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Artificial Neural Network to capture the Dynamics of a Dividing Wall Column

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Abstract

The forecasting ability of Artificial Neural Network (ANN) has made it received a widespread application in the field of engineering, biology, energy, and finance. One of the main advantages of ANN is its ability to capture complex dynamics, in fact, ANNs can approximate non-linear input-output relationships to any degree of accuracy in an iterative manner. Despite the forecasting ability of ANN, its application for the downstream process is still fragmented. This study applies an artificial neural network to model the dynamics of a dividing wall column that separates an effluent coming from fermentation producing acetone, butanol, and ethanol (ABE) for spark-ignition purposes. Considering the dynamic of the diving column simulated in Aspen Plus Dynamics, a 4-10-3 multi-layer perceptron with back-propagation algorithm was enough to reproduce the dynamics reported by the simulator. Two kind of dynamic studies were performed, an open-loop and closed-loop analysis. Four disturbances for six different percentages were applied in the open-loop policy; and three set point changes in the closed-loop policy. To ensure the reproducibility of the results, a dynamic simulation in Aspen Dynamics was performed. Results from the validated models show that the predicted versus actual values were bounded. Different input scenarios were evaluated promptly where the manipulated variables presented peaks in their values, and the result was relatively good. Between the two scenarios, the open-loop test, and closed-loop test, the closed-loop test showed a lower error percentage than the open-loop test. The largest error percentage values were close to 0.9%, however, the majority of errors were between 0.1 and 0.4%.

Keywords: Artificial Neural Network, Downstream process, ABE purification.

1. Introduction

The reproduction by simulation of chemical processes is associated with the reproduction of models; in such a way that the quality and reliability of said reproduction depends on the quality and certainty of the process model. Although the reproduction of these types of processes with variations in time can take a considerable period of. An interesting methodology to address complex models is that input and output data can be approximated as black boxes, with the main objective of obtaining reliable predictions. The problem then lies now in the quality of data with which the black box must be built. Artificial neural networks (ANN's) are a technique that can meet those requirements. The basic feedforward network is shown in Figure 1. The data enters the network at the input nodes, the data is propagated through the network through the hidden layers towards the output layer. Although ANNs have a relatively rudimentary structure, several studies conclude that any continuous and non-linear function can be successfully reproduced by an ANN (Cybenko 1989). One of the main advantages of using ANNs is the ability to initially use information to model complex systems, and predict results in a robust manner, since they can approximate non-linear input-output relationships of any degree of accuracy in an iterative manner (Safa and Samarasinghe 2011). Despite the great forecasting skills of the ANNs, their application to predict the behavior of separation processes is quite limited. One reason is the number of equations involved in the modeling of this kind of process, for example, considering that for each equilibrium stage and each component C, the total of MESH (mass and energy balance, thermodynamic equilibria, and purity constraint) equation solved are 2C +3. In addition, if the equations are modeling with variation in time the complexity increase. In the same way, the use of ANNs for more complex distillation systems has not been reported. That is, as far as the authors' knowledge is concerned, no work has been reported in which ANNs are used to model the dynamic behavior of intensified separation systems such as dividing wall columns (DWC). The interest of such intensified alternatives is the advantages that they represent over the conventional option regarding energy requirements and cost savings. In addition, due to the extra complexity it represents, no work has been reported that involves the handling of mixtures with high complexity relative to thermodynamic modeling. With this in mind, the aim of this work is to use an ANN to model and forecasting the dynamic behavior of a dividing wall column for the separation of a mixture composed of Acetone-Butanol-Ethanol and Water from a fermentation process. The modeling process was performed in two scenarios, *i)* modeling the dynamic behavior of the process under an open-loop analysis, *ii)* modeling the dynamic behavior of the process under a closed-loop analysis. The input data were obtained by means of Aspen Dynamics under both open-loop and closed-loop policy.

2. Case Study

Errico et al. (2017) presented a methodology to generate intensified alternatives to separate butanol from ABE fermentation. For the development of this methodology, they start from a hybrid design that considers a liquid-liquid extraction column and conventional distillation columns. Errico et al. (2017) apply a methodology to generate different intensified alternatives based on DWC. All the generated alternatives were evaluated and optimized by means of a robust optimization algorithm, differential evolution with tabu list (DETL), evaluating the total annual cost and the eco-indicator 99 as economic and environmental performance indices. As a result of their research, it was obtained several hybrid designs. Among those designs, the scheme in Figure 1 is considered as a case study. This scheme was initially simulated in Aspen Plus considering the NRTL-HOC as a thermodynamic model to describe phase equilibrium. The feedstream considered a mixture of Acetone, Butanol, Ethanol, and water in a proportion of 0.3018, 0.1695, 0.0073 and 0.5214 % wt respectively. Furthermore, the simulation was exported from Aspen Plus to Aspen Dynamics to obtain the dynamic behavior in both open-loop and closed-loop policy. The data from the dynamic simulation was used for being used as input data in the ANN.

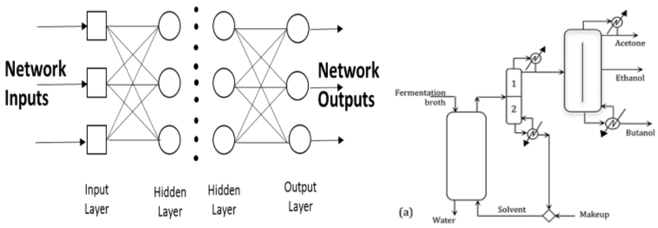

Figure 1. General topology of an ANN and DWC considered a case study

3. Methodology

3.1 Data Generation

The data to train the NNs were based on data using simulations for two cases, open-loop and close-loop policy in Aspen Dynamics. Regarding the open-loop, to generate the input data a step change of 5% every 5 hours in the manipulated variable was performed in a single manipulated variable until it reaches +20% of the nominal value. After that step change of -5% every 5 hours until reach again the nominal state, the other manipulated variables were kept as constant. The same procedure applied to the other variables in such a way that it was applied 3 different disturbances in 6 different percentages of the nominal point. Each manipulated variable was chosen according to each product stream, i.e., when a component was purified in the top of a distillation column, the manipulated variable was the reflux ratio; however, if the component purified remained in the distillation column as a bottom product, the manipulated variable was the reboiler heat duty, and so on. As output data, it was considered the composition profiles of all interest components obtained jointly the disturbances in Aspen Dynamics. Regarding the closed-loop test, the input data were obtained as follows. A setpoint change was implemented in the composition of each component of interest (Acetone-Butanol-Ethanol), in this way three changes of set points were performed and tuned at the same time. The analysis was based on the operation of a proportional-integral controller (PI). Because we considered PI controllers, the proportional gain (K_c) and the reset times (τ_i) were tuned up for each scheme studied here; in addition, we compared the dynamic performance by using the integral of the absolute error (IAE) criterion. To control the composition of distillate and funds, an LV structure was selected. As output data in this test, it was considered the composition profiles obtained. Once all input-output data was obtained, a 4-10-3 multi-layer perceptron with back-propagation algorithm was enough to reproduce the dynamics reported by the simulator.

3.2 Neural Network procedures

This subsection presents the procedures to establish the ANNs. The basic elements of the artificial neuron are: *i)* A set of synapses, or connecting links, each of which is characterized by weight or strength of its own. Specifically, a signal x_j at the input of synapse j connected to neuron k is multiplied by the synaptic weight w_{kj}. The first subscript in w_{kj} refers to the neuron in question, and the second subscript refers to the synapse's input end to which the weight refers. *ii)* An adder for summing the input signals, weighted by the respective synaptic strengths of the neuron; the operations described here constitute a linear combiner. *iii)* An activation function for limiting the amplitude of the neuron's output to the closed unit interval [0,1], or, alternatively, [-1,1]. However, there are exceptions like the linear activation function which covers the open range ($-\infty$, ∞). A neuron can be mathematically described by the following equations:

$$u_k = \sum_{j=1}^{m} w_{kj} x_j \quad \text{and} \quad u_k = \sum_{j=1}^{m} w_{kj} x_j \tag{1}$$

where $x_1, x_2, \ldots, x_m$ are the input signals; $w_{k1}, w_{k2}, \ldots, w_{km}$ are the respective synaptic weights of the neuron k. u_k is the linear combiner's output due to the input signals. b_k is the bias. $\varphi()$ is the activation function. y_k is the neuron's output signal. The use of bias b_k has the effect of applying an affine transformation to the linear combiner's output u_k as shown by

$$v_k = u_k + b_k \tag{2}$$

where v_k is the induced local field or activation potential. The activation function considered in this work is the logistic function:

$$\varphi(v) = 1 \big/ 1 + e^{-av} \tag{3}$$

where a is the slope parameter of the logistic function. Note that the previous equation ranges from zero to one in a strictly increasing fashion and exhibits a graceful balance between linear and nonlinear behaviors. The Feedforward Network (FFN) used in this work is the Multilayer Perceptron (MLP) which consists of full connected consecutive layers of neurons that can be classified as input, hidden and output layers. The input layer contains independent variables that are connected to the hidden layer for processing. Each of the hidden layers contains neurons with logistic activation functions. These are responsible for the nonlinear mapping between the network's inputs and outputs. The output layer, which in this work is composed of neurons with linear activation functions, finishes the prediction or the classification process and presents the results with a small estimation error. The Matlab neural networks toolbox allows the use of multiple network architectures. Each one of the NARX networks was constructed by means of the feedforward neural network's command of the Matlab toolbox *Feedforwardnet Toolbox*:*feedforward net(hiddenSizes,trainFcn).* This command creates a MLP with hidden layers. The hiddenSizes parameter is a row vector whose k_{th} element represents the number of neurons that compose the k_{th} hidden layer. Thus, the *hiddenSizes* vector length is the number of hidden layers composing the MLP. The parameter trainFcn defines the training algorithm for the new MLP. The algorithm backpropagation was considered in this work.

4. Results

4.1. Open-loop input data

Once the step changes in the manipulable variables were implemented, the variation of all of them in time was obtained. Despite all manipulated variables and all components were also monitored, Figure 2 A) shows only the variation of the reboiler duty over time, which together with the variation of the reflux ratio and the flow of the lateral current, were used as input data for the ANN. The composition profile of butanol in Figure 2 was used as output data together with the composition profiles of acetone and ethanol. With that input-output data, the neural network was trained. Both stages are shown in Figure 2. Regarding the closed-loop test, once the data for proportional gain (K_c) and the reset times (τ_i) were tuned with the minimum IAE. The values of the manipulated variables and the resulting composition profiles associated with those values of K_c and τ_i were considered as input-output data for training the ANN. Again, despite all variables were disturbed and the three components were studied, Figure 2 B) shows only the input and output data for Reboiler Heat duty and Butanol. According to Table 1, both AAN were able to reproduce the entire dynamic of the process with relatively good accuracy. Between both test, open-loop, and closed-loop, the ANN showed better accuracy to predict the complexity of the model under the presence of a PI controller. The K_c, τ_i and IAE values for all loops were 140/150/0.0677, 100/100/0.0183, 45/50/0.611 for acetone, butanol, and ethanol respectively.

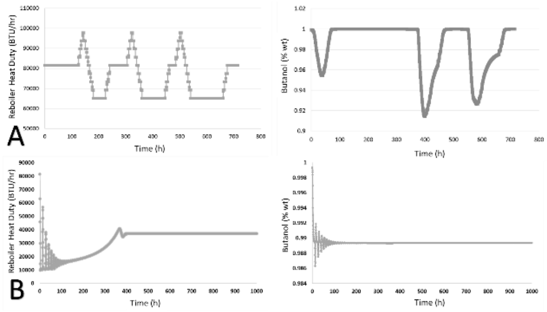

Figure 2. Input and output data Input and output data of the ANN in the open-loop test (A) and closed-loop policy (B).

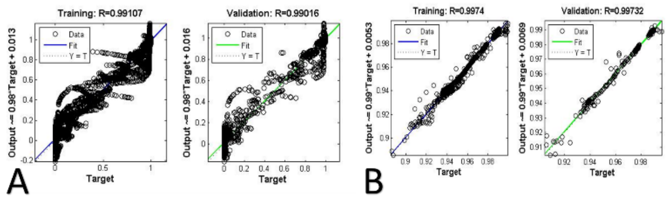

Figure 3. Training and validation data fit process for the open-loop test (A) and closed-loop policy (B).

Table 1. Data Validation for open-loop policy

INPUT		OUTPUT (%wt)			
			ANN	Aspen Dynamics	% Error
Time (h)	0.1	**Acetona**	0.9643	0.997	3.39106
Reb Duty (cal/s)	60413.5	**Butanol**	1.072	0.9992	6.79104
Reflux ratio (lb/lb)	24.3128	**Etanol**	0.9837	0.9864	0.27447
Side stream flow (lb/s)	0.724				
Time (h)	0.3	**Acetona**	0.8645	0.997	15.3268
Reb Duty (cal/s)	87014.5	**Butanol**	0.7313	0.9959	36.1821
Reflux ratio (lb/lb)	36.2144	**Etanol**	1.0488	0.9841	6.16895
Side stream flow (lb/s)	0.724				

Additionally, the computational time for reproducing in ANN was quite low (few seconds) in comparison with that in Aspen Dynamics (10-20 minutes). The values of the manipulated variables and the resulting composition profiles associated with those values of K_c and τ_i were considered as input-output data for training the ANN. Figure 2-3 shows the input and output data. According to Table 2, both AAN were able to reproduce the entire dynamic of the process with relatively good accuracy. Between both test, open-loop, and closed-loop, the ANN showed better accuracy to predict the complexity of the model under the presence of a PI controller. The K_c, τ_i and IAE values for all loops were 140/150/0.0677, 100/100/0.0183, 45/50/0.611 for acetone, butanol, and ethanol respectively. Additionally, the computational time for reproducing in ANN was quite low (few seconds) in comparison with that in Aspen Dynamics (10-20 minutes).

Table 2. Data Validation for closed-loop policy

INPUT		**OUTPUT**			
			Aspen Dynamics	**ANN**	**% Error**
Time (h)	3.6	ACETONE	0.995598	0.9889	0.672761496
Reflux ratio (lb/lb)	0	ETHANOL	0.959805	0.9686	0.916331963
Side stream flow (lb/s)	0	BUTANOL	0.992269	0.9902	0.208512006
Reb Duty (cal/s)	10555.8				
Time (h)	30	ACETONE	0.988805	0.9912	0.242211558
Reflux ratio (lb/lb)	0.617515	ETHANOL	0.970426	0.9724	0.203415819
Side stream flow (lb/s)	0.668623	BUTANOL	0.99086	0.9925	0.165512787
Reb Duty (cal/s)	11162				

5. Conclusions

Through de use of a 4-10-3 multi-layer perceptron with the back-propagation algorithm it was possible to reproduce the entire dynamic of a complex process to separate a highly nonideal mixture. The ANN showed the potential to reproduce the dynamic behavior of the process under two different test, an open-loop, and a closed-loop test. Between both tests, the ANN showed a minor error reproducing the closed-loop test in comparison with the open-loop test. Taking advantages of the capacities of ANN such as relative easy applications, computing time, and inferring on unseen data numerical convergence; it is possible to perform many studies considering the robustness, non-linearity, and complexity of the model involved in a divided wall column: controllability analysis, dynamic optimization, and model reduction for planning and scheduling works considering the application of the entire model of these complex schemes.

References

Cybenko, G., 1989, Approximation by Superpositions of a Sigmoidal Function. Mathematics of Control. Signals and Systems, 2, pp. 303-314.
Safa, M., & Samarasinghe, S.,2011,. Determination and modelling of energy consumption in wheat production using neural networks: “A case study in Canterbury province, New Zealand”. Energy, 36(8), 5140-5147.
Errico, M., Sanchez-Ramirez, E., Quiroz-Ramìrez, J. J., Rong, B. G., & Segovia-Hernandez, J. G., 2017,. Multiobjective optimal acetone–butanol–ethanol separation systems using liquid–liquid extraction-assisted Divided Wall columns. Industrial & Engineering Chemistry Research, 56(40), 11575-11583.