ARTIFICIAL NEURAL NETWORK IN THE ESTIMATION OF RHEOLOGICAL PARAMETERS FOR HIGH XANTHAN GUM PRODUCTION

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ABSTRACT

The production of the biopolymer xanthan gum by *Xanthomonas*, an aerobic microorganism, is directly dependent on the oxygenation of the cultivation broth. The bioproduct is widely used in the industry due to its high viscosity and stability properties. But this high viscosity is also one of the main obstacles to a proper mixing of the broth, therefore, leading to a poor oxygenation. A reliable correlation between gum concentration and viscosity would be a useful tool for a better control and strategy planning of a production process. It has only been reported simple and directly correlations of those two parameters in the literature. This work brings an artificial neural network (ANN) black box model to correlate gum concentration and apparent viscosity with great approximation with experimental data. The ANN was able to accurately represent the non-Newtonian behavior of the culture medium during the bioprocess in the bioreactor.

Keywords: Viscosity. Xanthan Gum. Xanthomonas. Neural Network. Artificial Intelligence.

1 INTRODUCTION

Xanthomonas campestris is well known for the secretion of a biopolymer widely used in the industry called xanthan gum. The main use is based on its high viscosity and high stability properties. *Xanthomonas* is an aerobic microorganism[1] and oxygenation is an important factor to the xanthan production[2]. During batch production the high viscosity shown by the broth, caused by the secretion of xanthan gum[3], is responsible for difficulties in the proper oxygen transportation to the cells due to mechanical limitations of proper mixing without harming the cells at high agitation speeds[4]. It has been reported in the literature that direct measured correlations between xanthan gum concentration and viscosity can be used to determine one or the other [4,5,6]. However, due to its non-Newtonian characteristics, the apparent viscosity of the solution containing xanthan gum can change drastically, necessitating the use of a non-linear model to represent this variation in order to make accurate predictions. In this work, a black box type of model based on an ANN is proposed, for a most reliable and easy correlation between these two important parameters.

2 MATERIAL & METHODS

Three different *Xanthomonas campestris pv campestris* modified strains (unpublished results), denoted as deH (3 times), PP (2 times), and XCC (1 time) were cultivated in 1 L benchtop bioreactors (Minifors® 2) with 900 mL of working volume, and a cultivation in a 5 L benchtop bioreactor (local manufacturing) containing 4 L of working volume was done for the strain deH (1 time). All cultivations were carried out at 28ºC using SYMP medium (in g.L-1: Sucrose, 35; Yeast extract, 4; Malt extract, 4; Peptone, 4; K_2HPO_4, 5.27; KH_2PO_4, 2.81; $MgSO_4$. $7H_2O$, 2; NaCl, 1; Urea, 0.4; and $FeSO_4$, 0.002). During the experiment in the larger bioreactor, 10 mL samples were taken throughout the cultivation and analyzed in terms of its rheology according to the power law and Metzner & Otto correlation for the shear rate for a Rushton impeller type, as follow the Equations 1-3 bellow[7], using the Brookfield DV III Ultra rheometer varying between Spindle 18 and 34, with stirring speed between 10 and 250 rpm. The experimental data obtained were interpolated using the Cubic Spline method for parameter *k* and Smoothing Spline for parameter *n*.

$$\tau = k * \gamma^n \tag{1}$$

$$\mu_{ap} = k * \gamma^{n-1} \tag{2}$$

$$\gamma = A * N \tag{3}$$

Where τ is the shear stress, *k* is the consistency index, γ the shear rate, *n* the flow index, *N* the agitation, *A*, constant relative to the impeller, and μ_{ap}, the apparent viscosity.

For the ANN, Figure 1, a Layered Recurrent Network type was selected, and it was trained individually for each of the two parameters, *k* and *n*, with the training following the Levenberg-Marquardt method. A log-sigmoid activation function was applied to the input and first hidden layers, while a linear activation function was applied to the second hidden and output layers. 500 training epochs were done, and a 5-cross validation process was carried out. The data were organized into 5 groups with equal distribution of points, preserving the structure of the product evolution curve.

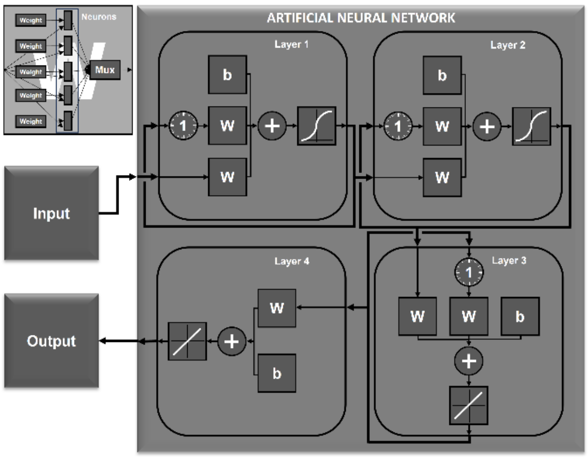

Figure 1 Operating scheme of the ANN used to describe the parameters *k* and *n* of the rheology of the medium. Each layer contains 'W' boxes for adding weights, one of which refers to retroactive data demonstrated with a delay of 1 sampling period, b' boxes for constants added, and the box representation of the transfer function applied.

3 RESULTS & DISCUSSION

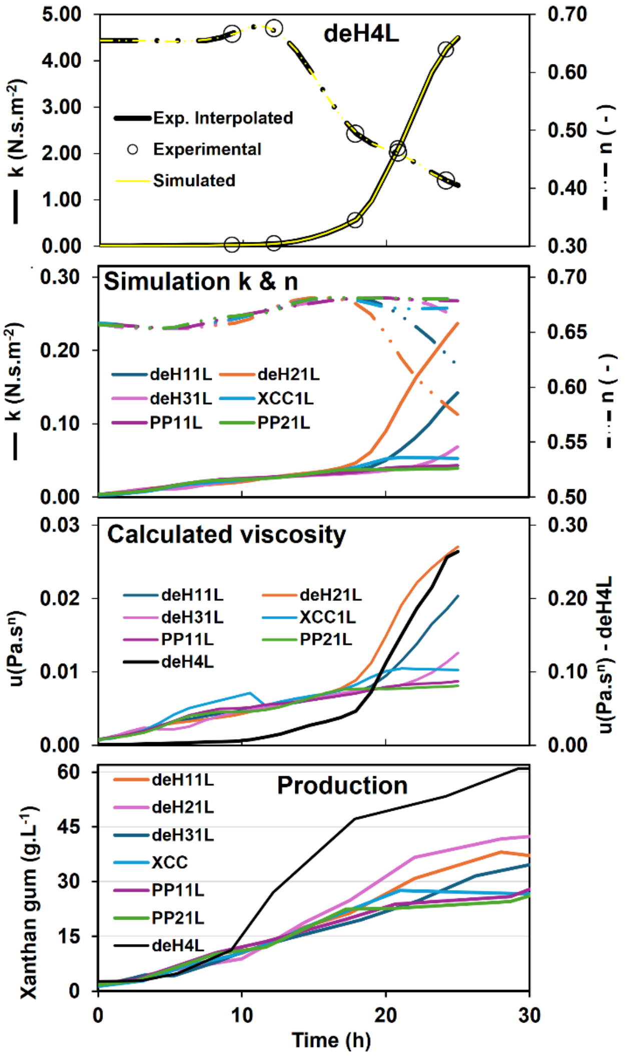

Figure 2: Curves from the ANN fitting process. The first graphic shows the interpolation performed on the experimental data of *k* and *n* utilized to train the ANN, along with the simulated curve generated. The second graphic depicts the simulated curves for the remaining cultivations, and the third illustrates the calculated viscosity. The final graphic shows the production data utilized as input for the ANN.

The fitting of the ANN to the 5 L bioreactor experimental data had great adjustment, with quadratic errors of 0.18 and 0.09 to the parameters k and n respectively (Figure 2 - deH4L). The simulations of the parameters to the 1 L bioreactor cultivations demonstrated consistent behavior, resulting in a high degree of approximation to the expected viscosity based on the observed cultivation production (Figure 2 - Calculated viscosity, Production). The viscosity does not have a linear correlation with the product concentration since it is not obeying a Newtonian behavior of a liquid. Consequently, an exponential increase in viscosity, observed in the experimental data, is initiated after a certain amount of product was reached, approximately 30 g/L of xanthan gum. The ANN was able to discern this behavior and replicated it in the other cultivations, where it is noted that the viscosity kept a linear tendency with the growth of the product and then an exponential growth begins when that product threshold is overcome (Figure 2 – Simulation k & n).

The result is seen with a greater difference in viscosity than what is observed in the product concentration. This ANN provides a correlation between the viscosity and the gum concentration that exhibits a higher affinity with the real-world behavior than the linear correlation commonly applied. This correlation can assist in the more effective management of the viscosity in a xanthan gum production cultivation.

4 CONCLUSION

A novel black box model based on an ANN was developed to correlate the xanthan gum concentration and its apparent viscosity over time in a cultivation broth. The fitting and adjustments made to the experimental data were deemed satisfactory for the purposes of this study. Moreover, the model demonstrated superior predictive capability in representing the actual viscosity evolution in comparison to a simple linear correlation with the product concentration.

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ACKNOWLEDGEMENTS

This work was supported by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES). The authors also acknowledge the Programa de Pós-Graduação em Engenharia Química (PPGEQ-UFSCar) and the Control, Optimization and Design for Energy and Sustainability (CODES-WVU) group for the technical and infrastructure support.