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APPLICATION OF ARTIFICIAL NEURAL NETWORKS TO ESTIMATE PERMEATED FLOW IN BIPHASIC MIXTURES OF WATER AND OLEIC ACID

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Abstract: The açaí (*Euterpe oleracea*) is a natural fruit from the Amazon, which has high nutritional values, being a food that is gaining national and international attention, because from it, it is possible to extract açaí juice. To guarantee the quality of the juice during storage, it is necessary to clarify it, thus facilitating other conservation processes and avoiding the generation of turbidity. The clarification process can be carried out by crossflow microfiltration using ceramic membranes. The use of this method for clarification has many benefits, among them are less energy use, in addition to not having to do thermal and chemical treatment. However, in addition to the benefits, this process also has the disadvantage of decreasing the permeate flux as a function of time, due to the obstruction of the membrane pores. In view of the above, this work presents a neural model capable of estimating the permeate flux of biphasic mixtures of water and oleic acid, from açaí, which can obstruct the pores of the membranes. The neural model results were satisfactory with a mean percentage error of 9.4%.
Keywords: Artificial neural networks. Crossflow microfiltration. Oleic acid. Learning algorithm.

INTRODUCTION

Açaí is an endemic fruit from the northern region of Brazil, which, although it has good nutritional qualities, cannot be consumed *in natura* because of its physical characteristics, and its pulp must be processed beforehand (CEDRIM; NASCIMENTO, 2018; CORRÊA et al., 2010).

Currently, there is a national and international interest in the consumption of açaí, which can be explained in part by its chemical composition, which has high nutritional values. However, both the fruit and its pulp are highly perishable, requiring the application of conservation methods for the export of these products to be possible. The clarification of açaí juice can facilitate the performance of some of these conservation processes (such as heat treatment and concentration of the juice), in addition to preventing the generation of unwanted turbidity in the juice during storage (COUTO, 2012; CEDRIM; NASCIMENTO, 2012; CEDRIM; NASCIMENTO), 2018; CORRÊA et al., 2010). Thus, clarification is a very important step in the storage of açaí juice.

The açaí juice can be clarified through the crossflow microfiltration process with ceramic membranes. The application of this process has some advantages such as low consumption and there is no need for thermal or chemical modifications of the juice to apply the method. Some advantages of using ceramic membrane in crossflow microfiltration is its resistance to high temperatures and organic solvents, in addition to not undergoing changes to biological attacks. Although, for these reasons, the use of this process is very promising in the food industry, this method has the disadvantage that the permeate flux passing through the membrane decreases as a function of time, due to the obstruction of membrane pores by materials retained in it (in the case of açaí juice, these materials are present in the açaí pulp, which has a complex composition) (CAMINOTO, 2012).

Thus, it is very useful to monitor the permeate flow throughout the microfiltration process and a methodology that has been drawing the attention of researchers for this purpose is artificial intelligence, more specifically, Artificial Neural Networks (ANNs), which have many advantages such as high accuracy, low computational cost, robustness, and the ability to generalize responses to data not used in your training.

Some interesting works that used ANNs to estimate the permeate flux are listed below:

Silva, Silva and Filletti (2021) used ANNs to estimate the permeate flux in a crossflow microfiltration process with ceramic tubular membranes for vinasse clarification, obtaining a good correlation between the estimated data and the experimental data, with an average percentage error of 1.62% using a membrane with 0.8 μm diameter pores, and an average percentage error of 4.66% for the data from the membrane with pores of 1.2 μm in diameter. Jokic et al. (2020) developed a neural model to monitor the permeate flux of a broth from the cultivation of Bacillus velezensis, in the microfiltration process. The ANN input variables were microfiltration time, surface feed velocity, transmembrane pressure, surface air velocity and the presence or absence of Kenics static mixer (a tool used to mix the broth). The results were satisfactory, showing that the neural model is able to provide the permeate flow values throughout the process. Proni, Haneda and Filletti (2020), proposed the application of ANNs using the Levenberg-Marquardt algorithm to estimate the permeate flux of an açaí-based beverage in crossflow microfiltration (two ceramic membranes with pores of 0 .8 μm and 1.2 μm). The input parameters of the neural models were the Reynolds number, the transmembrane pressure and the microfiltration time. The results obtained by the ANNs had low mean percentage errors, being 7.6% for the 0.8 μm membrane and 9.9% for the 1.2 μm membrane for the test data, thus validating the use of this tool.

Thus, the purpose of this work was to investigate the use of neural networks to estimate the permeate flux of a biphasic mixture of water and oleic acid from açaí, using the experimental data obtained by Caminoto (2012), and thus create a tool alternative computational tool to assist in the monitoring of the tangential microfitration process, in order to have more information at the time of evaluating whether obstructions are occurring in the pores of the ceramic membranes, through the observation of the decline of the permeate flux as a function of time.

ARTIFICIAL NEURAL NETWORKS

According to Braga, Carvalho and Ludermir (2000), Artificial Neural Networks are distributed parallel systems composed of simple processing units, called neurons, which calculate mathematical functions, normally non-linear. Neurons are arranged in one or more layers and interconnected by a large number of connections, which are associated with weights, which store the knowledge represented in the model and serve to weight the input received by each neuron in the ANN.

The development of a neural model initially goes through a learning phase, in which a set of examples is presented to the ANN, which automatically extracts the necessary characteristics to represent the information provided and generate answers to the problem, according to a learning algorithm. The ability to learn through examples and to generalize the information learned is the main advantage of problem solving through ANNs.

An algorithm widely used in the development of artificial neural networks is the Levenberg-Marquardt algorithm, which consists of a modification of the Gauss-Newton method (HAGAN and MENHAJ, 1994, BURKE and FERRIS, 1995), and uses the residual error function. quadratics. This algorithm calculates the function obtained by the difference between the desired response and the response obtained by the neural model, given by

$$e_i(x) = d_i(x) - y_i(x) \tag{1}$$

Where d_i is the desired response for neuron i, and y_i is the response obtained by the neural model and minimizes the error function in the iteration n given by

$$E_n(x) = \sum_{i \in C} e_i^2(x) \quad (2)$$

where C is the set of all neurons in the neural model and the vector $x=(x_1,\ldots,x_2)$ represents the weights associated with neurons. The Levenberg-Marquardt algorithm can be described by the following steps (CUSTÓDIO, FILLETTI and FRANÇA, 2019):

(i) All input variables with the corresponding output are presented to the neural model;

(ii) The neural model parameters (weights) are started with random values;

(iii) New values are calculated for the output, referring to the input variables;

(iv) The errors of equations (1) and (2) are calculated, and the root mean square error for the N training examples, given by

$$E_{med} = \frac{1}{N} \sum_{n=1}^{N} E_n\,(x). \quad (3)$$

(v) Calculate the Jacobian matrix

$$J(x) = \begin{bmatrix} \frac{\partial e_1}{\partial x_1} & \cdots & \frac{\partial e_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial e_N}{\partial x_1} & \cdots & \frac{\partial e_N}{\partial x_n} \end{bmatrix}. \quad (4)$$

and solve the equation

$$\Delta x = [\,J^T(x)\,J(x) + \mu I]^{-1} J^T(x) e(x) \quad (5)$$

where the parameter $\mu>0$ appears diagonally from $J^T(x)J(x)$ and is called the Levenberg-Marquardt parameter, I is the identity matrix, e(x) is the error, and J is the Jacobian matrix.

(vi) The neural model weights are modified according to the search direction of the Levenberg-Marquardt algorithm (equation (5));

(vii) It iterates from (iii) to (vi), successively modifying the neural model weights until a suitable stopping criterion is reached, such as, for example, the root mean square error reaches the desired value or the number of epochs reaches an established value.

The Levenberg-Marquardt parameter μ is multiplied by a factor β when propagation increases the value of the error function, but when there is a decrease in its value, μ is divided by the factor β. Thus, the parameter μ adjusts the approximation avoiding propagations that could lead to a convergence error, and therefore, a positive and significant value of μ will be enough to restore the matrix $J^T(x)J(x)$ and produce a good error search direction by the neural model (BENATTI, 2017; PRONI, HANEDA and FILLETTI, 2019).

DEVELOPMENT OF THE NEURAL MODEL

From the results presented by Caminoto (2012), a database was built to train the neural model. The input variables were the microfiltration time and the transmembrane pressure, and thus, the feedforward neural model had two neurons in the input layer, one for each of the variables. By trial and error, 7 neurons were defined in the intermediate layer, and the learning algorithm that provided the best results was that of Levenberg-Marquardt (PRONI, HANEDA and FILLETTI, 2020). The error backpropagation algorithm was also tested, but it did not provide satisfactory results. The output layer had only one neuron, which was responsible for estimating the permeate flux of the mixture of water and oleic acid.

For the development of the neural model, the database, which contained a total of 108 examples, was randomly divided into 3 sets, being one set for training (made up of 70% of the data, that is, by 76 examples), one set for validation (consisting of 15% of the data, that is, it contained 16 examples) and the third set for testing (also comprising 15% of the data). The neural model was developed in Matlab 2020a software with the tool *nnstart – fitting app.*

RESULTS AND DISCUSSIONS

In this section, the results provided by the neural model developed to estimate the permeate flux of the biphasic mixture of water and oleic acid will be presented. 30 epochs were performed during the training of the neural model and the best performance occurred at epoch 24, as shown in Figure 1. The average percentage relative error obtained for the training samples was 7.6%, for validation it was 6, 4% and for the test it was 14.3%. Thus, the average of percentage relative errors was 9.4%, which is a very satisfactory result.

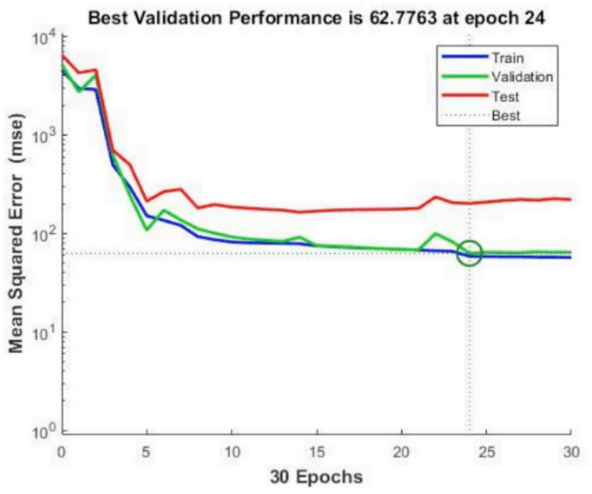

Figure 1 – Performance of the neural model during its training.

Source: Matlab 2020.

Figure 2 shows the distribution of errors (difference between the real values of the permeate flow and the values estimated by the neural model) of the training, validation and test sets. From this graph, it is possible to notice that the errors remain close to zero and present randomness, thus showing that the results obtained do not have trends. These observations can be confirmed by analyzing Figure 3, which contains the histogram of the errors obtained during the development of the neural model. Note a normal distribution of absolute errors centered on zero.

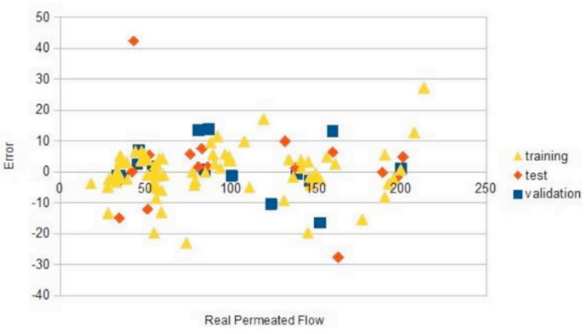

Figure 2 – Distribution of errors.

Source: The authors.

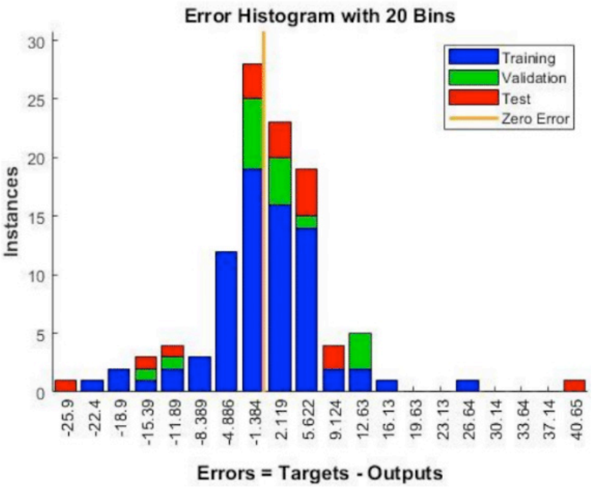

Figure 3 – Histogram of absolute errors for the best developed neural model.

Source: The authors.

Figure 4 shows the relationship between the values of the permeate flux of the real biphasic mixture of water and oleic acid and the values obtained by the neural model in the training, in the validation and in the test, whose coefficients of determination were 0.98, 0.98 and 0.95 respectively, values very close to the ideal value, which is equal to 1.

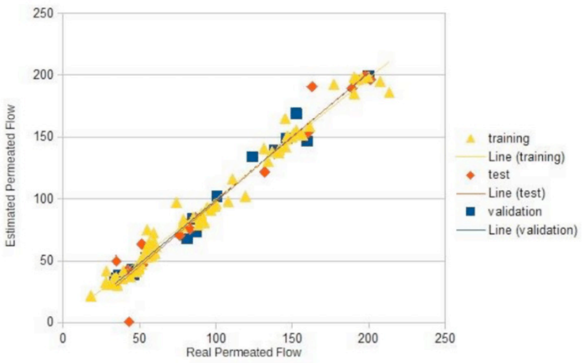

Figure 4 – Values of the permeate flow estimated by the ANN versus real values for the training, validation and test sets.

Source: The authors.

The equations that best fit the data are $y = 0.98\ x + 2.03$ for the training set, $y = 1.03\ x - 3.47$ for the validation set and $y = 1.04\ x - 6.69$ for the test set and, thus, it is possible to observe that the permeate flow values estimated by the neural model are very close to the real values, which were experimentally obtained by Caminoto (2012), showing that the developed neural model is capable of estimating the permeate flow of the biphasic mixture of water and oleic acid satisfactorily.

FINAL CONSIDERATIONS

This article showed that it is possible to use Artificial Intelligence to monitor the crossflow microfiltration process, in order to identify clogged pores of ceramic membranes due to encrustation of process residues. The neural model developed to estimate the permeate flux of the biphasic mixture of water and oleic acid provided satisfactory results, with an average percentage error of 9.4%, and also obtained coefficients of determination very close to 1, in addition to presenting a good approximation of the results with the central tendency line, evidencing once again that the results estimated by the ANN were close to the real values.

Given the above, future works include the application of Neural Networks, and other Artificial Intelligence methodologies, such as Random Forests, for example, to analyze the permeate flow of other solutions, as well as estimating other parameters of the crossflow microfiltration process, such as the Reynolds number or transmembrane pressure.

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