Modeling and Simulation of a Reactive Packed Distillation Column Using Delayed Neural Networks

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Abstract: The complex nature of a reactive packed distillation system due to the occurrence of both reactions and separations in a single unit demanded the need for a very robust tool of representing the process. In view of this, delayed neural networks are considered as one that can handle this problem effectively. As such, in this work, delayed neural networks Nonlinear AutoRegressive, Nonlinear AutoRegressive with eXogenous inputs and Nonlinear Input-Output models are developed and simulated with the aid of MATLAB R2010b to predict the top and bottom sections temperatures of the column. The predicted temperatures of the Input-Output models were found not to be satisfactory. However, the good agreements observed from the plots and the good values of the correlation coefficients and the mean squared errors between the predicted temperatures of NAR and NARX models and the experimental ones showed that these two models can be used to represent the process.
Keywords: Reactive packed distillation, Delayed neural network, Nonlinear AutoRegressive (NAR), Nonlinear AutoRegressive with eXogenous inputs (NARX), Nonlinear Input-Output (NIO), MATLAB/Simulink, Correlation coefficient (R), Mean squared error (MSE).

1 Introduction

In recent years, integrated reactive separation processes have attracted considerable attentions in both academic research and industrial applications, Völker et al., 2007 [1]. One of these processes which is known as reactive distillation is potentially attractive whenever conversion is limited by reaction equilibrium, Balasubramhanya and Doyle III, 2000 [2]. Reactive distillation combines the benefits of equilibrium reaction with a traditional unit operation (in this case, distillation) to achieve a substantial progress in not only promoting the reaction conversion through constant recycling of reactants and removal of products but also reducing the capital and operating costs in one way by reducing the number of equipment units. In addition, another advantage of reactive distillation is its ability to avoid azeotropes. However, the design of reactive distillation processes, especially when a packed column is involved, is still a challenge to chemical engineers because of the difficulties involved in obtaining process models capable of reliably describing the several complexes (such as the exhibition of multiple steady states) and the interrelated phenomena

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which includes simultaneous reactions and separations in the column. The complicated behavior of the process made the search for a very robust and powerful tool of modeling and simulating the dynamics of the reactive distillation a big task to chemical engineers. One of the strategies proposed for handling this kind of a task are the delayed neural networks because they can be trained to handle complex functions, Beale et al., 2010 [3].

Neural Networks modeling can be viewed as a nonlinear empirical model that are especially useful in representing input–output data, in making predictions in time, and in classifying data, Himmelblau, 2000 [4]. Neural Networks can be highly nonlinear, can learn easily, require little or no a priori knowledge of the structure, are fault-tolerant and can handle complex problems that cannot be satisfactorily handled by the traditional methods, MacMurray and D. M. Himmelblau, 2000 [5].

In this paper, a reactive packed distillation column is modeled and simulated using three different kinds of delayed neural network models and the equilibrium reaction for the production of ethyl acetate from the esterification reaction between acetic acid and ethanol was used as the case study.

2 The Model and Simulations

2.1 Data acquisition

The data used for the delayed neural networks modeling were acquired from the experiments performed in a pilot scale packed reactive distillation plant shown in Figure 1 below. The plant has, excluding the condenser and the reboiler, a height and a diameter of 1.5 and 0.05 m respectively, a cylindrical-shaped condenser having a height and a diameter of 22.5 and 5 cm respectively and a spherical-shaped reboiler with a volume of 3 Litre. The main column was divided into three parts of 0.5 m each. The upper, middle and lower sections were the rectification, reaction and stripping sections respectively. The rectification and stripping sections were packed with rasching rings while the reaction section was filled with Amberlyst 15 catalyst. The column was fed with acetic acid at the top (between the rectification section and the reaction section) whereas ethanol was fed at the bottom (between the reaction section and the stripping section) with the aid of peristaltic pumps which were operated via MATLAB/Simulink program. The top, reaction, stripping and bottom sections temperatures were measured and recorded on-line and in real-time using the thermocouples linked to the computer and also via the MATLAB/Simulink program. The reaction taking place in the column is given as:

$$CH_3COOH + C_2H_5OH \underset{k_b}{\overset{k_f}{\rightleftharpoons}} CH_3COOC_2H_5 + H_2O \tag{1}$$

Two different experiments were carried out using a reboiler duty of 560 W and applying step inputs unto the recycle ratio from total reflux to 5 and acetic acid to ethanol feed ratio from 0 to 1.25 to generate two sets of data. One set was used for training the models while the other was used to test the developed delayed neural network models.

(a)

(b)

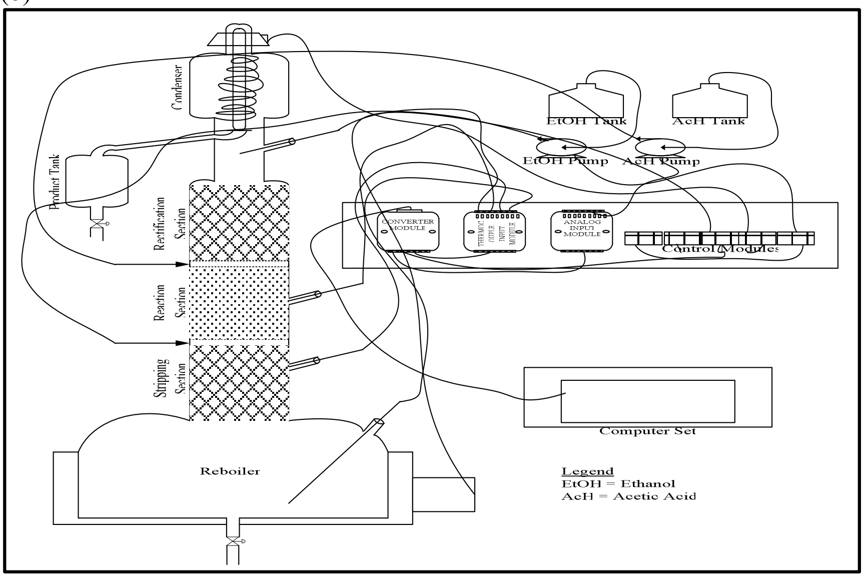

Fig. 1. Reactive Packed Distillation Pilot Plant: (a) Pictorial View; (b) Sketch View

2.2 Model development

In developing the models in the MATLAB environment, the sets of data generated from the experiments were pretreated by converting them to time sequence ones which were represented by a cell array because the delayed neural networks models to be developed required the data to be sequential in nature. The parameters used for the formulation of the models are as shown in Table 1 below:

Table 1. Neural network model formulation parameters

S/N	Parameter	Value/Description
1.	No. of inputs	2
	No. of outputs	2
2.	No. of layers	2
3.	No. of neurons	10
4.	No. of delays	5
5.	Training algorithm	Levenberg-Marquardt

The mathematical expressions for the three kinds of delayed neural networks (Nonlinear Autoregressive, Nonlinear Autoregressive with Exogenous Inputs and Nonlinear Input-Output) models developed for the reactive packed distillation column are:

NARX: $y(t) = f\left(u(t-1), u(t-2), ..., u(t-d), y(t-1), y(t-2), ..., y(t-d)\right)$ (2)

NAR: $y(t) = f\left(y(t-1), y(t-2), ..., y(t-d)\right)$ (3)

NIO: $y(t) = f\left(u(t-1), u(t-2), ..., u(t-d)\right)$ (4)

2.2 Results and discussions

The generated outputs recorded from the experiments carried out as described in Section 2.1 (that is, by applying step changes unto the recycle ratio from infinity to 5 and unto the feed ratio from 0 to 1.25) are as shown in Figure 2 below. Figure 2(a) shows the measurements taken from the pilot plant for the delayed neural networks training while Figure 2(b) contains another set of results taken from the plant for testing the models to be developed. The step changes applied unto the input variables (recycle ratio and feed ratio) are shown in Figure 2(c).

It could be observed from Figure 2 that, even though the responses of the training and testing results are not exactly the same for both the top section and reaction section temperatures, their trends were found to be similar. The discrepancies between them can be attributed to the unmeasured disturbances that normally affect the performances of chemical processes. Of course, these disturbances have to be taken into considerations when applying the delayed neural networks models in designing controllers for the plant in order to achieve stability and/or improve the performance of the system.

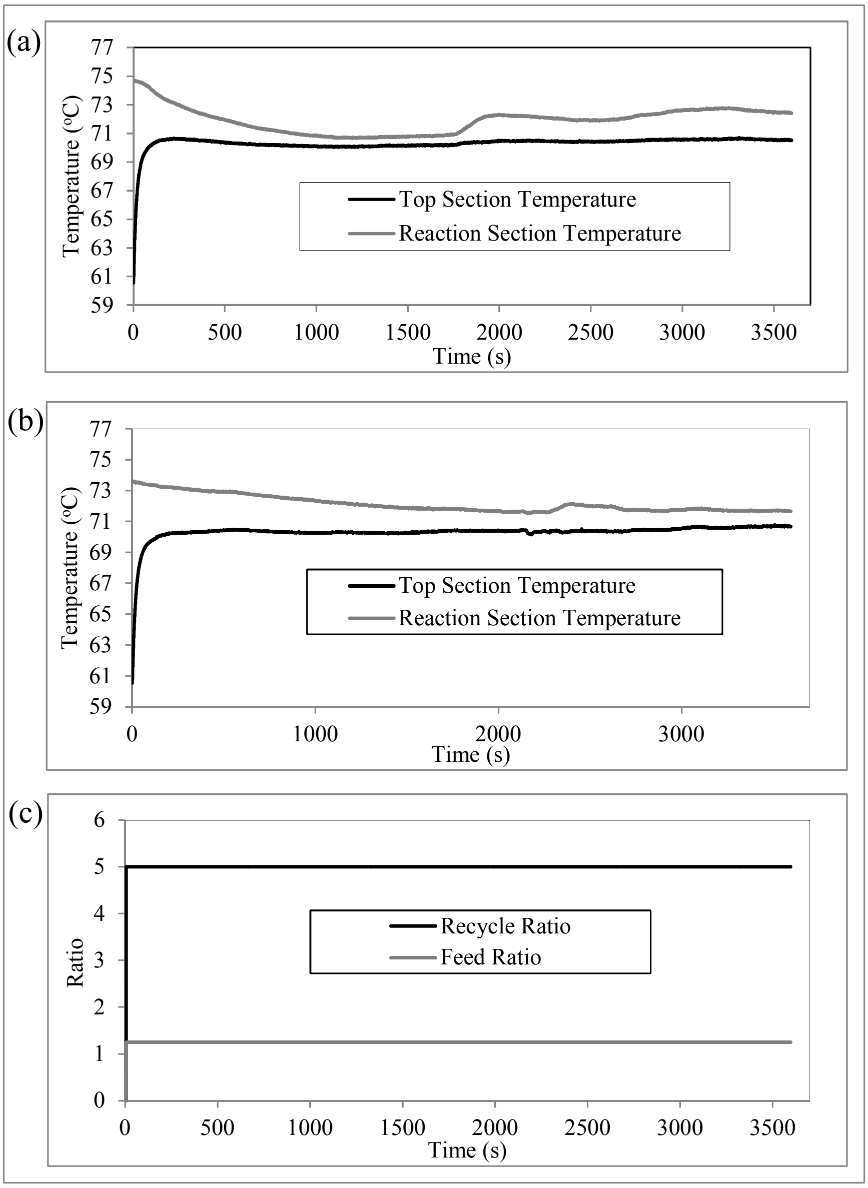

Fig 2. Input-Output Sampled Data: (a) Training Data; (b) Testing Data; (c) Applied Inputs

After using the data in Figure 2 to develop the neural networks models for the reactive packed distillation column, each of them (the models) was tested using the testing data shown in figure 2(b) in order to confirm the accuracy of the model in predicting the top section and the reaction section temperatures. Figure 3, 4 and 5 show the comparisons between the experimental and the predicted results of top section temperatures and the reaction section temperatures for the delayed neural networks NAR, NARX and NIO models respectively.

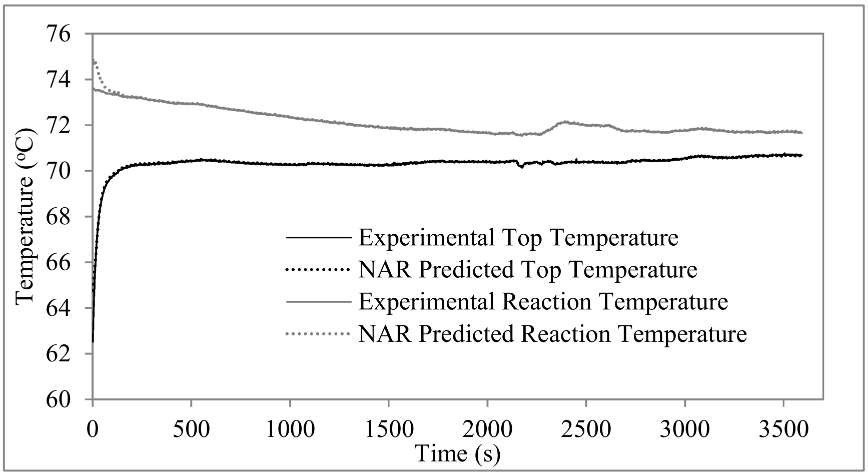

Fig. 3. Comparisons between Experimental Temperatures and Those Predicted Using Delayed Neural Networks NAR Model

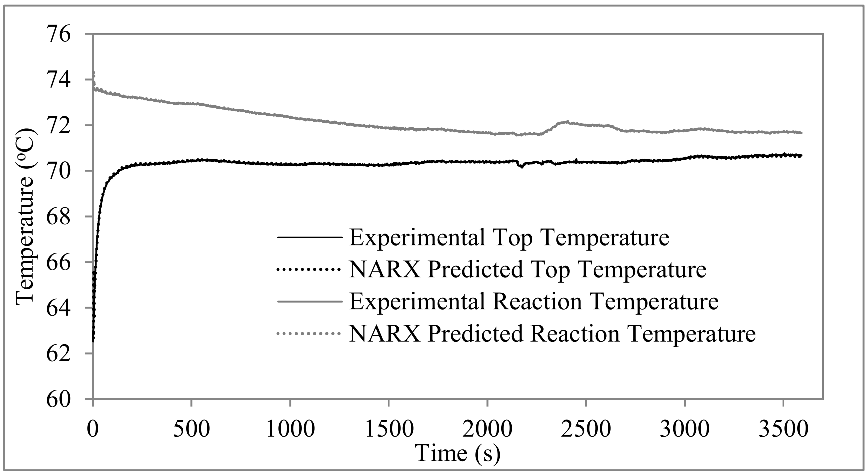

Fig. 4. Comparisons between Experimental Temperatures and Those Predicted using Delayed Neural Networks NARX Model

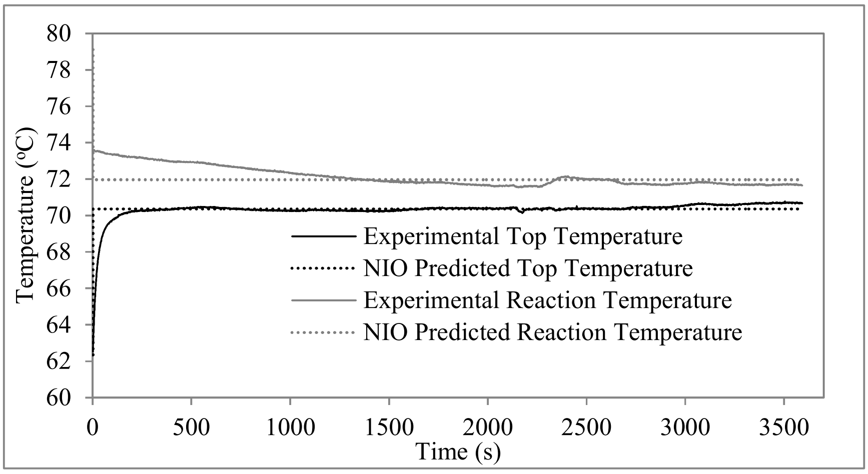

Fig. 5. Comparisons between Experimental Temperatures and Those Predicted Using Delayed Neural Networks NIO Model

From the results shown in Figure 3 and Figure 4, it was observed that there were good agreements between the experimental temperatures and those predicted using the developed delayed neural networks NAR and NARX. However, the predicted temperatures obtained using the Nonlinear Input-Output models were not in good agreements with the experimental ones, as seen in Figure 5.

The validities of the representations of the reactive packed distillation plant using the developed delayed neural networks models were further investigated by calculating the performance indices of the models. The performance indices used in this work are mean squared error (MSE) and correlation coefficient (R) and their calculated values are as tabulated below.

Table 2. Performance indices of the developed models

Model Type	**Top Section Temperature**		**Reaction Section Temperature**	
	MSE	**R**	**MSE**	**R**
NAR	0.0063	0.9927	0.0120	0.9852
NARX	0.0023	0.9952	0.0011	0.9984
NIO	0.2270	0.2642	0.3195	0.0454

From Table 2, it was observed that the correlation coefficients calculated when NAR model was used to predict the top section and reaction section temperatures were 0.9927 and 0.9852 respectively while those of the NARX model were 0.9952 and 0.9984 respectively for the top and reaction sections temperatures. Also, as seen from Table 2, each of the two (NAR and NARX) models was found to have a very low mean squared error. The low value of the mean squared error is another indication of a good model. The good performances showed by these models can be attributed to the use of some past outputs, as feedbacks, in their structures.

However, in the case of the Nonlinear Input-Output model, the situation was different because, apart from the fact that the curves produced by this model were not in good conformity with those of the experimental ones, its performance values were also bad, as seen from Table 2. For instance, the correlation coefficients obtained when this model was used to predict the top and reaction sections temperatures were 0.2642 and 0.0454 respectively. These values are too low for any model that is to be used to represent a reactive packed distillation plant. The poor performance of this model can be as a result of the fact that its structure does not make use of the past values of the output variables.

3. Conclusions

Three kinds of delayed neural networks models have been developed and simulated. The good closeness of the temperatures predicted using NAR and NARX models to the experimental ones has revealed that both of them can be used to represent the dynamics of the reactive packed distillation column.

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