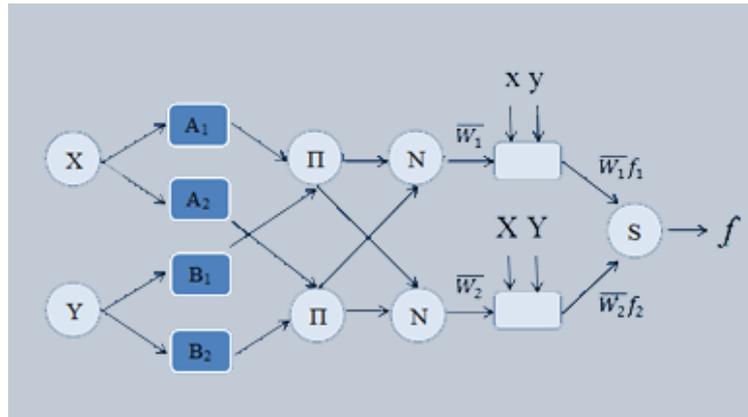


Fig. 2. a schematic of ANFIS structure [38].

ANFIS-SUB

Chiu by extending the mountain clustering method proposed the subtractive clustering method in order to subtract the optimization process [39,40]. This approach clusters data points based on an unsupervised learning method with respect to evaluating the potential of data in the feature vector. It is easy to apply for predicting a set of clusters and cluster centers when there is not a distinction associated with a given experimental point. The subtractive clustering approach presumes that each data point is a potential cluster center and estimates the potential function of density-based for each data point. Then the data point with the highest potential is selected as the first cluster grid, and the potential of data points nearby the origin grid is eliminated. The optimum point with the maximum remaining potential according to the center of the next cluster and the potential of point adjacent to the new cluster center is removed. In this method, the influential radius is very important for evaluating the number of clusters. The radius with a low value generated a higher number of clusters in the data space leading to the overestimation of a higher number of rule sets. Therefore, the influential radius is affecting clustering data space calculation. The next step is determining fuzzy rules and fuzzy membership functions. Then, a simple regression method and linear squares estimation (LSE) is used to evaluate the output MF as a result of valid FIS. According to explanation, ANFIS is one of the most powerful approaches to learn and refine the premise of fuzzy MF by using a combination of the least-squares estimation and backpropagation (BP) learning algorithm [39,40].

Methodology

In this study, the ANFIS was construct using MATLAB FUZZY TOOLBOX, and the subtractive clustering method was used to generate initial FIS. Predictions were done using data of a previous study on the modified surface force-pore flow model, some errors in this operation used to evaluate these systems are present here:

$$e_i = [P_m - P_e]_i \quad (23)$$

$$AAPE = \frac{1}{n} \sum_{i=1}^n |e_i| \quad (24)$$

$$MSE = \frac{1}{Q} \sum_{i=1}^Q e_i^2 \quad (25)$$

$$P_{av} = \frac{1}{n} \sum_{i=1}^n P_i \quad (26)$$

Correlation Coefficient or Pearson Coefficient:

$$R = \frac{\sum_{i=1}^n [(P_{m,i} - P_{m,av}) \times (P_{e,i} - P_{e,av})]}{\sqrt{\sum_{i=1}^n [(P_{m,i} - P_{m,av})^2] \times \sum_{i=1}^n (P_{e,i} - P_{e,av})^2}} \quad (27)$$

Where P_m is the target value and P_e is the value which are predicted by the model. In this case, data for train and test were chosen randomly (0.7 of data set for training and 0.3 for testing, effective parameters on ANFIS performance (subtractive clustering FIS) which consist of squash factor, accept ratio, reject ratios and Range of influence changed in their interval to obtain the best accuracy in prediction. Validation of ANFIS performance in this study is calculated by mean square error (MSE), correlation coefficient (R), and Absolute average percent error (AAPE) which are defined in formulas previously.

Result and Discussions

For all of membrane performance parameters, one ANFIS model was constructed, parameters which are effective on ANFIS performance were survived to find optimum condition. For all cases, it was observed that the squash factor, reject ratio, and accept ratio has no significant effect on ANFIS performance, so these parameters regulated as MATLAB default values. But for the range of influence parameters was very effective on ANFIS performance. Results showed that for all cases better performances achieved in situations when this parameter has a value of more than 0.5, as 0.86 for separation factor, 0.91 for net pre flux, and 0.83 for total flux.

Table 1 shows the result of ANFIS when optimum constructing parameters applied to it, this table shows that in all cases predictions are very accurate, and R^2 for all of them is more than 0.995 which is very desirable and accurate in comparison with numerical methods. Also, other errors have negligible values, so it concluded that ANFIS has modeled the RO membrane application accurately.

Table 1. Result of ANFIS

RO Parameter	AAPE	APE	R^2	MSE
f	0.01	2.9374	0.9973	1.1695×10^{-4}
N_p	0.029	10.93	0.9953	4.776×10^{-6}
N_t	0.0176	13.22	0.9988	2.0840×10^{-5}

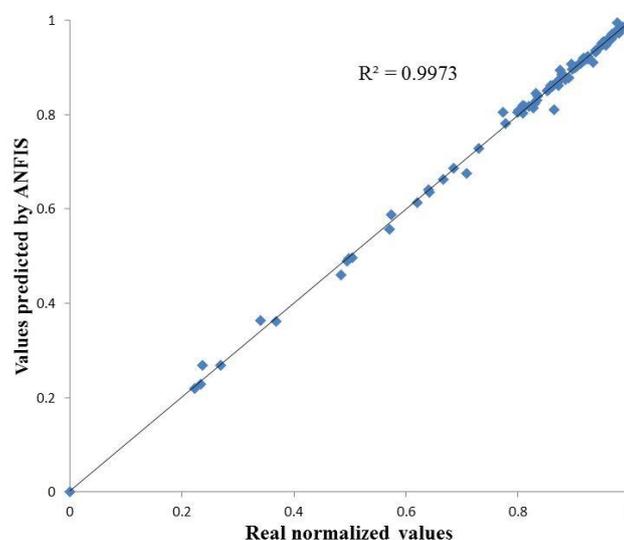


Fig. 3. Comparison among experimental and computed values by ANFIS for separation factor (f)

Fig. 3 shows the comparison between the normalized real value of separation factor and values predicted by ANFIS. This diagram which is developed for the test data set shows a good match between real and predicted values. So, it could be concluded that this model could be used to predict this parameter more accurately than numerical methods ($R^2 = 0.89$ for Golnari et al.).

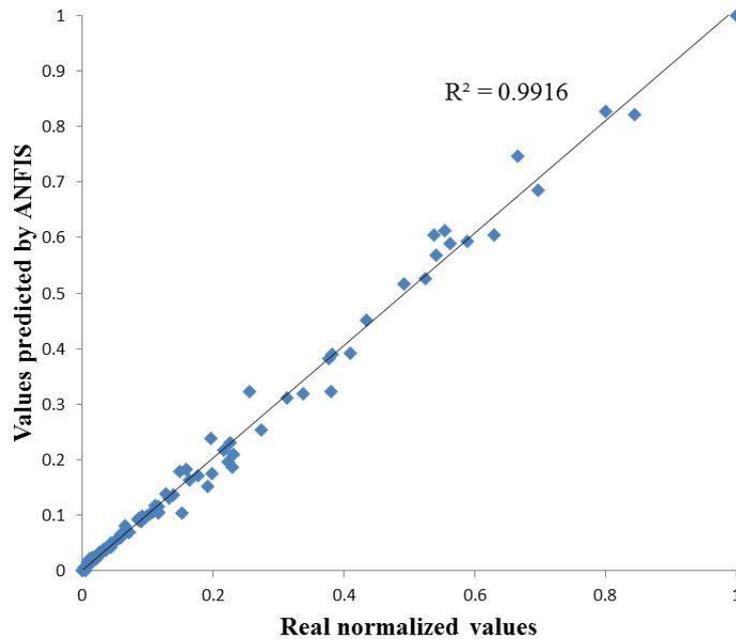


Fig. 4. Comparison among experimental and computed values by ANFIS for net pure flux (N_p)

Fig. 4 shows the comparison between the normalized value of real data and values which predict for net pure flux by ANFIS, this figure shows a good match too. The value of R^2 has the almost same value as numerical models, but because the ANFIS model is faster than the previous method, so it could be concluded that this model could be better and more useful.

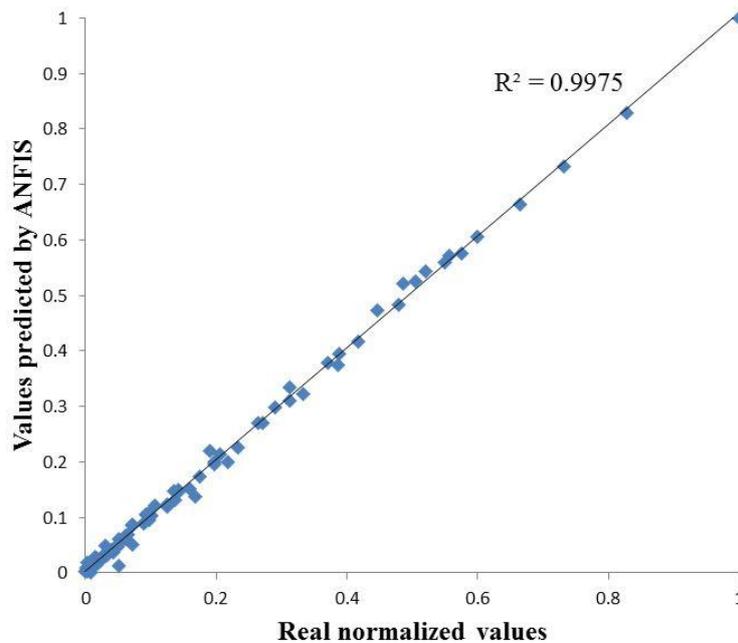


Fig. 5. Comparison among experimental and computed values by ANFIS for total flux (N_T)

Fig. 5 shows the comparison between the normalized value of real data and values which predict by ANFIS for total flux, in this case, a good match exists between real and predicted data too. The value of R^2 , in this case, has more value than the MD-SF-PF model. From the above result, it concluded that ANFIS could predict RO membrane performance better or the same mathematical models, but this method is very faster than previous models, so it can be used as powerful alternative methods to these models.

Conclusions

The present study focused on membrane performances such as separation factor (f), pure solvent flux (N_p), total flux passing through the membrane by use of an adaptive network-based fuzzy inference system, and comparing the result with a method which is based on CFD method. The results of this study show that the ANFIS enabled to predict the RO membrane performances faster and more accurate in comparison with mathematical models. The separation with R^2 equals to 0.9973, the pure solvent flux R^2 equals to 0.9916 and for total flux, R^2 equals to 0.9975. In all cases, the theoretical data can predict the input data and there is the best fit trend between outcomes of models and experimental values. These predicted data have more accuracy than mathematical models, Also, this method takes less time than one minute to model the RO membrane, which is very fast in comparison with mathematical methods.

Nomenclature

$b(\rho)$	Friction function, dimensionless
$C_A(r, z)$	Concentration of solute inside a pore, (kmole/m ³)
$J_{A,r}(r)$	Radial component of solute flux through a single pore, (kmole/m ² -sec)
$J_{A,z}(r)$	Axial component of solute flux through a single pore, (kmole/m ² -sec)
l_1 & l_3	Definite integral, dimensionless
N_i	Flux of i through membrane, (kmole/m ² -sec)
f'	Theoretical separation, dimensionless
C	Molar density of solution, (kmole/m ³)
P	Hydrostatic pressure, (kPa)
D_{AB}	Solute diffusivity in free solution, (m ² /sec)
D_{AM}	Solute diffusivity inside the pore, (m ² /sec)
r	Cylindrical coordinate normal to the pore wall, (m)
R	Gas constant, (kJ/kmole-K)
T	Temperature, (K)
$k^*(\rho)$	Ratio of local partition coefficients at the ends of a pore for solute
$U_i(r)$	Velocity of i inside the pore, (m/sec)
z	Cylindrical coordinate parallel to the pore wall, (m)
OF	Objective function
RMSD	Parameter

Greek letters

$\alpha(\rho)$	Velocity defined, dimensionless
β_1	Parameter defined, dimensionless
ΔP	Pressure drop across the membrane, (kPa)
ε	Fractional pore area of membrane, dimensionless
ρ	Radial coordinate, dimensionless

τ	Average pore length taking tortuosity into account, (m)
$\Phi(\rho, \zeta)$	Potential function, dimensionless
η	Solution viscosity, (kPa-sec)
θ_1	Potential parameter, (m)
θ_2	Potential parameter, dimensionless
λ	Parameter defined, dimensionless
ζ	Axial coordinate, dimensionless
$\sigma_2(\rho)$	Local Staverman (reflection) coefficient at the feed-membrane interface
$\sigma_3(\rho)$	Local Staverman (reflection) coefficient at permeate-membrane interface
V_A	Partial molar volume of solute (m ³ /kmole)
$\omega(\rho)$	Parameter

Subscripts:

1	feed solution
2	feed at the membrane interface
3	permeate solution.
A	solute
B	solvent
M	membrane
P	pure solvent (pure water)
T	total solution
W	pore wall

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