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Prediction of the clogging of ultrafiltration membranes by neural networks

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***Abstract* –** One of the important aspects affecting the overall effectiveness of membrane filtration systems is pore clogging. Pore blockage results in significant filtration resistance and a dramatic reduction in the filtrate flux rate at constant pressure conditions and a significant rise in pressure for membrane filtration operation under constant flux conditions clogging filtration. This work investigates the use of neural networks in modelling the clogging of ultrafiltration membranes. A feed-forward neural network (NN) model characterized by a structure (three neurons in the input layer, ten neurons in the hidden layer, and one neuron in the output layer) are constructed with the aim of predicting the clogging of the ultrafiltration membrane.

A set of 175 data points was used to test the neural networks. 70%, 15%, and 15% of the total data were used respectively for the training, the validation, and the test. For the most promising neural network model, the predicted clogging values were compared to measured rejections clogging ultrafiltration membrane values, and good correlations were found (R =0.99095 for the training phase, R =0.99180 for the validation phase, and R =0.9844 for testing phase). The mean squared errors were (MSE =0.0577938 for the training phase, MSE =0.063348 for the validation phase, and MSE =0.109035 for the testing phase).

Keywords – Prediction; Clogging; ultrafiltration; Membranes; Neural Networks

I. Introduction

Membrane filtration, including microfiltration and ultrafiltration, is a crucial step in producing drinking water, treating home and industrial effluents, creating water that is appropriate for reuse, clarifying beverages, and other processes. Membrane fouling, which always results in a substantial reduction in water quality, is one of the main obstacles to the widespread use of membrane systems for water treatment. Decrease in filterability as filtration is being done. Such a decline in filterability may be brought about by membrane surface cake production or pore blockage. The pore walls of membrane pores may accumulate foulants smaller than membrane pores, which can result in pore constriction and dramatically reduce the cross-sectional area for flow. Larger foulants, however, have the potential to clog pore entrances, significantly increasing the filtration resistance before helping to create a continuous cake layer. Mechanisms that cause the membrane to get fouled during membrane filtration operations as a result of the build-up of foulants, greatly increase the filtration resistance. The fouling qualities of the feed solution affect the filter's capacity. Clarifying the underlying mechanisms influencing membrane fouling during membrane filtration operations is crucial for the practical implementation of the filtration procedures [1].

Artificial neural networks (ANN) have gained great popularity in the last decade as an attractive alternative to the previous approach due to their high parallelism, robustness [2] and for their inherent ability to extract from experimental data the highly non-linear and complex relationships between the variables of the problem [3].

The goal of this research work, we improved a neural networks (NN) model to predict the clogging of ultrafiltration membranes by neural networks.

II. MATERIALS AND METHOD

In this study, a procedure based on the design and optimization of the architecture of the neural network is advanced as described in Figure 1.

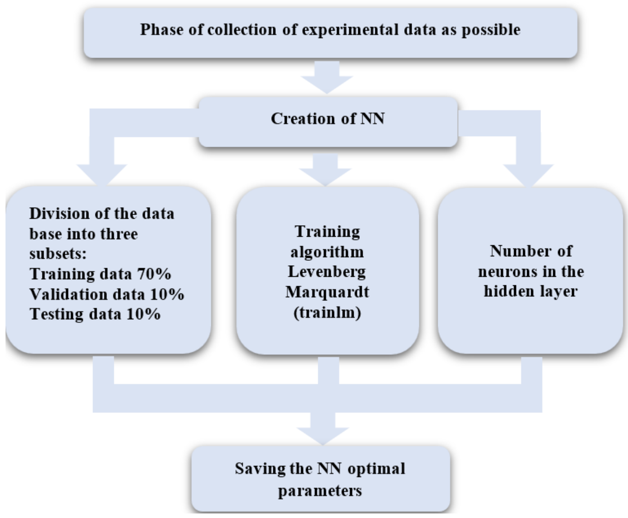


Fig. 1 Procedure of the design and optimization of the architecture of neural network.

The values of the minimum, the mean, the maximum, and the standard deviations (STD) for the inputs and output data are shown in table 1.

Table 1. Statistical analysis of inputs and output.

	Min	Mean $*10^{+3}$	Max $*10^{+3}$	STD $*10^{+3}$
Volume (L)	0.0050	0.0002	0.0001	0.0001
Time (h)	91.0000	8.0400	2.0963	3.2289
Concentration (mol/L)	1.0000	0.0400	0.0149	0.0115
Permeat flow (mg/l)	18.5400	0.0429	0.0058	0.0320

In the present study, we have used data available in the literature [4] of 175 data points. The total database collected from the literature was divided into three parts 70% for training phase (123 data points), 15% for validation phase (26 data points), and 15% for test phase (26 data points). The training algorithm used in this work is the Levenberg-Marquardt (trainlm). The neural networks contains three layers of neurons or nodes: one input layer with three neurons, one hidden layer with ten neurons, and one output layer with one unit that generated the estimated value of permeate flow, is advanced as described in Figure 2. The tangent sigmoid (tansig) transfer function was used in the hidden layer. The pure-linear (purelin) transfer function was used in the output layer. The ANN modeling of the permeat flow by ultrafiltration membranes was performed using MATLAB.

III. RESULTS AND DISCUSSION

Results According to the previous discussion, a neural network model was developed with the aim of predicting the permeat flow by ultrafiltration (UF) membranes. Figure 2 shows the total agreement plots for the permeat flow with agreement vectors approaching the ideal [linear equation: $y^{cal} = \alpha y^{exp} + \beta$, with $\boldsymbol{\alpha}$=slope, $\boldsymbol{\beta}$=y intercept, ***R***=correlation coefficient][5], [α, β, R] = [1, 0.042, 0.9991] for training phase; [α, β, R] = [1, 0.11, 0.9992] for validation phase, [α, β, R] = [0.99, 0.11, 0.9984] for testing phase, and [α, β, R] = [1, 0.027, 0.9990] for total phase. we have observed that the calculated permeate flux values predicted by the ANN approach are close to the experimental values, with a correlation coefficient R close to one, considered excellent so the model is acceptable.

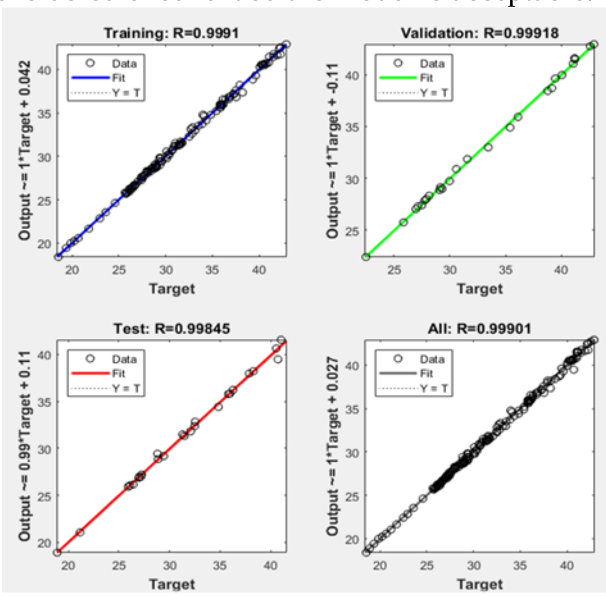
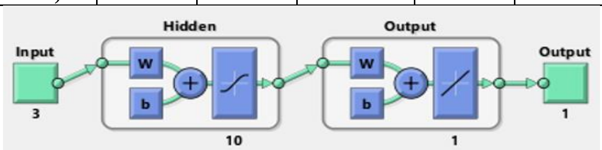


Fig. 2 Comparison between the experimental values and the values calculated by nftool: (blue) the trining phase, (green) the validation phase, (red) the test phase, (black) the total phase.

Table 2 shows the structure of the optimized QSAR-NN models.

Table 2. Structures of the optimized NN models.

Training Algorithm	Input layer	Hidden layer		Output layer	
	Neurons number	Neurons number	Activation function	Neurons number	Activation function
Levenberg - Marquardt (trainlm)	1	10	tansig	1	purlin



From the optimized neural networks (NN) shown in Figure. 3, assimilation of the clogging of ultrafiltration membranes by neural networks can be expressed by a mathematical models incorporating all inputs E_i (volume, time, concentration) within it as follows:

The instance outputs Z_j of the hidden layer:

$$Z_j = f_H\left[\sum_{i=1}^{3} w_{ji}^{I}E_i + b_j^{H}\right] = \frac{exp\left(\sum_{i=1}^{3} w_{ji}^{I}E_i + b_j^{H}\right) - exp\left(-\sum_{i=1}^{3} w_{ji}^{I}E_i + b_j^{H}\right)}{exp\left(\sum_{i=1}^{3} w_{ji}^{I}E_i + b_j^{H}\right) + exp\left(-\sum_{i=1}^{3} w_{ji}^{I}E_i + b_j^{H}\right)} \quad (2)$$

j=1, 2… 10

Output pearmeat flow:

$$J_p = f_0\left[\sum_{j=1}^{10} w_{1j}^{H}Z_j + b_1^{o}\right] = \sum_{j=1}^{10} w_{1j}^{H}Z_j + b_1^{o} \quad (3)$$

The combination of equations (2) and (3) results in the following mathematical formula that, taking into consideration all inputs, depicts permeate flow assimilation.

$$J_p = \sum_{j=1}^{11} w_{1j}^{H} \frac{exp\left(\sum_{i=1}^{10} w_{ji}^{I}E_i+b_j^{H}\right)-exp\left(-\sum_{i=1}^{10} w_{ji}^{I}E_i+b_j^{H}\right)}{exp\left(\sum_{i=1}^{10} w_{ji}^{I}E_i+b_j^{H}\right)+exp\left(-\sum_{i=1}^{10} w_{ji}^{I}E_i+b_j^{H}\right)} + b_1^{o} \quad (4)$$

Where w_{ji}^{I} represents the synaptic weight of the connection of neuron i of the input layer to neuron j of the hidden layer, w_{1j}^{H} represents the synaptic weight of the connection of the neuron j of the hidden layer to the neuron of the output layer, b_j^{H} represents the biases of neuron j of the hidden layer, b_1^{o} represent the bias of neuron j of the output layer.[5]

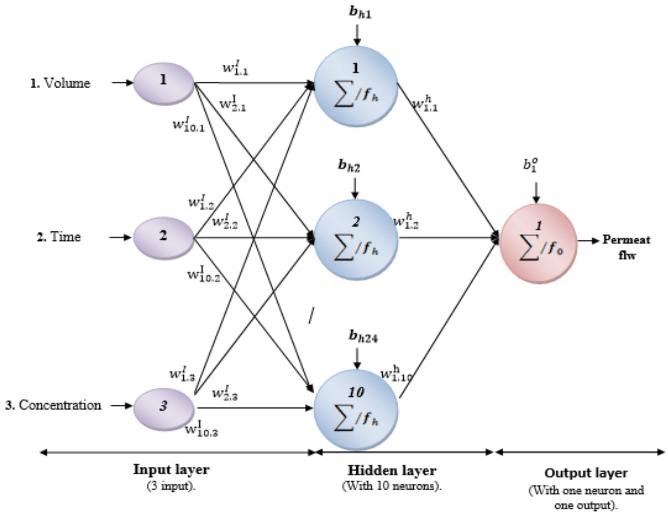


Fig. 3. Schematic representation of the optimized NN.

IV. CONCLUSION

The present paper illustrates the use of the neural network model that were developed with the aim of predicting the clogging of ultrafiltration membranes processes. For the most promising neural network model, the predicted clogging values were compared to measured rejections clogging ultrafiltration membrane values, and good correlations were found (R =0.99095 for the training phase, R =0.99180 for the validation phase, and R =0.9844 for testing phase). The mean squared errors were (MSE =0.0577938 for the training phase, MSE =0.063348 for the validation phase, and MSE =0.109035 for the testing phase).

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