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Modeling the Prediction of Flux and Fouling Parameters of PVDF Nanocomposite Ultrafiltration Membranes with Carbon Nanotubes using Artificial Intelligence Networks

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INTRODUCTION

Membrane processes have been proposed in recent years as efficient methods for separation and purification. Since the hydrophilicity membranes with functional carbon nanotube have higher resistance to fouling than hydrophobic materials, the increase in hydrophilicity of polymer membranes is one of the basic solutions for membrane modification. In addition, carbon nanotubes have been considered by many researchers because of their desirable properties such as low mass density, high flexibility and effective interaction between carbon nanotube bonds and functional groups which have the proper properties to improve the performance of polymer membranes. Moreover, four intelligent systems (MLP, RBF, LSSVM, and ANFIS) and three optimization algorithms (GA, PSO, and SA) for modeling flux and fouling parameters have been used by us. Artificial neural networks have been successfully used to prevent membrane fouling during microfiltration and ultrafiltration of colloidal compounds, proteins as well as urban and industrial water treatment [1-5].

PREPARATION OF NANOCOMPOSITE MEMBRANE

For manufacturing ultrafiltration membranes by phase inversion, a certain amount of nanotubes based on previous experiences and studies (0.05, 0.1, 0.2, 0.3, 0.5 wt.% compared to polymer)[6-7] has been distributed for half an hour in normal methylpyrrolidone solvent using ultrasonic bath and then Polyvinylidene fluoride polymer with a 15 wt.% (compared to the weight of the polymer) is solved in solution. Then cavity-causing polymer of polyvinylpyrrolidone in the amount of 1 wt.% (compared to the weight of the polymer) for pitting is added to the solution. After stirring the solution for 24 hours, it is placed in an oven of 55 °C for de-bubbling for 6 hours. After passing of the solution through a smooth glass substrate to reach ambient temperature, membrane layer thickness by a video cache with a thickness of 150 micrometers and at a constant speed was spread on the bed and immediately, immersed in the coagulation bath water. After about 10 minutes, the membrane is removed from the water bath and stored in a container which contains distilled water.

MODELING

In this paper, modeling using artificial intelligence networks has been used to create a predictive model of fouling and flux parameters that uses 4 smart networks and three optimization algorithms.

FOULING PARAMETER MODELING:

In this research, 80% of the modeling data for training and 20% for network testing were selected randomly.

MLP MODELING:

At this stage, a 3-layer neural network was used to simulate . This three-layer neural network contains 5 neurons in the input layer and 1 neuron in the output layer. For both hidden and output layers, the tansig activation function was used. The objective function was also considered as the least mean squared error (LMSE). To find the optimal number of hidden neurons, several neural networks have been constructed and their function has been investigated. To do this, a neuron number of 2 to 30 has been hidden in the layer, and finally, after comparing the results of the constructed networks, the optimal value for the number of hidden layer neurons has been 15. After the network has been built using the data set devoted to training, test data has been also provided to the network. The function of the MLP network has been constructed, and the function is shown in Figures 1 and 2.In addition, the related statistical parameters have been presented in Table 1.

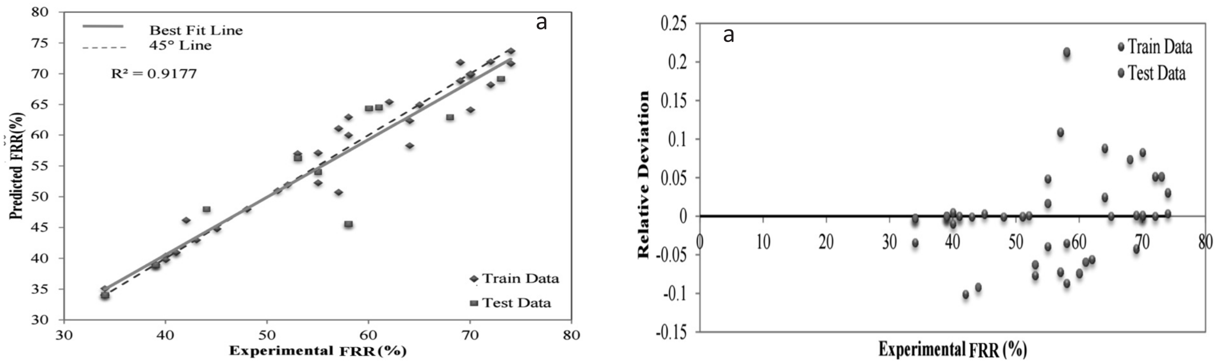

Figure 1: (a) The cross-sectional graph shows the correlation coefficient between predicted values and actual data by the MLP network for training and testing data. (b) The graph shows the relative error for the training and testing data for the MLP designed network.

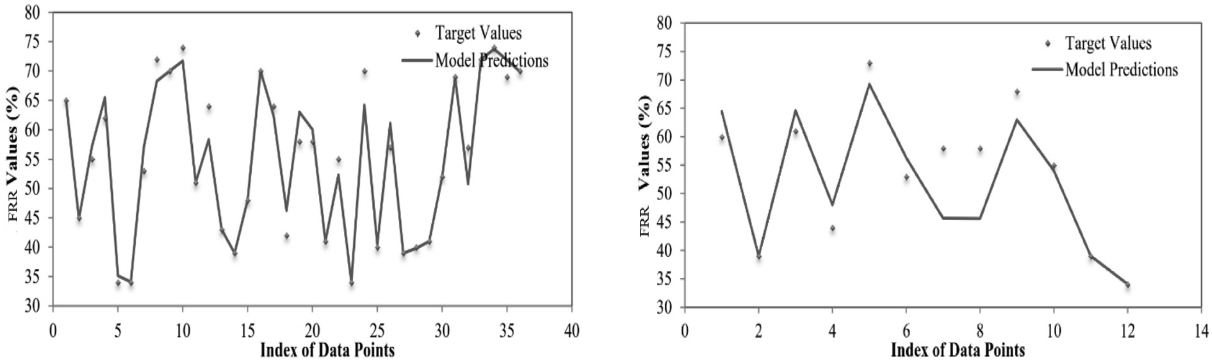

Figure 2: Comparison between the values predicted by the MLP network with actual data (a) training data, (b) test data.

Table 1: Statistical Parameters for the MLP Neural Network.

N	RMSE	STD	AARD	R^2	
36	2.587527	0.04496	2.807025	0.960509	Training data
12	5.815536	0.101796	7.149236	0.775561	Test data
48	3.671047	0.063741	3.892577	0.917662	Total data

The modeling which has been achieved for other networks RBF, LSSVM, and ANFIS is similar to the above table and figures.

Comparison of Models for fouling Parameters are following in Table 2. Modeling which has been simulated are similar to fouling parameter.

Comparison of the models with each other for finding the flux parameter are shown in Table 3.

Table 2: General results of modeling using different methods.

		R^2	AARD	STD	RMSE	N
MLP	Train data	0.960509	2.807025	0.04496	2.587527	36
	Test data	0.775561	7.149236	0.101796	5.815536	12
	All data	0.917662	3.892577	0.063741	3.671047	48
GA-RBF	Train data	1	8.23E-14	1.61E-15	7.87E-14	36
	Test data	0.932464	4.171744	0.053156	3.403937	12
	All data	0.982956	1.042936	0.028026	1.701968	48
LSSVM	Train data	0.81951	7.365815	0.116697	5.686178	36
	Test data	0.92654	5.513205	0.06567	3.229177	12
	All data	0.838147	6.902663	0.1056	5.182313	48
Conjugate-ANFIS	Train data	1	2.04E-15	6.26E-17	3.13E-15	36
	Test data	0.963835	4.038988	0.048845	3.531359	12
	All data	0.983726	1.009747	0.028506	1.76568	48

Table 3: General outcomes of modeling using different methods.

		R^2	AARD	STD	RMSE	N
MLP	Train data	1	0.000147	4.15E-06	0.001188	36
	Test data	0.929902	6.102074	0.089494	25.19476	12
	All data	0.970603	1.525629	0.045198	12.59738	48
GA-RBF	Train data	0.999671	0.303117	0.004457	1.212818	36
	Test data	0.991598	1.952475	0.027128	7.287811	12
	All data	0.99709	0.715457	0.013693	3.792261	48
LSSVM	Train data	0.998006	0.662018	0.010907	3.024102	36
	Test data	0.919262	4.488421	0.070189	21.93118	12
	All data	0.973731	1.618618	0.035357	11.274	48
Conju-gate-ANFIS	Train data	1	1.9E-14	2.59E-16	6.48E-14	36
	Test data	0.981002	2.705384	0.036376	10.98454	12
	All data	0.993869	0.676346	0.018683	5.492272	48

FIND OPTIMAL LABORATORY PARAMETERS

In this section, the goal is to obtain optimal values for the conditions at which the fouling reaches its minimum, while the flux values are high. For this, the best models made last season for both outputs will be used. Moreover, a combination of genetic and particle swarm algorithms is working to find optimal values. At first, a random population of 300 responses was possible. Then, after 50 generations, it converges to optimal conditions. The target function is the least squared FRR and flux. Finally, convergence to the optimal values for the 15% PVDF membrane and 18% PVDF membrane are shown in Table 4.

Table 4: Estimated optimal values.

polymer	nanoparticle %	contact angle	porosity	BSA Rejection	FRR%	(Flux(L/m^2.hr
15	0.069212835	88.13671097	0.72680354	81.7703366	100.00	252.7
18	0.171222113	79.90790664	0.75124799	98.86853228	63.47	454.2

CONCLUSIONS

In the present study, PVDF ultrafiltration membranes with two concentrations of 15 and 18% have been prepared by phase inversion using NMP solvent. In order to improve the hydrophilic properties and to reduce the fouling of these membranes, various acidic, basic, and amine carbon nanotubes with different concentrations have been used. The modeling results have been performed using four artificial intelligence networks. Finally, using optimization algorithms, the optimal parameters have been obtained according to the goals of the most flux and the minimum fouling for both PVDF (15 wt.% and 18 wt.%) polymers. The overall outcomes of this research can be summarized as follows: For modeling flux and fouling parameters, four intelligent multi-layer neural network (MLP), radial basic function (RBF), least squared support vector mechine (LSSVM) and adaptive neuro fuzzy interference systems (ANFIS) have been used. Errors have been calculated and compared with each other for each neural network system. According to the correlation coefficient obtained for each system and the correlation coefficient (> 0.85) is a good accuracy for neural networks, it can be concluded that for flux and fouling parameters, the best model are GA-RBF and Conjugate-ANFIS. In the next section, modeling has been used to obtain the optimal values of the best models which have been made for both outputs. Afterward, by using the combination of genetic algorithm with particle swarm optimization algorithim, optimal values have been obtained.

Finally, for 15% PVDF polymer, optimum nanoparticle content is 0.6% with flux 252.7% L/m2h, 100% fouling, 88° contact angle and 73% porosity; moreover, for 18% PVDF polymer, optimum nanoparticle content is 0.17% with flux volume 454.2 L/m2h, fouling 63.5%, contact angle 80° and porosity 75%.

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