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PREDICTION OF PORE SIZE OF ULTRAFILTRATION MEMBRANE BY USING ARTIFICIAL NEURAL NETWORK (ANN)

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Abstract. The objective of this research is to develop a neural network model to predict the pore size of ultrafiltration membrane. Usually, the pore size of ultrafiltration membrane was determined experimentally using permeation and rejection rate experiments, followed by empirical equations. Therefore, in this study, Artificial Neural Network (ANN) has been proposed as an alternative method to predict the pore size of flat sheet ultrafiltration membranes. Experimental data were collected from the previous research whereby the polyethersulfone (PES) polymeric membranes were fabricated with lithium bromide (LiBr) additive. The membranes were tested by using various polyethylene glycol PEG molecular weights solution. The neural network has a pyramidal architecture with three different layers which consists of an input layer, hidden layer and output layer. Feed-forward Backpropagation (FFBP) network was constructed in MATLAB version 7.2 environment by using Levenberg-Marquardt algorithm (*trainlm*) training method. In addition, Bayesian regularization method was introduced to improve the neural network generalization. The simulated results obtained from this study were then compared to the experiment results so as to obtain the best model with the smallest Root-Mean Square (RMS) error. The results revealed that the constructed networks were able to accurately estimate the pore size of ultrafiltration membrane.

Keywords: Artificial neural network; feed-forward backpropagation; ultrafiltration membrane modelling; pore size estimation

Abstrak. Objektif penyelidikan ini adalah untuk membangunkan sebuah model rangkaian saraf buatan bagi meramal saiz liang membran turasan ultra. Saiz liang membran turasan ultra biasanya ditentukan secara eksperimen dengan menggunakan eksperimen kadar penelapan dan kadar penolakan, diikuti oleh persamaan empiris. Dalam kajian ini, rangkaian saraf buatan (ANN) telah dicadangkan sebagai satu kaedah alternatif untuk meramal saiz liang membran keping rata turasan ultra. Data eksperimen diperoleh daripada eksperimen lalu di mana membran polimerik polyethersulfone (PES) dibuat dengan additif litium bromida (LiBr). Membran itu telah diuji dengan menggunakan pelbagai larutan polietilena glikol PEG. Rangkaian saraf mempunyai seni bina berpiramid yang terdiri daripada tiga lapisan berbeza, iaitu lapisan input, lapisan tersembunyi dan lapisan output. Rangkaian suap depan *backpropagation* (FFBP) telah dibina dalam persekitaran MATLAB 7.2 dengan menggunakan kaedah latihan algoritma Levenberg Marquardt (*trainlm*). Tambahan pula, kaedah *bayesian regularization* telah diperkenalkan bagi meningkatkan pengitlakan rangkaian saraf. Keputusan simulasi yang diperoleh daripada kajian ini kemudiannya dibandingkan dengan keputusan eksperimen agar model terbaik dengan ralat punca min kuasa dua (RMS) yang

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paling kecil dapat diperoleh. Keputusan menunjukkan bahawa rangkaian yang dibina berupaya menganggar saiz liang membran turasan ultra dengan tepat.

Kata kunci: Rangkaian saraf buatan; suap depan; permodelan membran turasan ultra; penganggaran saiz liang

1.0 INTRODUCTION

In this study, Artificial Neural Network (ANN) is selected to predict the pore size of ultrafiltration membrane. The network used is Feed-Forward Back Propagation (FFBP) with Levenberg-Marquardt algorithm (*trainlm*). The networks and algorithm were selected due to its ability in prediction or forecasting. The applications of ANNs in prediction were proven in recent papers elsewhere [1-9]. ANN also clearly shows the existence or the truth to be an effective predictive instrument for modeling the behavior of non-linear dynamic systems. In general, ANN is a black box type of correlation method with no physical laws involved. However, ANN offers nearly the same predictability as with the mass transfer model and requires shorter computing time [10].

In developing the neural model, data from experiments performed by Idris and Ahmed [11] were used. The experiments were carried out to investigate the influence of various concentrations of additive and preparation method towards the ultrafiltration morphology. Polyethersulfone (PES) was used as the polymer in the experiment due to its excellent membrane forming properties. A mixture of two solvents was used in preparation of dope solutions, which are dimethylformamide (DMF) and acetone. In addition, various concentrations of lithium bromide (LiBr) were used as an additive in order to improve the rejection and permeation rates of the membranes.

The dope solutions were prepared by using two methods which are microwave technique (MW) as well as conventional electrothermal heating (CEH) method. The performances of the various membranes are evaluated in terms of solute permeation fluxes and solute rejection rates in a stainless steel cross flow test cell. Solute rejection of membranes is evaluated with various molecular weight polyethylene glycol (PEG) solutions ranging 200 – 36000 kDa at 3.5 bar. The concentration of PEG solution used is 500 ppm. The pore sizes of flat sheet membrane are calculated using the solute transport data from ultrafiltration experiments.

2.0 MATERIALS AND METHODS

In this study, MATLAB version 7.2 was used to develop a neural network process as an alternative method to predict the pore size. First, experimental data was analysed and elaborated. This is a very important step in order to determine the independent variables as the input and output of neural network model. The hidden layer also can be approximated according to the number of inputs. Certain data was chosen for training while the rest was used to test the model. Next, the neural model was

built, which consists of input layer, hidden layer and output layer. The effects of the number of training points, hidden neurons and training data arrangements on the simulation correctness were investigated elsewhere. Then, root mean square (RMS) error was calculated to determine the accuracy of the network.

A neural network was developed by using permeation rate, solute rejection, various concentration of additives and various molecular weight of polyethylene glycol as inputs in order to the predict the pore size of ultrafiltration membrane. The selected network developed was feed-forward backpropagation (FFBP). The developed network was then simulated. The best neural network was selected based on the comparison between the simulated results and the data from literature. The comparison was based on the RMS error.

3.0 RESULTS AND DISCUSSION

A neural network model was successfully developed in order to predict the pore size of ultrafiltration membrane. A set of experimental data was used for training and testing in feed-forward backpropagation model. The results of the simulation were compared to experimental data and the errors were calculated. The best model with the least root mean square error was generated.

For the training of the weight parameters, four inputs and one output were used. Various sizes of neural networks with one hidden layer were trained and tested. The node in hidden layer will do the actual processing. Therefore, the number of nodes was selected using systematic trial and error. Since the network consists of four inputs, four to twelve nodes was tested. Over-fitting occurs if the number of nodes is too high.

For the MW membrane results, a network with five hidden nodes was found to be the most suitable and accurate. For MW, the inputs were permeation rate, solute rejection, additives concentration and PEG molecular weight. The used network had 40 weight parameters and the total number of data sets was 36. Of these, 29 were used for training the network and the rest were used to prove the predictivity of the network.

For CEH membrane results, the inputs were permeation rate, solute rejection, additives concentration and PEG molecular weight. However, four hidden nodes was found out to give a very good predictive. The network used 32 weight parameters and the total number of data sets was 36. Of these, 29 were used for training the network while the rest were used for testing the network to predict the pore size.

After testing the data between the nodes of four to twelve, it was proven that the best number of nodes used was four for both MW and CEH. The RMS errors were 0.0018517 and 0.0035354 for MW and CEH respectively. These values proved that this model is able to predict the pore size of ultrafiltration membrane accurately as shown in Table 1 and Table 2. For the best model, graph of literature data versus simulated results were plotted. The predicted data are very accurate because a perfect

Table 1 The comparison of pore size between experimental data with predicted results for MW membranes

Experimental data	Simulated data
1.738	1.7385
1.053	1.0522
0.75	0.74981
2.573	2.5641
0.856	0.85597
0.979	0.97896
2.573	2.5724

Table 2 The comparison of pore size between experimental data with simulated results for CEH membranes

Experimental data	Simulated data
2.727	2.7268
2.324	2.3239
0.8106	0.8322
3.526	3.5294
1.831	1.8437
3.256	3.2546
3.526	3.5278

fit is obtained as in Figure 1 and Figure 2. This can be proven by the correlation coefficient (R-squared) value obtained. To prove that the model is accurate, the correlation value must converge to 1 and the RMS error value approaches 0. An

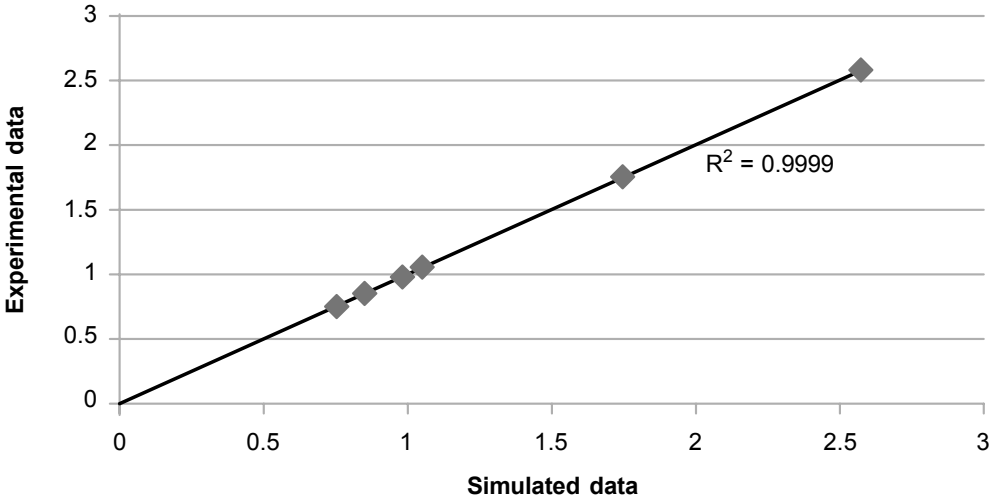

Figure 1 Correlation coefficient (R^2) of pore size for MW membranes

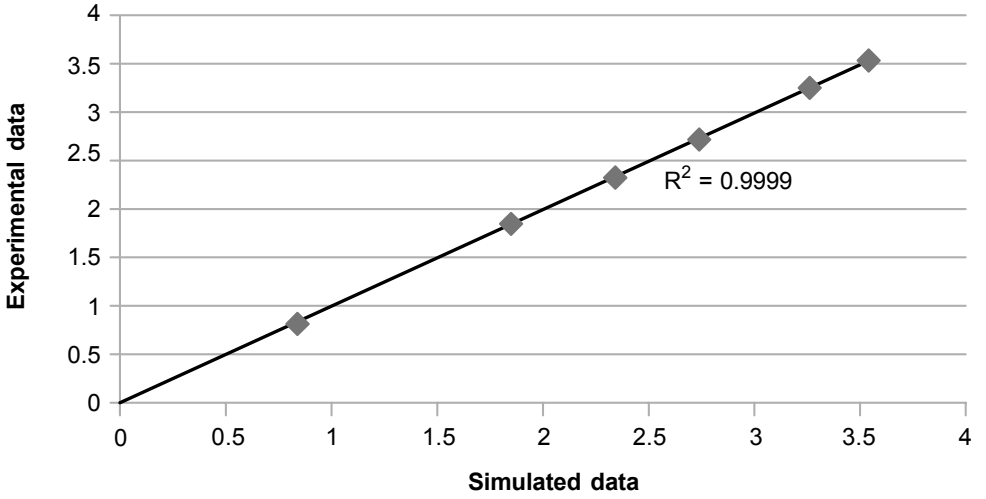

Figure 2 Correlation coefficient (R^2) of pore size for CEH membranes

accurate model must achieve its correlation at least 0.99 with RMS error lowered than 0.1. From the graph, the value of R-squared is 0.99999 for both MW and CEH. The parameters and architecture of FFBP was summarized in Table 3.

There was no specific rule to obtain the number of layer and hidden layer nodes of a network. Obviously, many hidden nodes are redundant, but this kind of overparametrized network is easy to train. Trial and errors were done to identify the best represented architectures of each network type. The complexity of the structure increases as the number of nodes increase. This is most likely caused by the over trained network due to the complexity of the network (high number of hidden layer

Table 3 The parameters and network architecture for MW and CEH membranes

Parameters	Network architecture (MW)	Network architecture (CEH)
Input	Permeation rate	Permeation rate
	Solute rejection	Solute rejection
	Additives concentration	Additives concentration
	PEG molecular weight	PEG molecular weight
Output	Pore size	Pore size
Transfer function	Log-sigmoid, pure-linear	Log-sigmoid, pure-linear
Training method	Levenberg-Marquardt	Levenberg-Marquardt
Number of hidden layer	1	1
Number of nodes in hidden layer	5	4
RMS error	0.0018517	0.0035354
Correlation	R^2 = 0.99999	R^2 = 0.99999

nodes and interconnection weights) that require too many iterations.

On the basis of the above described considerations, a neural model, called feed-forward backpropagation (FFBP) is finally chosen based on the trial and error procedure with, maximum relative error lower than 5%. The neural model has a pyramidal architecture with three different layers:

(i) An input layer with four neurons and a logistic sigmoid activation function;
(ii) One hidden layer having five and four neurons for MW and CEH membranes respectively with a logistic sigmoid activation function;
(iii) An output layer with only one neuron and a logistic sigmoid activation function.

However, one of the problems that occur during neural network training is called overfitting. The error on the training set is driven to a very small value, but when new data is presented to the network the error is large. The network has memorized the training examples, but incapable to generalize to new situations. Therefore, in this study, Bayesian regularization method was introduced to improve the neural network generalization. The weights and biases of the network are assumed to be random variables with specified distributions. It is also important to train the network until it reaches convergence when using Bayesian regularization. The sum squared error, the sum squared weights, and the effective number of parameters should reach constant values when the network has converged.

4.0 CONCLUSION

In this work, the neural networks were applied to simulate the determination of membrane pore sizing process. The pore sizes of ultrafiltration membrane were calculated using the weight parameters of the neural network based on experimental results. The results were compared with the corresponding results obtained by mass transfer model. The model predictions, obtained with a network architecture consisting of one input layer with four modes, one hidden layer having five and four nodes for MW and CEH respectively and one output layer composed by only one node are shown to be in remarkable agreement with the actual experimental results. The RMS error of the FFBP network developed for MW and CEH are 0.0018517 and 0.0035354 respectively. It proves that the networks are reliable and could be implemented in membrane industries to optimize the membrane separation processes.

REFERENCES

[1] Ou, S. and L. E. K. Achenie. 2005. A Hybrid Neural Network Model for PEM Fuel Cells. *J. Power Sources* 140(2): 319-330.

[2] Shetty, G. R. and S. Chellam. 2003. Predicting Membrane Fouling during Municipal Drinking Water Nanofiltration using Artificial Neural Networks. *J. Membr. Sci.* 217(1-2): 69-86.
[3] Aydinera, C., I. Demira and E. Yildizb. 2004. Modeling of Flux Decline in Crossflow Microfiltration using Neural Networks: The Case of Phosphate Removal. *J. Membr. Sci.* available on-line 11 November 2004.
[4] Chellam, S. 2005. Artificial Neural Network Model for Transient Crossflow Microfiltration of Polydispersed Suspensions. *J. Membr. Sci.* 258(1-2): 35-42.
[5] Rai, P., G. C. Majumdar, S. DasGupta and S. De. 2005. Modeling the Performance of Batch Ultrafiltration of Synthetic Fruit Juice and Mosambi Juice using Artificial Neural Network. *J. Food Eng.* 71(3): 273-281.
[6] Curcio, S., G. Scilingo, V. Calabrò and G. Iorio. 2005. Ultrafiltration of BSA in Pulsating Conditions: An Artificial Neural Networks Approach. *J. Membr. Sci.* 246(2): 235-247.
[7] Bowen, W. R., M. G. Jones and H. N. S. Yousef. 1998. Dynamic Ultrafiltration of Proteins—A Neural Network Approach. *J. Membr. Sci.* 146: 225-235.
[8] Razavi, M. A., M. Mousavi and A. Mortazavi. 2003. Dynamic Prediction of Milk Ultrafiltration Performance: A Neural Network Approach. *Chem. Eng. Sci.* 58: 4185-4195.
[9] Razavi, M. A., A. Mortazavi and M. Mousavi. 2003. Dynamic Modelling of Milk Ultrafiltration by Artificial Neural Network, *J. Membr. Sci.* 47-58.
[10] Shahsavand, A. and M. P. Chenar. 2007. Neural Network Modeling of Hollow Fiber Membrane Processes. *Journal of Membrane Science*. 297: 59-73.
[11] Idris, A. and I. Ahmed. 2008. "Microwave Assisted Polyethersulfone Asymmetric Membranes using Two Solvents and Halogenated Lithium Bromide as Additive."