ISSN 2176-5480

22nd International Congress of Mechanical Engineering (COBEM 2013)
November 3-7, 2013, Ribeirão Preto, SP, Brazil

PREDICTION OF THE PERMEATE FLUX IN CROSSFLOW MEMBRANE FILTRATION MODELED BY ARTIFICIAL NEURAL NETWORK

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Abstract. *The filtration process has the potential for expansion in important sectors, as in the processing of edible oils and sugarcane industry, where the trade expansion demands better technologies. In this work a methodology based on artificial neural networks is developed for estimate of permeate flux of mixtures in suspension of xanthan gum in a tubular membrane. The neural network has been trained through a selected set of experimental data already published. The experimental data were obtained for the concentration of complex macromolecular suspensions (non-Newtonian fluid) in turbulent flow with ceramic membrane of nominal pore size of 0.4 μm. Few experimental series were considered to construct a database applied to neural model parameters that could be adjusted. The input variables of neural model were transmembrane pressure, flux velocity and microfiltration time. The results shown that the neural model can be trained in a reasonable computational time and it is able to predict of real values of the permeate flux with errors of the order 10^{-3}.*

Keywords: *Artificial neural networks, Crossflow filtration, Tubular membrane, Macromolecular suspension, Modeling*

1. INTRODUCTION

In the last decades, the crossflow membrane filtration process has been widely adopted by various industries. In food industries, applications include clarification of wines, juices and vinegar, removal of yeast beer and separation of bacteria and fat the milk. In chemical industries, applications are relevant to the processing of paint and oil derivatives, among others. The filtration process has the potential for expansion in important sectors, as in the processing of edible oils and sugarcane industry, where the trade expansion demands better technologies (Zeman and Zydney, 1996). However, the biggest obstacle, inherent to the process, is the permeate flux decline that occurs due to the polarization and fouling effect. Therefore, an extensive study of the transport phenomena is necessary to better understand the mass transfer mechanisms in this process. Evaluating parameters related with the transport phenomena, often request complex mathematical equations with adjustable parameters that are difficult to determine experimentally and that the analytical solution cannot be obtained. In this context, artificial neural networks (ANNs) have attracted attention as new approach for determining complex relationships between input and output variables on analysis of experimental data.

Amongst the several advantages of neural network models, it can emphasize that they are easy to use and to update, possess large degree of freedom and accurate prediction at high speed (Nafey, 2009, Valle and Araujo, 2011, Niemi, *et al.*, 1995). Besides, ANNs can also include available theoretical knowledge about the process. As a consequence, several researchers have devoted to study the application of neural networks models in crossflow filtration process. Razavi, *et al.*, 2004 applied neural networks for the dynamic simulation of permeate flux and total hydraulic resistance. The methodology was used to the case of milk concentration by crossflow ultrafiltration as a function of physicochemical conditions (pH and fat per cent). The results were satisfactory with average error less than 1.06%. Curcio, *et al.*, 2006 presented ANN methodology for the control of permeate flux decay, on the basis of the experimental results collected,

ISSN 2176-5480

during ultrafiltration of BSA solutions. Liu, *et al.,* 2009 used ANN models to predict the performance of microfiltration systems for water treatment. Five input variables were used in order to construct a database for development neural model to predict and/or simulate membrane fouling behavior. Guadix, *et al.*, 2010 develop an ANN that predicts the time evolution of the milk permeate flux through a ceramic membrane submitted to operational cycles of filtration and cleaning with different degrees of aggressivity. The results show satisfactory with an error of 10%. Authors as Niemi *et al.* 1995, Shetty *et al*. 2003, Curcio e*t al.* 2005, Chellam (2005), Shahoo and Ray (2006), Silva and Flauzino (2008) and Hilal *et al*. 2008 also worked with the applicability of ANNs to describe membrane processes.

The aim of this research is to investigate the possibility of employing ANNs models to predict permeate flux and, consequently, to obtain an other tool to estimate parameters of crossflow filtration process. In particular, ANN was developed to estimate the permeate flux during the microfiltration of mixture in suspension of xanthan gum as a function of process operating parameters. In order to construct a database for development neural model, the experimental data in turbulent flow with ceramic membrane of nominal pore size of 0.4 *m* were obtained of the literature (Queiroz and Fontes, 2008). The results obtained by the artificail neural network have shown to be satisfactory, with average error of 8%.

2. ARTIFICIAL NEURAL NETWORK

This section introduces the basic concepts of artificial neural networks, describes the back-propagation algorithm and the experimental data and defines the neural model developed for estimate of permeate flux.

2.1 Theory and training algorithm

A artificial neural network can be defined as a nonlinear mapping of an input onto an output vector space. This is achieved through layers of activation functions or neurons in which the input coordinates are summed according to specific weights and bias to produce single output or firing values. In this work, a feed forward network was used for which there is no recursiveness, i.e., the input vector of a specific neuron layer is formed only by the firing values of the preceding layer, as shown in Fig. 1.

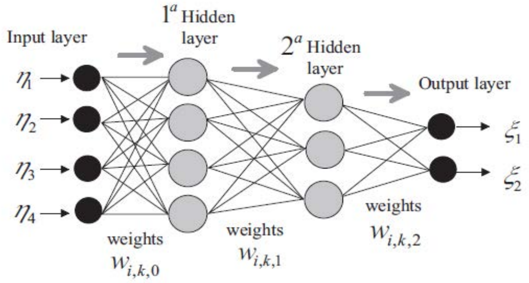


Figure 1. Schematic representation of a feed forward neural network mapping a four-coordinate input vector onto a two-coordinate output vector.

Formally, if the activation function of ***i***-th neuron in the ***j***-th layer is indicated by $F_{i,j}(.)$, its output $s_{i,j}$ can be calculated from the outputs of the preceding layer $s_{i,j-1}$ and the corresponding bias $b_{i,j}$ and weights $w_{i,k,j-1}$ (the second subscript ***k*** indicates the neuron in the (***j***-1)-th layer from which the connection is being established), according to the Eq. (1)

$$s_{i,j} = F_{i,j}\left(b_{i,j} + \sum_k w_{i,k,j-1} s_{k,j-1}\right) \quad (1)$$

After denoting the networks input and output values, respectively, by $_i$ and $_i$, the mapping relation of one onto another can be calculated by successively applying the Eq. (1), which for the example in Fig. 1 results

$$_i = F_{i,3}\left(b_{i,3} + \sum_{k=1}^{2} w_{i,k,2} F_{k,2}\left(b_{k,2} + \sum_{m=1}^{3} w_{k,m,1} F_{m,1}\left(b_{m,3} + \sum_{n=1}^{4} w_{m,n,0} \; _m\right)\right)\right) \quad (2)$$

Equation (2) makes it clear that the relation between $_i$ and $_i$ is unambiguously defined by choosing the activation

ISSN 2176-5480

functions and by setting the bias and weights. Among many, a very important characteristic of neural networks is the so-called learning potential, i.e., the possibility of adjusting the bias and weights through a convenient training rule to closely reproduce pre-assigned pairs of input/output values.

There are different learning algorithms. The technique most used in feedforward neural network is the back-propagation because of its mathematical strict learning method to train the network and guarantee mapping between inputs and outputs (Nafey, 2009, Haykin, 1999). It is based on the iterative application of a discrete gradient descent algorithm, computed from the first derivatives of a conveniently defined error function whose arguments are the parame-ters of the network (weights and bias). A more complete text can be found at Haykin (1999) and Hagan, *et al.*, 1996.

In general lines the basic steps of the back-propagation procedure implemented in this work are the following (Filletti, 2007, Filletti and Seleghim, 2010):

1. initialize the parameters of the network $b_{i,j}$ and $w_{i,k,j}$ with random numbers;
2. from a training data set with pre-assigned input/output pairs take the ***p***-th (${}_i^p$, Δ_i^p) pair, calculate the outputs of the network with the same input and form the pair (${}_i^p$, ${}_i^p$);
3. calculate the error between the desired and the obtained output values according to the Euclidean norm

$$e = \sqrt{\sum_i (\Delta_i^p - {}_i^p)} \tag{3}$$

4. calculate the derivatives of error ***e*** with respect to $b_{i,j}$ and $w_{i,k,j}$;
5. modify the network parameters according to the steepest descent strategy and a specified learning rate

$$b_{i,j} \leftarrow b_{i,j} - \frac{\partial e}{\partial b_{i,j}} \tag{4}$$

$$w_{i,j} \leftarrow w_{i,k,j} - \frac{\partial e}{\partial w_{i,k,j}} \tag{5}$$

and

6. iterate from 2 to 5, successively modifying $b_{i,j}$ and $w_{,k,,j}$, until a defined number of learning epochs (cycles) or a convenient stopping criterion has been achieved.

The performance of a artificial neural network is profoundly affected by its internal architecture (number of hidden layers and number of neurons in each one) and the type of interconnections (feed-forward, recursive, winner-take-all, etc). The exact shape of the activation function has limited effects on the overall performance and is usually set according to the needs of the training heuristics (a sigmoid function in the case of back-propagation method). There is no general mathematical theory but rather a number of empirical rules to be considered when constructing such models.

2.2 Experimental data

As previously mentioned, the experimental method and data set used in this research were described by Queiroz and Fontes (2008). In order of elucidate, in this subsection, a brief summary of the method is reported.

Figure 2 shows a schematic drawing of the experimental equipment used to analyze the concentration process by microfiltration.

The experimental system was manufactured by Netzsch do Brazil Ltda, with one ceramic tube modules with a 1000 *mm* (4, Fig. 2) long, 7 *mm* diameter each a surface area of 0.022 m^2. The solution in the feed tank (1, Fig. 2) was made to circulate using a positive-displacement pump (2, Fig. 2) and the transmembrane pressure was maintained constant by a frequency in versor. The retention flux was returned to the feed tank, whereas the permeate outflow was volumetrically measured (5, Fig. 2) as a function of time (Fontes, *et al.*, 2005). Data series were made for xanthan gum solution of high molecular weights (xanthan gum = $4{\times}10^6 Da$). The commercial ceramic membrane used in this research has nominal pore size of 0.4 *m*.

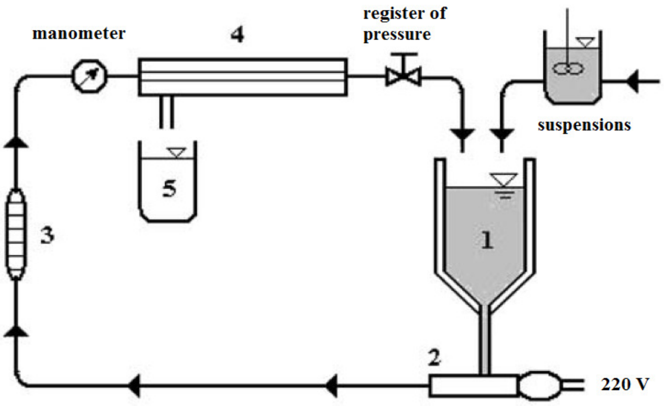


Figure 2. Schematic drawing of the experimental apparatus: (1) jacketed fluid container; (2) pump; (3) flowmeter; (4) covering module with membrane tubular; (5) permeate outflow.

2.3 Neural network model for xanthan gum filtration

The neural network implemented in this work has three inputs and one output. Various architectures were trained and tested. The neural model that had the best result, obtained by trial and error, has two hidden layers with six and three neurons, respectively. The activation functions used in the neural network are the tangent sigmoid in the hidden layers and the linear function in the output layer, given, respectively, as follow

$$(v) = \frac{2}{(1+\exp(-2v))} - 1 \tag{6}$$

$$(v) = v, \tag{7}$$

where $v = b_{i,j} + \sum_k w_{i,k,j-1} s_{k,j-1}$ is the activation potential of the above functions.

The training procedure comprehended the acquisition the transmembrane pressure, the flux velocity and the microfiltration time selected set of experimental data already published (Queiroz and Fontes, 2008), which are described in section previous. Few experimental series were considered to construct a database applied to artificial neural network parameters that could be adjusted.

The input data matrix has 3 lines for 95 columns, where 3 is the number of inputs (transmembrane pressure, flux velocity and microfiltration time), and 95 is the number of examples used in the training of the neural network. Each example corresponds to a known and fixed value of permeate flux of mixtures. The output matrix has 1 line for 95 columns, where 1 is the number of desired output and 95 is the number of examples. The neuron of the output layer is responsible for estimating the permeate flux of mixtures. For the generalization, 48 examples different from those used in the training were presented to the neural network. Therefore, 143 pairs of input/output values were obtained for to compose the database from which the parameters supplied to the ANN were extracted. The division of the examples in training and test sets was made randomly and was obtained a good coefficient of correlation among the data.

3. RESULTUS AND DISCUSSION

This section is divided into two parts. The first part presents the results of training of neural networks implemented in this paper. In the second part, experimental data of the average permeate flux obtained of Queiroz and Fontes (2008) are compared with values estimated by neural network.

3.1 Training of ANN

Figure 3 shows the error of the training of the ANN as a function of the epochs. The technique of learning algorithm used in this work is the back-propagation, which was described earlier. The results of the training of the neural network showed that it is capable of reproducing the input/output relation of the data of the training set. As can be observed in Fig. 3, the error of the training was the order of 10^{-3}.

To determine the values of the learning rate, the number of epochs as well as the number of neurons in the

ISSN 2176-5480

intermediate layers of the neural networks, an optimization of the parameters of the neural networks was performed by trial and error, in an attempt to diminish the error in a reasonable time. Thus, the neural network architecture implemented in this work was 3-6-3-1, the learning rate used in the neural network was 0,1 and the training time was 1 hour and 200000 epochs were performed during the training.

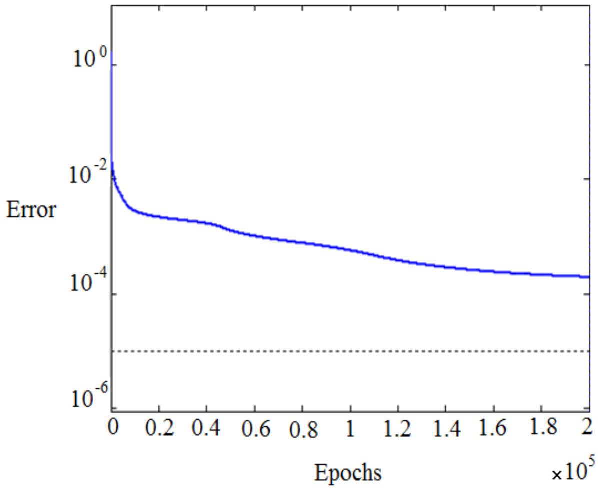


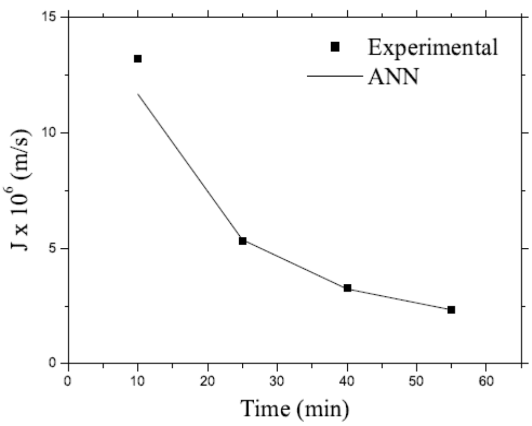
Figure 3. Decrease of the error during the training of the neural network to estimate the permeate flux.

3.2 Verification of the ANN

To evaluate the generalization capacity of ANN, new experimental data were presented to the neural networks. It is good to emphasize that these data were unknown to the ANN. A good correlation among the input and output data could be observed for the test set.

Figure 4 shows comparison of the experimental data with of the results calculated by neural network, concerning the examples contained in the test set, for the average permeate flux of mixture in suspension of xanthan gum as a function of the time. The neural network results presented in this figure showed good agreement with the experimental data with average relative error equal to 3.5% in the case of u = 2.6 *m/s* and ΔP = 400 *kPa* (Fig. 4 (a)), 3.9% for u = 3.7 *m/s* and ΔP = 300 *kPa* (Fig. 4 (b)), 5.5% for u = 4.7 *m/s* and ΔP = 400 *kPa* (Fig. 4 (c)) and 4.5% for u = 5.7 *m/s* and ΔP = 500 *kPa* (Fig. 4 (d)).

(a)



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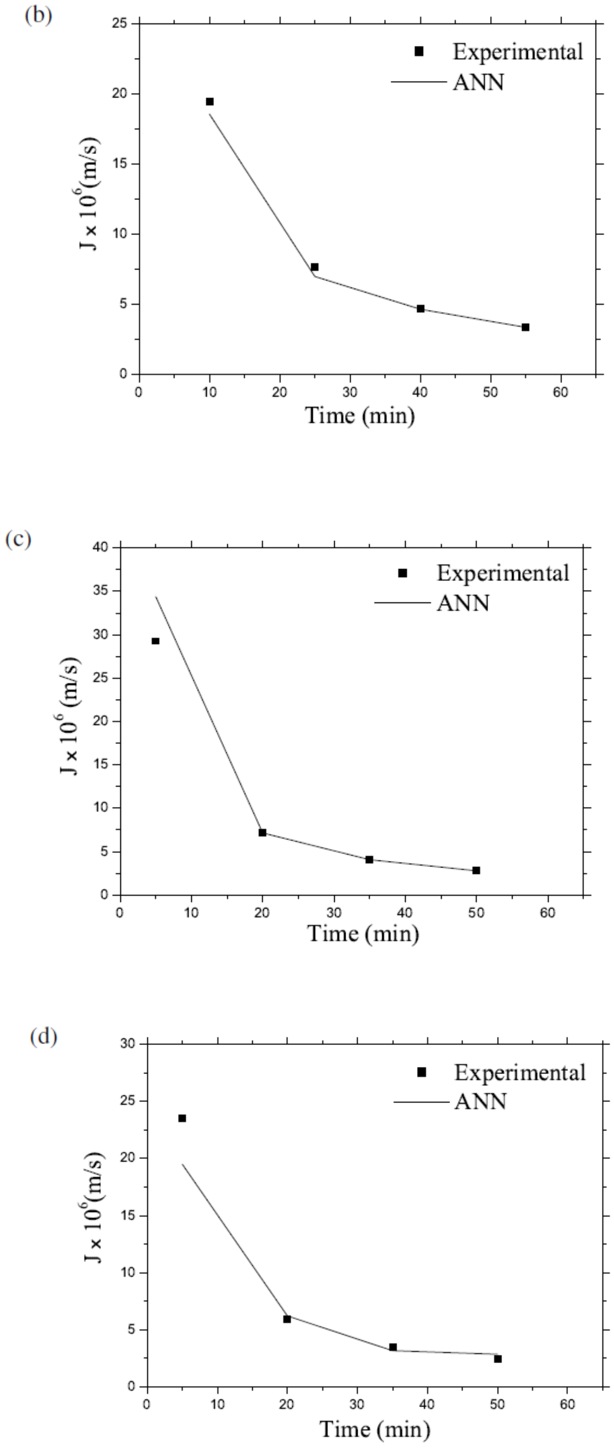

Figure 4. Average permeate flux as function of the time: (a) u = 2.6 *m/s* and ΔP = 400 *kPa*; (b) u = 3.7 *m/s* and ΔP = 300 *kPa*; (c) u = 4.7 *m/s* and ΔP = 400 *kPa*; (d) u = 5.7 *m/s* and ΔP = 500 *kPa*.

Table 1 presents some of the neural network responses to average permeate flux (J) of some examples contained in the test set.

As can be observed in the Tab. 1, even with a few experimental data for training, the results obtained by ANN for the test examples are quite satisfactory, with correlation coefficient between the values equal to R^2 = 0.94 (see Young, 1962, Doebelin, 1990). Besides, an average relative error of 8% was observed.

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Table 1. Response of the neural network to the permeate flux.

Flux velocity [*m/s*]	Pressure [*kPa*]	J_{exper}	J_{ANN}
2.6	300	4.34	4.6935
	300	2.99	2.9418
	400	3.27	3.2412
	400	2.35	2.3718
	500	3.11	2.9455
	500	2.38	2.4051
3.7	300	4.71	4.6474
	300	3.40	3.3598
	400	2.72	2.5348
	400	2.00	2.2077
	500	5.16	5.1269
	500	3.35	3.1655
4.7	300	9.40	10.080
	300	3.10	3.0946
	400	7.21	7.1409
	400	4.09	4.0656
	500	5.73	5.9968
	500	3.40	3.1414
5.7	300	5.93	6.2138
	300	3.48	3.1638
	400	3.98	3.3267
	400	2.39	2.7764
	500	5.72	5.7688
	500	3.28	3.1437

The relative error was calculated for equation

$$J_{error} = \frac{\left|J_{\mathrm{exper}} - J_{ANN}\right|}{J_{\mathrm{exper}}} \times 100\% \tag{8}$$

where J_{ANN} is the value of *J* obtained by J_{exper} is the experimental value of *J*.

4. CONCLUSIONS

The neural network was trained with experimental data already published. A small number of examples were considered to construct a database, from which the parameters of the neural network (weights and bias) could be adjusted. More specifically, the neural models were constructed to map parameters of crossflow membrane filtration process, estimating the corresponding permeate flux of mixtures in suspension of xanthan gum. These parameters correspond to transmembrane pressure, flux velocity and microfiltration time.

After concluding this stage, the implementation of artificial neural network and preliminary studies were carried out aiming to obtain architecture optimized regarding the problem. After that, the training of the best model with examples extracted from the database was performed to determine the permeate flux of mixtures.

The results of the artificial neural networks were quite satisfactory, as it showed to be capable of estimating the values of the permeate flux of mixtures for examples that were not presented to it in the training, with average error of 8%.

The simplicity and efficiency of the developed neural approach indicates that the proposed methodology can be used as an efficient method to estimate parameters related to the crossflow membrane filtration process.

5. ACKNOWLEDGMENTS

The authors wish to express their thanks to CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico) grants no. 475390/2011-3 for the financial support.

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7. RESPONSIBILITY NOTICE

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