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Modeling water flux in osmotic membrane bioreactor by adaptive network-based fuzzy inference system and artificial neural network

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Abstract

Osmotic Membrane Bioreactor (OMBR) is an emerging technology for wastewater treatment with membrane fouling as a major challenge. This study aims to develop Adaptive Network-based Fuzzy Inference System (ANFIS) and Artificial Neural Network (ANN) models in simulating and predicting water flux in OMBR. Mixed liquor suspended solid (MLSS), electrical conductivity (EC) and dissolved oxygen (DO) were used as model inputs. Good prediction was demonstrated by both ANFIS models with R^2 of 0.9755 and 0.9861, and ANN models with R^2 of 0.9404 and 0.9817, for thin film composite (TFC) and cellulose triacetate (CTA) membranes, respectively. The root mean square error for TFC (0.2527) and CTA (0.1230) in ANFIS models was lower than in ANN models at 0.4049 and 0.1449. Sensitivity analysis showed that EC was the most important factor for both TFC and CTA membranes in ANN models, while EC (TFC) and MLSS (CTA) are key parameters in ANFIS models.

Keywords: OMBR; Water flux; Membrane process; Modeling; ANFIS, ANN

1. Introduction

Water borne diseases are the main cause of 3.4 million human death, mostly children, based on the World Water Development Report 2018 (Yanar et al., 2020). Providing clean water for all people is therefore critical to protect human wellbeing. However, considering water scarcity in the world and necessity to treat water and wastewater including desalination to provide the required clean water, the major problem is the energy consumption required for the water and wastewater treatment processes (Liu et al., 2020; Yanar et al., 2020). In order to provide clean drinking water from wastewater and saline water sources, membrane-based purification systems are considered as promising technologies (Luo et al., 2018). These include microfiltration, nanofiltration, ultrafiltration, reverse osmosis, forward osmosis (FO), membrane distillation and membrane bioreactors (MBRs) (Aftab et al., 2017; Tow et al., 2018; Wu et al., 2020).

The integration of FO systems into the traditional biological processes has been proposed as an emerging technology in wastewater treatment, which is known as Osmotic Membrane Bioreactor (OMBR). In this process, the osmotic pressure differences between feed and draw solutions (DS) in both internal and external sides of a semi-permeable FO membrane extract water from feed solution (Cornelissen et al., 2008). However, DS reverse permeation causes salinity build-up detected by mixed liquor electrical conductivity (EC) as a challenging problem in OMBR, which can be adjusted by installing a microfiltration system in FO-MBR process not to adversely affect the biological process (Pathak et al., 2018). Mixed liquor suspended solid (MLSS) is another important parameter in such combined membrane and biological processes affecting wastewater treatment as well as membrane fouling (Aftab et al., 2017). In comparison to MBRs, OMBRs take advantage of better-quality product water, more fouling reversibility and less tendency of membrane fouling (Wang et al., 2016). It is worth highlighting that there are advantages for all of the membrane technologies such as higher purification efficiency, lower sludge production, less chemical additives, more flexibility and

less footprint than conventional biological methods (Chen et al., 2020a; Ibrar et al., 2020; Wu et al., 2020). However, the main restriction of these technologies is membrane fouling (Chen et al., 2020b; Ibrar et al., 2020). Fouling minimization and consequently augmentation of water flux are considered as the most important targets in the OMBR process (Tran et al., 2019). The presence of particulate, colloid and dissolved substances coupled with water-borne microorganisms in the influent is the main cause of the membrane fouling (Kochkodan and Hilal, 2015; Kwan et al., 2015; She et al., 2016; Zhao et al., 2012). Membrane fouling can be classified into four main categories, i.e. microbial, organic, inorganic or mineral and colloidal fouling (She et al., 2016; Tijing et al., 2015). However, in FO part of the OMBR process, concentration polarization (CP) is regarded as the main reason for the reduction in water flux compared to theoretical calculation. CP can be classified into dilutive external and internal CP, and concentrative external and internal CP. Among all types of CPs, dilutive internal concentration polarization (DICP) has the most detrimental effect on the performance of the FO process and is the main reason for sharp reduction in water flux. This is due to the fact that the more diluted the draw solution, the more diminution in osmotic driving force will occur (Arjmandi et al., 2020). Besides, aeration has demonstrated a critical role for fouling prevention in membrane processes, due to the great shear force induced on the membrane surface by air bubbles. The shear stress increases with the aeration rate, hence reducing membrane fouling (Johir et al., 2012). Regarding the effect of MLSS on membrane fouling, it is notable that due to the diversity and complexity of the biological sludge, the effectiveness of this parameter depends on other factors such as biomass properties and polymer components. However, there is an overall direct relationship between the concentration of MLSS and fouling in membrane biological systems (Le-Clech et al., 2003). Thus, these parameters play important roles in the evolution of the OMBR process. The effects of fouling on membrane treatment technologies include lower water quality, less water permeability, shorter membrane life and higher transmembrane pressure (Liu et al., 2020; She et al., 2016;

Sun et al., 2015). In addition, fouling increases both the operational and capital costs in membrane technologies (Fenu et al., 2010). Different methods have been applied to mitigate membrane fouling such as application of various nanomaterials in membrane structures (Guo et al., 2019; Wen et al., 2019), chemical treatment, hydraulic cleaning like backwashing and membrane relaxation (Cai and Liu, 2016; Guo et al., 2019; Linares et al., 2016; Woo et al., 2015), air scouring (González et al., 2018), optimization of operating conditions (Bunani et al., 2018), anti-biofouling membrane development (Karkhanechi et al., 2014) and process design modification (Stoller et al., 2013). Therefore, the control of membrane fouling resulting in stable production of the water flux has great importance for maintaining OMBR performance.

As the OMBR process is highly complex, its performance is very difficult to predict due to the lack of sufficient knowledge about different parameters. Therefore, more efficient options are needed to predict the membrane process performance, in particular OMBR (Sargolzaei et al., 2012; Zuthi et al., 2017). To date, studies on modeling the OMBR process are scarce.

As a flexible and effective modeling method, Artificial Neural Network (ANN) can learn the linear and nonlinear correlations between different variables from a set of data. In addition, this procedure is able to model various processes without the full understanding of mathematical background and nature of complicated mechanisms of various processes (Hosseinzadeh et al., 2020). Furthermore, Adaptive Network-based Fuzzy Inference System (ANFIS), which is a combination of fuzzy logic and ANN, benefits from the learning ability of ANN and is proposed as a more powerful procedure to generate results that are more accurate than ANN (Rego et al., 2018). In fuzzy logic applications, a group of IF-THEN rules is generated by the knowledge of the user; however, the group of these rules in ANFIS application is produced from the pairs of input-output in the dataset by the system based on the learning ability of ANN in ANFIS. Several studies applied ANFIS and ANN models

simultaneously to predict different parameters in various fields and showed different performances in different applications (Dashti et al., 2018; Rahmanian et al., 2012); however, there has been no such study in using these two models to assess the performance of membrane technologies for water and wastewater treatment. Currently, cellulose triacetate (CTA) and thin film composite (TFC) are the most widely used membranes in the FO process (Pathak et al., 2018; Ibrar et al., 2020). This study aims to develop ANFIS and ANN models to simulate and predict the water flux by these two popular membranes in the OMBR process under various conditions of MLSS, EC and DO. In addition, the performance of ANN and ANFIS models was compared in their application, and the importance of the key parameters was determined using sensitivity analysis.

2. Materials and methods

2.1. Data collection and processing

In this work, results from published studies are used for model development and simulation. After a detailed literature review regarding the OMBR process, only four relevant datasets (Zhang et al., 2017; Zhu et al., 2018; Luo et al., 2015) were found with comparable conditions in terms of the aerobic condition, application of both FO and microfiltration in MBR for controlling the salinity, use of NaCl solution as draw solution, having suspended MLSS without any media and FO mode. Of the four datasets extracted from various studies on OMBR, two of which were regarding the performance of CTA membrane (Luo et al., 2015; Zhang et al., 2017) and the others were for TFC membrane (Zhang et al., 2017; Zhu et al., 2018). It should be stressed that all of the extracted data were for the same period of OMBR process from the beginning up to membrane cleaning. For data processing, all of the input data were randomized in the range of 0.1 to 0.9 using equation 1 (Hosseinzadeh et al., 2020):

$$x_i \text{ normalized proportion} = \frac{x_i - \text{data minimum value}}{\text{data maximum value} - \text{data minimum value}} \times (0.9 - 0.1) + 0.1 \quad (1)$$

Data normalization was carried out to prevent over-training and to decrease the computational complexity. However, the output data were not normalized.

2.2. Artificial neural network

In this study, a feed-forward ANN model was used to simulate water flux in the OMBR process. During model structure design, the number of neurons in input and output layers were determined according to the number of input and output variables. With loading different neurons in hidden layer of ANN model along with various training procedures, a large number of neural networks were designed and evaluated. The accuracy of these models in training, validation and test phases was calculated by R^2 and mean square error (MSE) as statistical indices based on which the best model was selected. For modeling, all data were divided into two sections of 80% and 20%; the first section (i.e. 80%) was used for training, validation and test with portions of 70%, 15% and 15%, respectively; and the rest (20%) was applied for an additional test. To choose the best training algorithm, four backpropagation training algorithms including Levenberg-Marquardt (trainlm), resilient back-propagation (trainrp), scaled conjugate gradient (trainscg) and gradient descent with momentum (traingdm) were applied with the same initial input data. In addition, a linear transfer function (purelin) and tangent sigmoid transfer function (tansig) were employed in output and hidden layers, respectively. Using MSE equation (Table 1), the values of MSE were calculated. To obtain the most appropriate number of neurons applied, the neurons with different numbers ranging from 1 to 20 in the hidden layer of the neural networks were studied. In addition, this modeling was performed with ten replications in all three phases of training, validation and testing of the network to mitigate the errors and to increase the estimation accuracy of the network weights as well as output predictions.

2.3. Adaptive neuro fuzzy inference system

The fuzzy system reasoning ability along with the ANN learning ability is combined by ANFIS. There are six layers in ANFIS structure including input, fuzzy, product and normalized, defuzzy, total output and output layers. There are adaptive nodes in the layers of defuzzy and fuzzy, for example, some of the applied factors in these adaptive nodes are verified at training stage. However, the nodes of the third and fourth layers, product and total output layer, are constant. The training procedure is the same as that in the ANN (Souza et al., 2018).

The function *genfis1* of Matlab with use of Gaussian (*gaussmf*), which is considered a membership function (MF), was applied to develop the fuzzy interference system for ANFIS. A hybrid optimization procedure, based on which the back-propagation algorithm is combined with the least-squares estimation, was applied to implement and simulate the network (Souza et al., 2018).

2.4. Sensitivity analysis

Garson (1991) first introduced sensitivity analysis as an equation-based procedure (equation 2), which is applied to evaluate the effective portion of various inputs on output. In ANN models, the importance of MLSS, EC and DO in water flux produced by CTA and TFC membranes in OMBR was assessed.

$$I_j = \frac{\sum_{m=1}^{N_h} \left(\left(\frac{|W_{jm}^{ih}|}{\sum_{k=1}^{N_i} |W_{km}^{ih}|} \right) \times |W_{mn}^{ho}| \right)}{\sum_{k=1}^{N_i} \left\{ \sum_{m=1}^{N_h} \left(\frac{|W_{km}^{ih}|}{\sum_{k=1}^{N_i} |W_{km}^{ih}|} \right) \times |W_{mn}^{ho}| \right\}} \times 100 \quad (2)$$

where I_j , N_i and N_h are correspondingly the importance of parameter (%), number of input parameters, and number of hidden layer neuron; W is ANN weight; m , k and n are respectively the number of hidden neurons, the number of input parameters, and the number of output parameters; and o , i and h are related to the output, hidden and output layers of ANN model (Baziar et al., 2017).

In order to verify the key independent parameter in ANFIS models, three single parameter models were developed for each of the MLSS, DO and EC variables under the best conditions of the constructed models. The assessment of the constructed models was carried out using the R^2 , the value of which determined the importance of the relevant independent parameters.

2.5. Comparison of ANN and ANFIS models

The root mean squared error (RMSE), R -squared (R^2), adjusted R^2 ($Adj-R^2$) and sum squared error (SSE) were applied to evaluate the goodness of fit and prediction accuracy of the developed models. As a principle, a model is deemed to be effective with high values of R^2 and $Adj-R^2$ and small values of RMSE and SSE. The equations applied to calculate the mentioned statistical indices are listed in Table 1 (Hosseinzadeh et al., 2018; 2020). It is notable that all extracted data for CTA and TFC water flux were applied in comparison, which were 58 and 76 extracted experimental data points, respectively.

3. Results and discussion

3.1. ANN models of CTA and TFC water fluxes

3.1.1. Backpropagation training algorithm choice

To obtain the best backpropagation training algorithm, the smaller the value of the MSE for each number of neurons in different training algorithms, the better the performance of the algorithms. Therefore, the trainlm was selected as the best one for ANN models of CTA and TFC performance.

3.1.2. Optimization of neuron number

In order to optimize the number of neurons in ANN models, the neurons with the lowest MSE proportions were selected in all three phases of training, validation and testing (Yetilmezsoy and Demirel, 2008). According to the obtained results, the neurons with the number 11 in trainlm algorithm showed the smallest MSE, and hence were chosen as the best one for TFC

membrane. Similarly, the neurons with the number 8 in trainlm algorithm showed the smallest MSE and were selected as the best one for CTA membrane. Therefore, the optimized topologies for ANN models of TFC and CTA were 4-11-1 and 4-8-1, in which the 4 and 1 are the number of neurons in input and output layers correspondingly.

3.1.3. Model validation and test

In total, 30% of the data were applied in validation and test phases (15% each). Using the ANN model and actual water flux data, the predicted water flux results were obtained by using equation 3. The obtained scatter plots (Figs 1 and 2), which depict the predicted values of the water flux versus the actual ones, demonstrate the correlation coefficient of these models in all three phases and for all data. As shown in Fig. 1, the R^2 values of the CTA membrane for three phases of training, validation and test were 0.9931, 0.9223 and 0.9440, respectively, while the R^2 for the whole dataset was 0.9842. Fig. 2 shows the proportions of 0.9317, 0.9917, 0.9600 and 0.9411 were the R^2 of train, validation, test and all data models for TFC water flux correspondingly.

According to the obtained results, the constructed models can predict the proportions of TFC and CTA membranes water fluxes up to 94.1% and 98.42%, respectively. It is notable that the MSE proportions for training, validation and testing phases were 0.1833, 0.0351, and 0.1354 for TFC membrane and 0.0093, 0.0146 and 0.0595 for CTA membrane, respectively.

The ANN model for water flux prediction is shown in equation 3:

$$ANN\ equation = Purelin\{W2 \times tansig(W1 \times [MLSS; DO; EC; Time] + b_1) + b_2\} \quad (3)$$

The equations for the best linear fit and R^2 regarding the built ANN model for all data of water flux of CTA membrane are consecutively presented in equations 4 and 5:

$$y = 1.0029x + 0.0052 \quad (4)$$

$$R^2 = 0.9842 \quad (5)$$

where y and x are the predicted and actual values of water flux, respectively. The equations for the best linear fit and R^2 regarding the built model of ANN for all data of water flux of TFC membrane are presented in equations 6 and 7:

$$y = 0.9507x + 0.3151 \quad (6)$$

$$R^2 = 0.9411 \quad (7)$$

In addition, the additional tests were conducted to predict water flux produced by CTA and TFC membranes using ANN models. Based on the obtained results (Fig. 3), the R^2 and MSE values were 0.9852 and 0.0301 for TFC membrane, and were 0.9730 and 0.2030 for CTA membrane, respectively.

In studying membrane fouling in an anoxic-aerobic MBR, Schmitt et al. (2018) showed high potential of ANN models with development of an ANN model with R^2 of 0.850 demonstrating that the developed ANN models in the present study take advantage of greater prediction strength (Schmitt et al., 2018). In another study, Tsompanas et al. (2019) applied the ANN to simulate the polarization of cylindrical microbial fuel cells (MFC) with two different types of membranes and electrode configurations and predict the voltage as an MFC output. The final developed ANN model possessed a topology of 4-10-1 exhibited R^2 of 0.9932 (Tsompanas et al., 2019). These promising prediction strengths of the ANN models in different studies reported as well as the present study demonstrate that the ANN is able to model a wide range of processes effectively.

3.2. ANFIS models of water fluxes in CTA and TFC membranes

Regarding the fact that in comparison to the structure of Mamdani fuzzy inference system (FIS), the Sugeno FIS demonstrates better performance in mathematical datasets; therefore, the latter one was applied in the present work to model the water flux in OMBR. In this method, the hybrid neural network optimization procedure was applied to model the response variable in both CTA and TFC membranes.

In this study, 80% and 20% of all data were used for training and testing correspondingly. Figs 4 and 5 show the train and test outputs of ANFIS models in water flux models of both TFC and CTA membranes. R^2 of the train and test datasets for developed ANFIS models were 0.9816 and 0.9625 for TFC membrane and MSE of these models were 0.044 and 0.150 respectively. This statistical parameter (R^2) for the constructed ANFIS model of CTA water flux was 0.9836 and 0.9934, and the MSE of the train and test datasets models was 0.016 and 0.009 correspondingly. The FIS generalization capacity is assessed by the testing data at each epoch. Error sizes of training and testing phases, which are representative of mapping function compatibility in ANFIS are shown in Figs 4 and 5. In fact, this parameter demonstrates the differences between experimental and predicted results. Besides, the membership function factors (MFFs) were adjusted somewhat to mimic well with the actual results during this modeling procedure.

Different MF types including triangular (trimf), Gaussian (gassmf), generalized bell-shaped (gbellmf), and trapezoidal (trapmf) were investigated to construct the best ANFIS models. Based on the results, two MF types of gassmf and trapmf were selected as the best models for TFC and CTA membranes, respectively. It is worth highlighting that two membership functions were assigned for each input variable to apply fuzzy rules under all the mentioned MF types. Besides, the output MF of the models were evaluated in two linear and constant forms. The obtained results for TFC and CTA membranes models are exhibited in Tables 2 and 3 respectively.

As can be seen in Tables 2 and 3, there was a high dependence between the training and testing errors and the optimization procedures and MF of the variables (input and output). The obtained residual errors for these procedures in TFC and CTA ANFIS models as well as the actual and predicted proportions of water flux are depicted in Figs 4 and 5. As observed in Tables 2 and 3, the gassmf and trapmf from the hybrid optimization procedure with the

output type of linear were the best compatible MF for TFC and CTA membranes water fluxes, respectively.

Vural et al. (2009) studied the prediction strength of ANFIS model for the performance of a proton exchange membrane applied in an MFC. The developed ANFIS model could predict the produced voltage of the MFC with R^2 of 0.9894 and RMSE of 0.015 (Vural et al., 2009). Furthermore, Rahimzadeh et al. (2016) modelled the permeate volume of a membrane process by which water and oil were separated. According to the reported results, the developed ANFIS model by three inputs including time, the concentration of oil and transmembrane pressure could predict the permeate volume with high accuracy ($R^2 = 0.99$). Therefore, as most of the reported results, the developed ANFIS models in the present study demonstrated promising prediction strength.

3.3. Sensitivity analysis

3.3.1. Sensitivity analysis of ANN models

The importance of different effective independent variables like MLSS, DO, and EC in the ANN models of water flux of TFC and CTA membranes in the OMBR was analyzed by the sensitivity analysis. The connection weights of the constructed models were used by this approach. The matrix of the neural network weights for the TFC and CTA membrane water fluxes achieved is presented in Tables 4 and 5 correspondingly.

According to Fig. 6, all mixed liquor EC, DO and MLSS show significant importance in response to variables in both CTA and TFC membranes. Nevertheless, the greatest proportions of effectiveness belonged to the mixed liquor EC in both membranes with values of 48% and 42%, respectively. While, MLSS and DO were known as the second effective parameter for these two membranes with 35% and 34%, respectively.

3.3.2. Sensitivity analysis of ANFIS models

With each of the EC, DO and MLSS inputs, the ANFIS models were developed under the best conditions. Based on the results obtained for CTA membrane, the R^2 values of the single parameter models based on MLSS, DO and EC were 0.768, 0.444 and 0.230 consecutively. In comparison, the R^2 values for TFC membrane were 0.715, 0.326 and 0.250 based on EC, MLSS and DO as input parameter, respectively.

According to the results obtained, all of the parameters (EC, DO, MLSS) showed considerable effects on the output. For TFC membrane, the most important parameter was the mixed liquor EC with R^2 of 0.715 followed by MLSS with R^2 of 0.326. While for CTA membrane, the most important parameter was MLSS, followed by DO and mixed liquor EC. The differences between the sensitivity analysis results of these two models can be related to the dispersion of the data for each factor. Data dispersion can cause induce different effects to response prediction in these two analysis processes owing to their different natures. Therefore, according to the results of these sensitivity analyses performed by ANN and ANFIS models, the mixed liquor EC appears to be the most important factor for both type of membranes.

3.4. Comparison of ANN and ANFIS models

The strengths of the developed ANN and ANFIS models for prediction of water flux produced by CTA and TFC membranes in OMBR processes were compared using the RMSE, R^2 , Adj- R^2 and SSE. In contrast to the input data, the output data were not normalized, the obtained errors are on an actual scale. Figs 1-5 exhibit the actual and predicted values of the water flux by both CTA and TFC membranes under different conditions. In addition, the obtained values of the aforementioned statistical indices for the developed models are presented in Table 6.

Based on the statistical errors like SSE and RMSE, slightly greater deviation is demonstrated in ANN models predictions compared with the ANFIS ones. In addition, the

values of the R^2 and Adj- R^2 demonstrated that the developed ANFIS models mimic the water flux trend in both CTA and TFC membranes slightly better than the ANN models. In general, both the ANN and ANFIS models predictions for the water flux of these membranes fitted well with the experimental data. Dashti et al. (2018) modeled the performance of a H₂-selective nano-composite membrane in separation of H₂ from CH₄, CO₂ and C₃H₈ using different types of models. Their obtained results demonstrated that the developed ANFIS and ANN models with R^2 of 0.9990 and 0.9994 had almost similar performances. In contrast to the present study, the developed ANN models demonstrated a little better performance than the ANFIS model (Dashti et al., 2018). In another study, Rahmanian et al (2012) compared the strength of ANN and ANFIS models in prediction of lead ions separation from aqueous solutions. The constructed ANFIS models could predict the permeate volume and rejection with R^2 of 0.976 and 0.992, respectively. These R^2 values for ANN models were 0.925 and 0.981 correspondingly, which are so close to the obtained prediction strength of the built models in the present study (Rahmanian et al., 2012).

4. Conclusions

OMBR is gaining popularity as a membrane technology for water and wastewater treatment, but the decrease of water flux in OMBR is a key challenge to overcome. The present study focused on modeling the water flux by using ANFIS and ANN models in the OMBRs with TFC and CTA membranes. Four different datasets were extracted from published research studies and applied to develop computer models under various operating conditions.

According to the sensitivity analysis, mixed liquor EC was shown as the most important parameter in most of the tests. In addition, four statistical indices including RMSE, SSE, Adj- R^2 and R^2 were used to compare the developed models, with the ANFIS models demonstrating better prediction strength than ANN.

Appendix: Supplementary Information

E-supplementary data of this work can be found in online version of the paper.

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