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Neural models for monitoring the transmembrane flux in the vinasse clarification process by crossflow microfiltration

Modelos neurais para monitorar o fluxo transmembrana no processo de clarificação de vinhaça por microfiltração tangencial

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Abstract

Artificial Neural Networks (ANN) were used for estimating the transmembrane flux in a crossflow microfiltration process with ceramic tubular membranes to clarify the vinasse. The prevision was accomplished through the training of ANN feedforward using the experimental database generated in the work of Trevisoli (2010). The results showed a good correlation between the estimated data and the experimental data of transmembrane flux. For the microfiltration process with the membrane nominal pore size of 0.8 µm, the test subset presented maximum percentage error of 5.21% and average percentage error of 1.62%. For the membrane nominal pore size of 1.2 µm, the test subset had maximum percentage error of 28.51% and average percentage error of 4.66%. Therefore, it is feasible to use the ANN technique to estimate future data, helping to study membranes in microfiltration processes.
Keywords: Neural models, Levenberg-Marquadt algorithm, Microfiltration, Vinasse.

Resumo

Redes Neurais Artificiais (RNA) foram utilizadas para estimar o fluxo transmembrana em um processo de microfiltração tangencial com membranas tubulares cerâmicas para clarificação da vinhaça. A predição foi realizada através do treinamento de RNA *feedforward* utilizando o banco de dados experimental gerado no trabalho de Trevisoli (2010). Os resultados mostraram uma boa correlação entre os dados estimados e os dados experimentais de fluxo transmembrana. Para o processo de microfiltração com o tamanho nominal dos poros da membrana de 0,8 µm, o subconjunto de teste apresentou um erro percentual máximo de 5,21% e um erro percentual médio de 1,62%. Para o tamanho nominal do poro da membrana de 1,2 µm, subconjunto de teste teve erro percentual máximo de 28,51% e erro percentual médio de 4,66%. Portanto, é viável o uso da técnica de RNA para estimar dados futuros, auxiliando no estudo de membranas em processos de microfiltração.
Palavras-chave: Modelos neurais, algoritmo de Levenberg-Marquadt, microfiltração, vinhaça.

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1 Introdução

Vinasse is the residue from the production of alcohol and sugar with a high agricultural value as a fertilizer (UYEDA, 2009). In Brazil, a common practice for the problem of the destination of vinasse is the application directly to the soil as a fertilizer and source of potassium. However, with the higher productivity of alcohol, consequently, of vinasse, the sugar and alcohol mills increased the application of the residue in the soil, which generated problems such as contamination of groundwater close to the surface and saturation of some nutrients such as potassium. Clarifying vinasse before disposal can reduce the harmful action on the soil. An alternative to the treatment of liquid waste is crossflow microfiltration, which can concentrate and retain unwanted substances (TREVISOLI, 2010).

Crossflow membrane filtration technology (microfiltration, ultrafiltration and nanofiltration) has been researched and used widely in industry because it has a great potential for removing particles. During filtration processes, fouling is the main problem causing loss of productivity, because reduces equipment efficiency with permeate flux decline, which increases production cost by repetitive cleanings and can cause contamination problems due to the growth of microorganisms at the membrane surface. 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 Network (ANN) has attracted attention as new approach for determining complex relationships between input and output variables on analysis of experimental data (FILLETTI; SILVA, 2015).

ANN model has drawn attention over the past decades as a new approach to determining complex relation between many input and output variables. In previous studies, the ANN model has been demonstrated to perform better than the conventional modeling methods in addition besides it offers the advantage of being easy to use. ANN has attracted much interest in certain membrane processes because it has potential to describe highly non-linear behaviors, such as decreased flow or increased resistance under different conditions.

A few works have been done with the application of ANN model in membrane crossflow filtration. Razavi, Mortazavi and Mousavi (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, Calabro and Iorio (2006) presented ANN methodology for the control of permeate flux decay, on the basis of the experimental results collected, during ultrafiltration of BSA solutions. Chen and Kim (2006) investigated the capability of a radial basis function neural network to predict long-term permeate flux decline in crossflow membrane filtration. They used transmembrane pressure and filtration time along with feed water parameters such as particle radius, solution pH, and ionic strength were used as inputs to predict the permeate flux. The results observed indicated that a single radial basis function neural network accurately predicted the permeate flux decline under various experimental conditions of colloidal membrane filtrations. Liu, Kim and Lee (2009) used ANN model to predict the performance of microfiltration systems for water treatment using a hollow fiber membrane module. The effects of operating parameters on membrane performance were evaluated based on the comparison of transmembrane pressure (TMP) as a function of operating time. The ANN model used five input variables for predicting corresponding TMP. The modeling results indicated that there was an excellent agreement between the experimental data and predicted values. Liu *et al* (2014) developed an ANN model to model the turbulence promoter-assisted during crossflow microfiltration process of particulate suspensions. Using the trained ANN model, the effects of microfiltration operation conditions on the flux improvement efficiency were studied, and the relative importance of each operation condition to the flux improvement efficiency was analyzed. Jokic *et al* (2020) analyzed a non-recurrent feed-forward ANN with one hidden layer for microfiltration modeling using Bacillus velezensis cultivation broth as the feed mixture. The results presented of application of the ANN model for prediction of permeate flux during microfiltration of Bacillus velezensis cultivation broth were satisfactory. Authors as Chellam (2005), Curcio *et al* (2005), Delgrange *et al* (1998), Guadix *et a*l (2010), Hilal, Ogunbiyi and Al-Abri (2008), Niemi, Bulsari and Palosaari (1995), Shahoo and Ray (2006), Shetty and Chellam (2003) and Silva and Flauzino (2008) also worked with the applicability of ANN to describe membrane processes.

Research group of the authors of this work used ANN to estimate the permeate flow of a beverage based on açai through the crossflow microfiltration process using two ceramic membranes (PRONI; HANEDA; FILLETTI, 2020). The results provided by the ANN was very satisfactory, which motivated to extend this study to other solutions.

Therefore, the aim of this research work was the development of a neural model to predict the performance of microfiltration applied to clarify the vinasse originated from the processing of sugarcane, with tubular ceramic membranes with nominal pore size of 0.8 μm (M08) and 1.2 μm (M12). The results were compared with those obtained by Trevisoli (2010).

2 Neural network model

The ANN developed in this work was implemented in the MATLAB R2018a Neural Networks Start Toolbox (NNSTART) library on an Intel (R) Core (TM) i7-3630QM computer with 2.40GHz and 6.0 GB of RAM with the Levenberg-Marquadt algorithm (HAGAN; MENHAJ, 1994).

The experimental data set (TREVISOLI, 2010) used in the development of ANN was randomly divided into three subsets as follows: 70% of the data were used in ANN training, 15% formed the validation subset and the remaining 15% constituted the test subset. For both models, 144 experimental data were used, which were divided into training, validation and test.

The ANN was multilayer perceptron of the type feedforward. To work with the membrane M08 data, ANN had a hidden layer with five neurons as shown in Figure 1 and the ANN for M12 had a hidden layer with six neurons. In order to obtain accurate results for the transmembrane flux, the number of neurons in each ANN was defined by trial and error.

ANN received three characteristics from which they should extract information for their responses: Reynolds number, pressure (bar) and filtration time (min). The ANN output layer was composed of a neuron, which was responsible for estimating the transmembrane flux ($L.h^{-1}m^{-2}$).

The training process was interrupted with few epochs to avoid ANN from losing its generalization capacity caused by overtraining. When this happens, ANN memorizes the training subset instead of mapping the main aspects of it, generating little or no reproducibility of the results of the validation and test subsets.

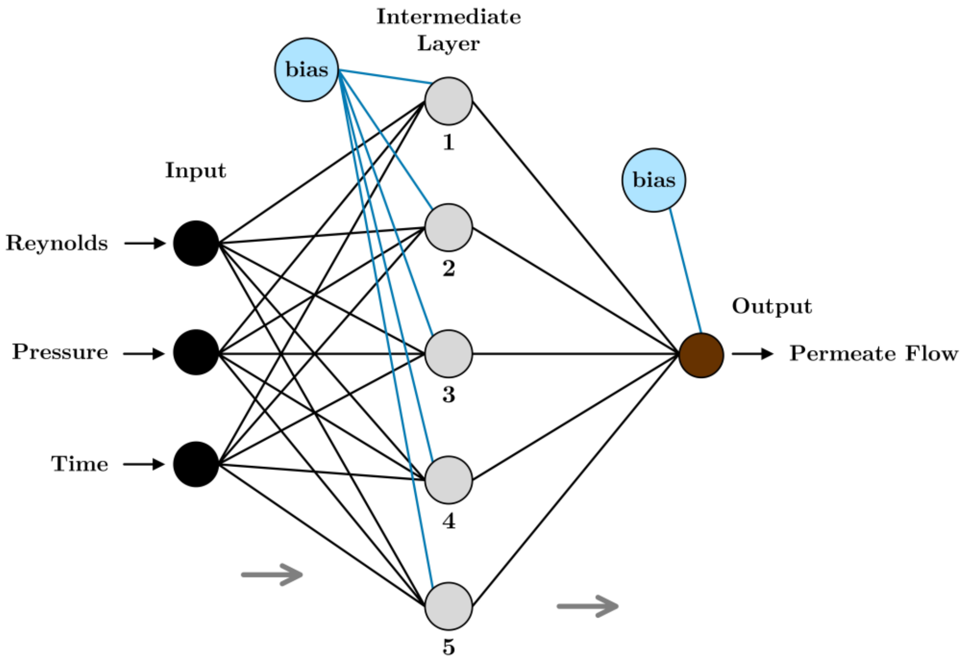


Figure 1: ANN architecture used to estimate the permeate flux of the membrane M08.

3 Results and discussion

The proposed ANN for membrane M08 showed excellent convergence in its results. For the training subset, a maximum percentage error of 5.20% and an average percentage error of 1.06% were obtained; for the validation subset, the maximum percentage error was 12.26%, with an average percentage error of 1.62%; for the test subset, the maximum percentage error was 5.21% and the average percentage error was 1.62%. Table 1 shows the permeate flux values estimated by ANN compared to the experimental values for the membrane M08 in the test subset, and the average percentage error calculated for each value obtained.

Table 1: Comparison between the permeate flux values estimated by ANN and the experimental values for the membrane M08 in the test subset.

Experimental values	Values estimated by ANN	Percentage error
31.40	33.04	5.21%
31.04	30.94	0.32%
31.20	30.61	1.88%
30.49	29.83	2.17%
29.48	29.25	0.76%
29.21	29.08	0.45%
28.91	29.02	0.37%
29.40	29.82	1.42%
40.24	40.04	0.48%
36.79	36.43	0.98%
36.35	36.01	0.92%

31.70	31.65	0.17%
39.69	40.68	2.48%
37.80	37.45	0.91%
37.61	36.96	1.73%
36.08	36.54	1.26%
35.83	36.47	1.77%
36.16	36.19	0.08%
40.73	42.61	4.62%
39.91	39.03	2.20%
37.31	38.14	2.23%
41.33	42.68	3.26%
Average percentage error		**1.62%**

Figure 2 shows the good correlation between the experimental values and the values estimated by the ANN in which the abscissa axis represents the experimental values and the ordinates axis represents the results provided by the ANN. The good results are reinforced by the linear regression equations and by the correlation coefficients: $y = 0.98x + 0.61$ and $R = 0.99$ (training subset), $y = 0.89x + 3.93$ and $R = 0.96$ (validation subset) and $y = 1.04x - 1.38$ and $R = 0.99$ (test subset).

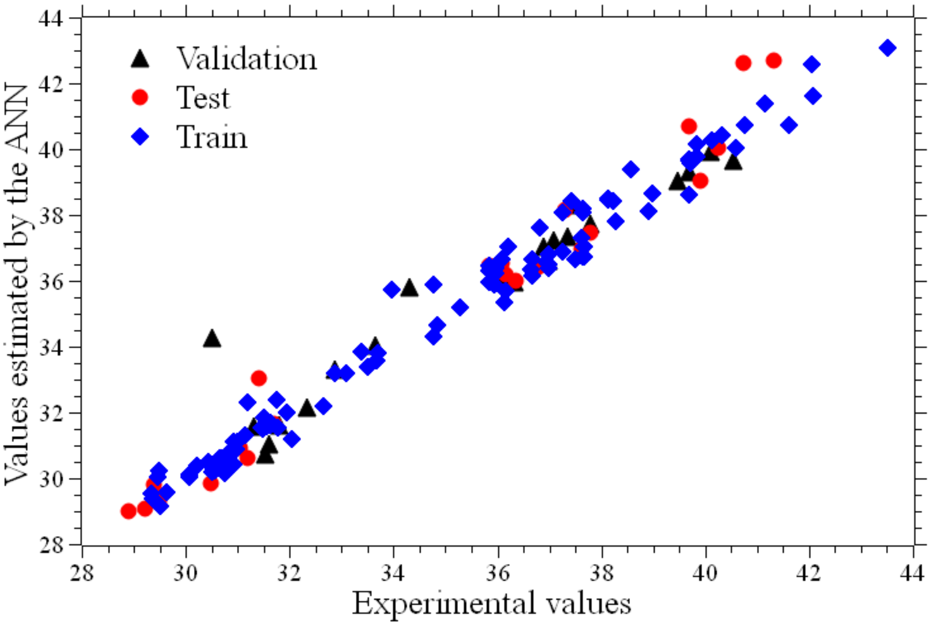


Figure 2: Permeate flux estimated by ANN versus experimental values for the training, validation and test sets of the membrane M08.

Figure 3 presents a comparison between permeate flux estimated by ANN (output) and experimental values (target) for the test subset of the membrane M08 for different Reynolds with pressure of 2 bar (Figure 3a) and 5 bar (Figure 3b). Note that, for both pressures, the output and target values practically coincide at all points that were experimentally collected during the microfiltration process. In this case, the Reynolds number values used were: 11500, 22500, 33500.

The performance of the ANN model for the membrane M08 can be seen in Figure 4, which shows that the training stage stopped at 66 epochs, with a mean squared error (MSE) of approximately 0.25. The established stopping criterion was check validation, that is, the training is interrupted if the performance of the validation set deteriorates for 6 consecutive epochs. Thus, it is avoided excessive adjustment by ANN that could cause poor generalization performance. The best performance of ANN was obtained with sigmoid transfer function in the hidden layer and with a linear transfer function in the output layer.

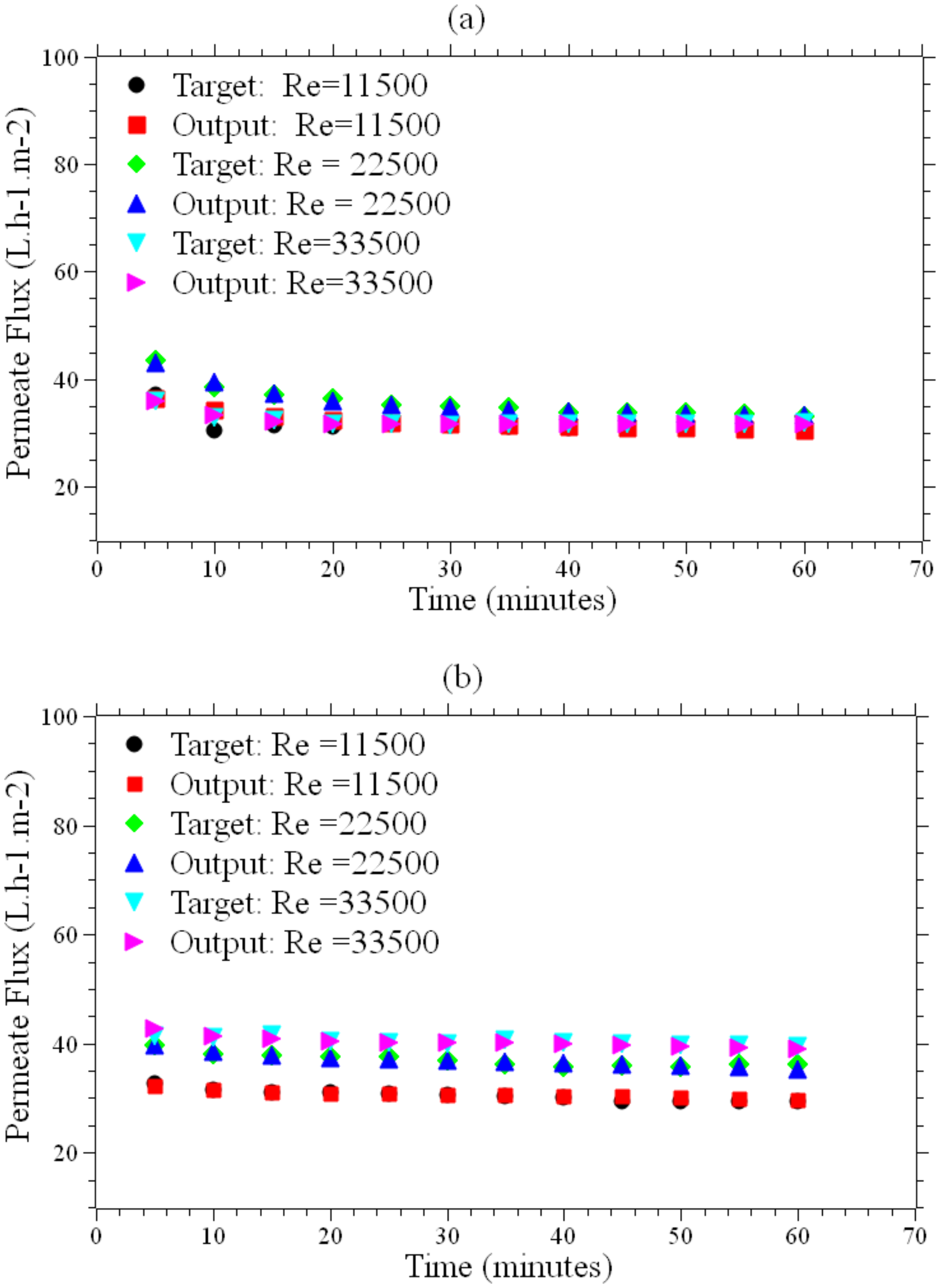


Figure 3: Permeate flux estimated by ANN (output) and experimental values (target) for the test subset of the membrane M08 for different Reynolds: (a) 2 bar and (b) 5 bar.

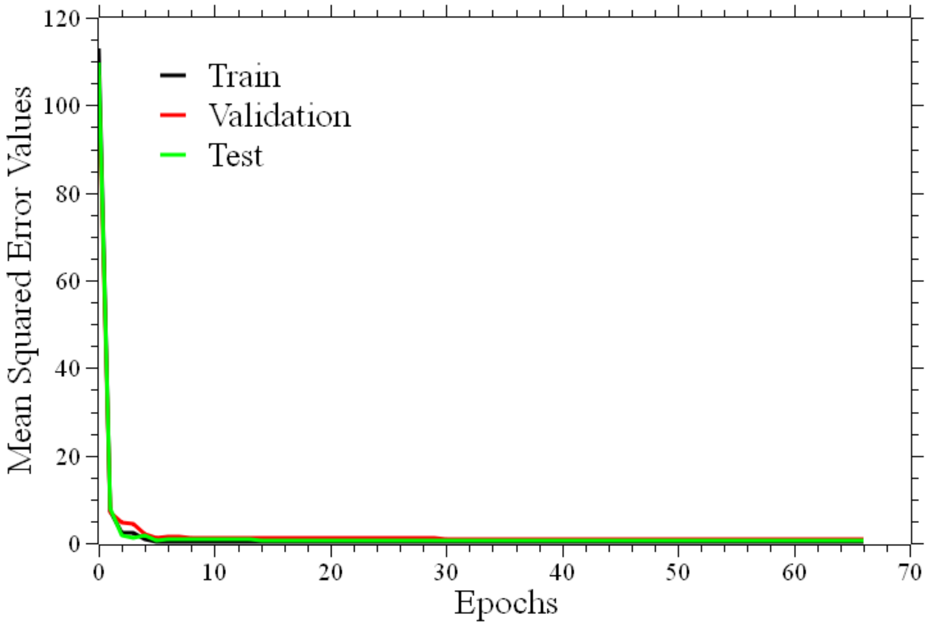


Figure 4: ANN performance during training for membrane M08 data.

The ANN developed for the membrane M12 also showed good generalization from the experimental data. In this case, the structure differs from the previous one, because it has six neurons in the hidden layer. This adjustment was necessary due to the difficulty of converging the solution during training.

The maximum percentage error was 40.58% in the ANN training. However, it is worth noting that the transmembrane flux supplied to the ANN network was 4.34 $L.h^{-1}m^{-2}$, while the value estimated by ANN was 6.12 $L.h^{-1}m^{-2}$. As it is a small value, a small variation causes a considerable percentage error. In addition, the experimental value differs considerably from the other data of the training subset, configuring an outlier and, therefore, little representative as an ANN efficiency parameter. Furthermore, the average percentage error for this subset was 3.11%, demonstrating considerable linearity between the experimental data and the data estimated by the ANN. For the validation subset, the maximum percentage error was 30.02% and the average percentage error was 4.91%. For the subset of tests, ANN presented a maximum percentage error of 28.51% and an average percentage error of 4.66%.

Table 2 shows the permeate flux values estimated by ANN compared to the experimental values for the membrane M012 in the test subset, and the average percentage error calculated for each value obtained.

Table 2: Comparison between the permeate flux values estimated by ANN and the experimental values for the membrane M12 in the test subset.

Experimental values	Values estimated by ANN	Percentage error
31.31	30.27	3.31%
30.30	31.14	2.76%
35.83	34.76	2.99%
31.34	31.84	1.61%

31.48	31.47	0.02%
15.33	16.12	5.15%
33.83	30.21	10.70%
27.40	27.54	0.50%
30.77	30.75	0.06%
28.19	30.17	7.02%
11.14	7.96	28.51%
11.66	12.21	4.69%
11.91	12.59	5.72%
12.37	12.14	1.82%
23.35	21.20	9.22%
21.21	20.46	3.52%
19.32	19.73	2.10%
19.76	19.57	0.98%
19.43	18.65	4.00%
24.85	25.42	2.28%
24.01	25.05	4.33%
28.93	28.54	1.35%
Average percentage error		**4.66%**

Figure 5 shows the good correlation between the experimental values and the values estimated by the ANN developed for the M12. The linear regression equations and the correlation coefficients were: $y = 0.96x + 0.97$ and R = 0.99 (training subset), $y = 1.06x – 1.32$ and R = 0.97 (validation subset) and $y = 0.99x − 0.02$ and R = 0.98 (test subset).

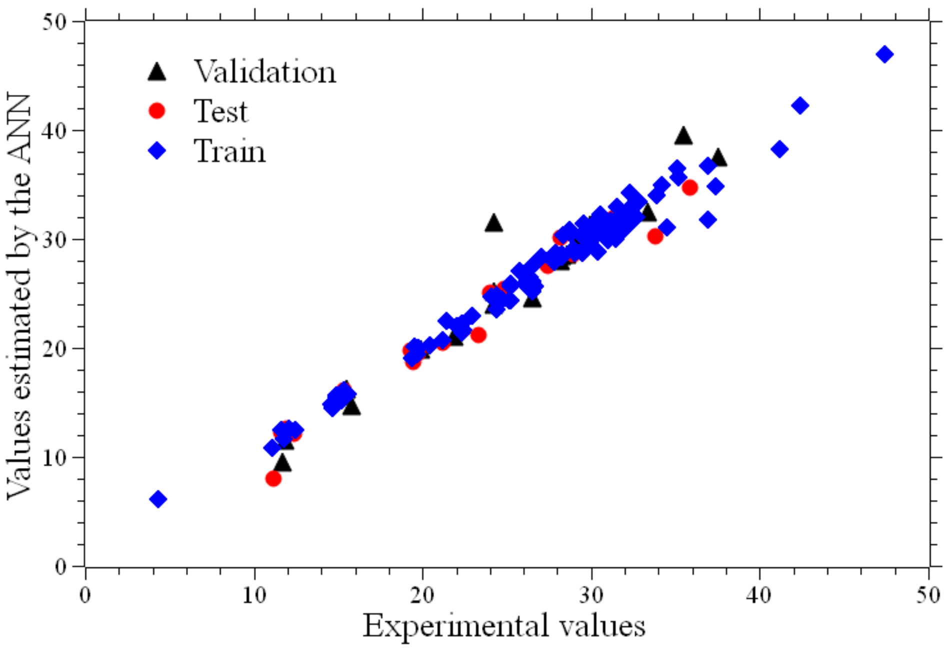


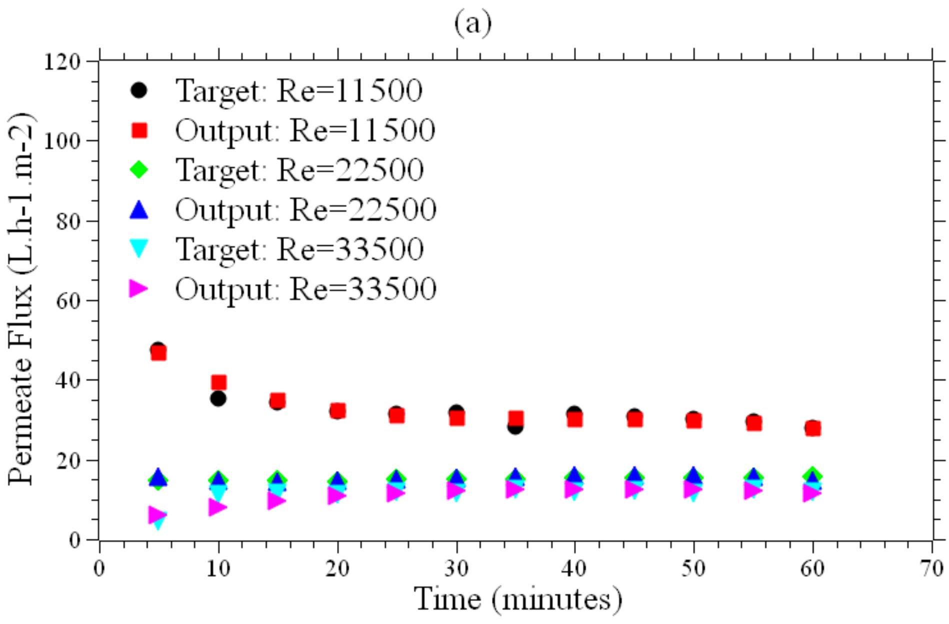
Figure 5: Permeate flux estimated by ANN versus experimental values for the training, validation and test sets of the membrane M12.

It is noted that the relative percentage errors were greater in the case of the membrane M12 when compared to the values of the membrane M08. It is believed that this happened because the filtrations in both membranes happened differently, because according of the Trevisoli (2010) work, it was observed that for the membrane M12 the permeation rate resulting was more susceptible to tangential velocity and transmembrane pressure variations and the transmembrane flux was unstable with variations during the 60 minutes of the process. This is due to the pore obstruction phenomena not having stabilized during the process. The membrane M08 showed the lowest resistance results and was less affected by the change in tangential velocity when compared to the membrane M12 under the same conditions.

Thus, it is clear that the crossflow microfiltration process using the membrane M12 generated an irregular experimental database with respect to permeate flows, due to the unstable process. This hindered the training of the ANN, which estimated some values of the transmembrane flux with greater errors than in the case of M08.

One can see from Figure 6 a comparison between permeate flux estimated by ANN (output) and experimental values (target) for the test subset of the membrane M12 for different Reynolds with pressure of 2 bar (Figure 6a) and 5 bar (Figure 6b). Again, it can be noted that the output and target values coincide, which helps to confirm the good results provided by ANN to estimate the permeate flux in the vinasse microfiltration process.

The training stage was interrupted in 22 epochs, with an MSE of approximately 1.11, as it is shown in Figure 7. In this case, the same stopping criterion was used for training, that is, check validation. Other transfer functions were tested, but the best result was also a sigmoid transfer function in the hidden layer and a transfer function linear in the output layer.



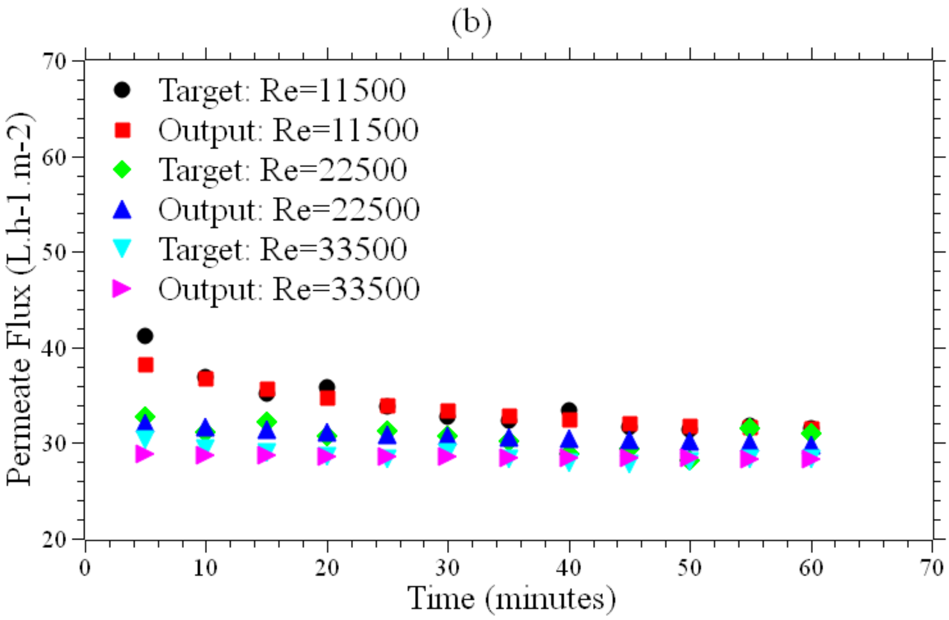


Figure 6: Permeate flux estimated by ANN (output) and experimental values (target) for the test subset of the membrane M012 for different Reynolds: (a) 2 bar and (b) 5 bar.

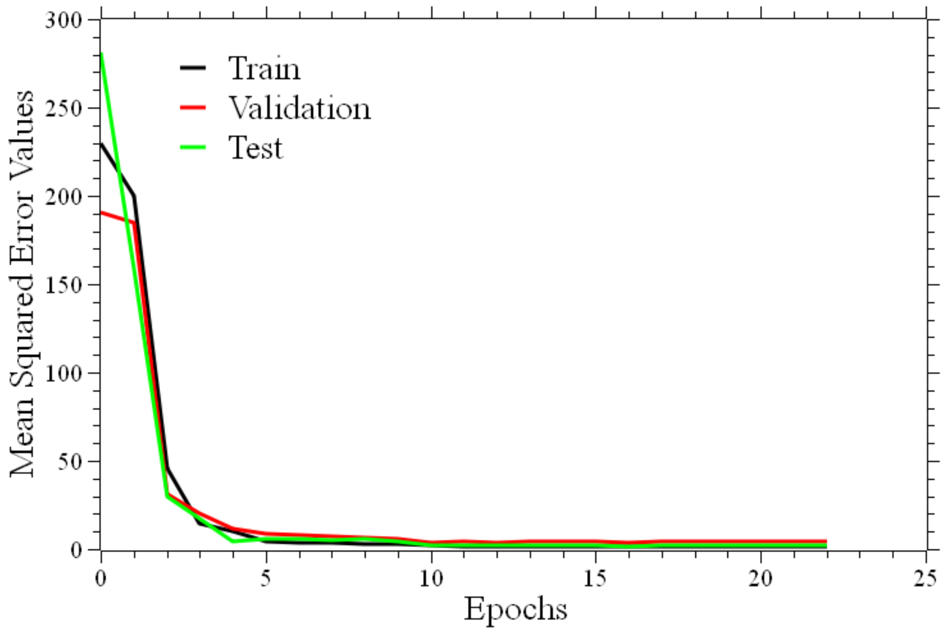


Figure 7: ANN performance during training for M012 membrane data.

4 Conclusions

In this work of numerical investigation, two neural models, which were based on the experimental database generated in the work of Trevisoli (2010), were developed with the Levenberg-Marquadt algorithm to estimate the transmembrane flow in a crossflow microfiltration process with ceramic tubular membranes for clarification of vinasse. The input variables supplied to ANN were Reynolds number, pressure and filtration time.

The two ANN models had good generalization of their experimental data, despite the different fluid-dynamic conditions in which the experiments were carried out (TREVISOLI, 2010). A correlation in both situations was satisfactory, demonstrating that the methodology is promising and suitable for the solution of this problem and can be used as a tool to estimate the transmembrane flux. Once again, ANN have demonstrated the ability to process information with high speed and accuracy， showing itself able to simulate the transmembrane flux data from the vinasse of the crossflow microfiltration process. This can contribute to the experimental research in the area, as it was found that this computational tool has the potential to be used in helping to define which membrane is most suitable for the process, thus saving costs with simulations. Therefore, it can be concluded that Artificial Neural Networks are capable of estimating transmembrane flux values for different operational conditions in the crossflow microfiltration process.

Can stand out that, due to few experimental data, the ANN tests were performed for two types of ceramic membranes. Thus, it is suggested as future work to analyze ANN for other types of membranes, to have greater ANN versatility.

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