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Layer-Recurrent Neural Network Modelling of Reactive Distillation Process

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Abstract: Reactive distillation is one of the complex processes encountered in process industries as a result of the integration of both reaction and separation in a single unit. Nowadays, the modelling of this process has become a big challenge to Process Engineers. The use of a reliable model that can handle complex functions is very necessary to represent this complex process. It has been discovered that Neural Network can be used to handle complex functions very well. Therefore, the modelling of the reactive distillation process considered in this work has been carried out with the aid of a dynamic neural network known as Layer-Recurrent Neural Network. The simulated results obtained from the developed Neural Network models were compared with the measured results to confirm the validities of the developed models.

Keywords: Neural Network, Reactive distillation, Modelling, Simulation.

1. Introduction

In recent years, integrated reactive separation processes have attracted considerable attentions in both academic research and industrial applications (Völker et al., 2007; Giwa and Karacan, 2012a). 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; Giwa and Karacan, 2012a).

Reactive Distillation (RD) 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 unconverted materials and removal of products but also reducing the capital and operating costs in one way by reducing the number of equipment units (Giwa and Karacan, 2012a). Moreover, its other advantages include improved selectivity, lower energy consumption, scope for difficult separations and avoidance of azeotropes (Jana and Adari, 2009). However, due to the integration of reaction and separation, reactive distillation exhibits complex behaviours (Khaledi and Young, 2005) such as steady state multiplicity, process gain sign changes (bidirectionality) and strong interactions between process variables (Jana and Adari, 2009). These complexities have

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made the modelling of Reactive Distillation Process extremely difficult (Giwa and Karacan, 2012b; Giwa and Giwa, 2012). As such, a robust tool that can handle complex functions very well is needed to represent this complex process. One of these tools has been discovered to be Neural Network model because, according to Beale et al. (2010), Neural Network can be trained to handle complex functions.

Neural Network model can be viewed as a nonlinear empirical model that is especially useful in representing input-output data, in making predictions in time, and in classifying data (Himmelblau, 2000). Neural Network can be highly nonlinear, can learn easily, requires little or no a priori knowledge of model structure, is fault-tolerant and can handle complex problems that cannot be satisfactorily handled by the traditional methods (MacMurray and Himmelblau, 2000). There are many kinds of Neural Network models available in the literature. For instance, a simple classification can be: Static Neural Network and Dynamic Neural Network. It is perceived that a dynamic network, especially Layer-Recurrent Network (LRN), will be better in representing this complex Reactive Distillation Process because of the presence of a delay ensuring proper dynamics in each of its layers except in the last one.

According to the information gathered from the literature, Giwa and Karacan (2012a) used three different types of delayed neural network (Nonlinear AutoRegressive (NAR), Nonlinear AutoRegressive with eXogenous inputs (NARX) and Nonlinear Input-Output (IO)) models to represent a reactive distillation column in predicting the temperatures of the top and the bottom sections of the reactive distillation column used for the production of ethyl acetate and they were able to obtain very good results from both NAR and NARX models while the results given by IO models were found not to be satisfactory. Also, Giwa and Karacan (2012c) developed two nonlinear black-box (treepartition and sigmoid network NARX) models for the Reactive Distillation Process used for the production of ethyl acetate from the esterification reaction between acetic acid and ethanol and found that sigmoid network NARX model was better than treepartition NARX model for the reactive distillation process studied in their work.

In this work, Reactive Distillation Process is aimed to be modelled with the aid of Layer-Recurrent Neural Network using the metathesis reaction of trans-2-pentene to trans-2-butene and trans-2-hexene as the case study.

2. Procedures

The methods used for the accomplishment of this work are as outlined below.

2.1 Data Acquisition

The diagram of the metathesis reactive distillation column, developed with the aid of Aspen HYSYS (Aspen, 2011), used for the production of trans-2-butene (obtained in high purity at the top segment of the column) and trans-2-hexene (obtained in high purity at the bottom segment of the column) from trans-2-pentene, and from which the measured data used for the neural network model development were generated is as shown in Figure 1 below. As can be seen from the figure, the column had one feed stream and two product streams. The olefin metathesis reaction that occurred in the column was a reversible type given as shown in Equation 1.

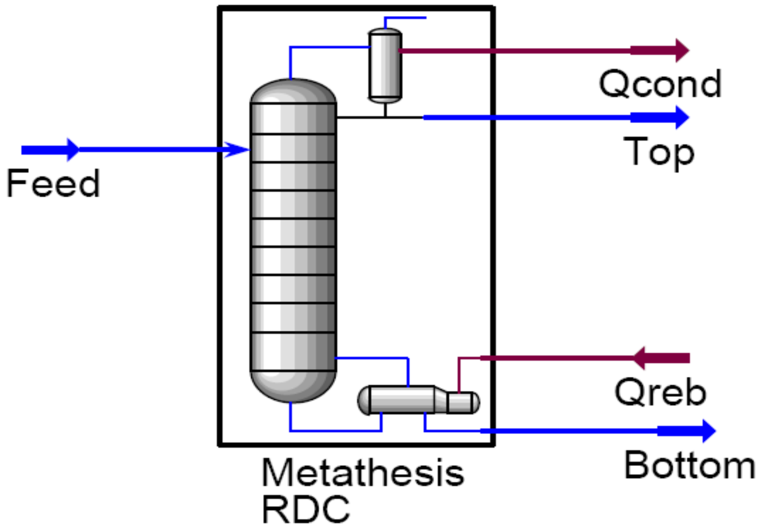

Fig. 1. Process flowsheet for metathesis reactive distillation process

$$2C_5H_{10} \xleftrightarrow{K_{eq}} C_4H_8 + C_6H_{12} \tag{1}$$

The data used for the development of the process in Aspen HYSYS environment are as given in Table 1.

Table 1. HYSYS metathesis reactive distillation process development data

Parameter	**Value**
Feed	
Flow rate (mL/min)	35
Temperature (K)	298.15
Pressure (atm)	1.11
Feed Composition (Mole fraction)	
trans-2-pentene	0.999998
trans-2-butene	1.00E-06
trans-2-hexene	1.00E-06
Fluid Package	UNIQUAC

Column	
Type	Packed
Packing type	Raschig Rings (Ceramic) 0.25 inch
No. of segment	15
Feed segment	8
Reaction	
Type	Equilibrium
Segment	6 - 10 and reboiler
K_{eq} source	Gibbs Free Energy
Basis	Molar concentration
Phase	Liquid

In the process development, reflux ratio and reboiler duty were chosen as the manipulated (input) variables while top segment and bottom segment temperatures were selected as the process (output) variables. By using the random data set values of the manipulated variables built with the aid of Parametric Utility of Aspen HYSYS, the column was run and the top segment and the bottom segment temperatures were obtained as the measured values of the output variables. Two different data sets were generated from the Aspen HYSYS system of the process. One was used for the training while the other was used for the testing of the Layer-Recurrent Neural Network models.

2.2 Modelling and Simulation

In the modelling of the Reactive Distillation Process in MATLAB (Mathworks, 2012) environment, the data sets obtained from Aspen HYSYS system of the process were converted from concurrent types to sequential ones because those were the types required by the dynamic Layer-Recurrent Neural Network. The parameters used for the formulation of the Neural Network models of the process considered in this work are as given in Table 2.

Table 2. Layer-Recurrent Neural Network model formulation parameters

Parameter	**Value**
Number of inputs	2
Number of outputs	2
Number of layers	2
Number of neurons in hidden layer	7
Hidden layer transfer function	*tansig*
Output layer transfer function	*purelin*
Training algorithm	*Levenberg-Marquardt*

Owing to the fact that there were two outputs, and even with two inputs, the structure of the neural network had two models in it – one for each process variable; that is, one model was for top segment temperature and the other was for bottom segment temperature. The structure of the developed models is shown below in Figure 2.

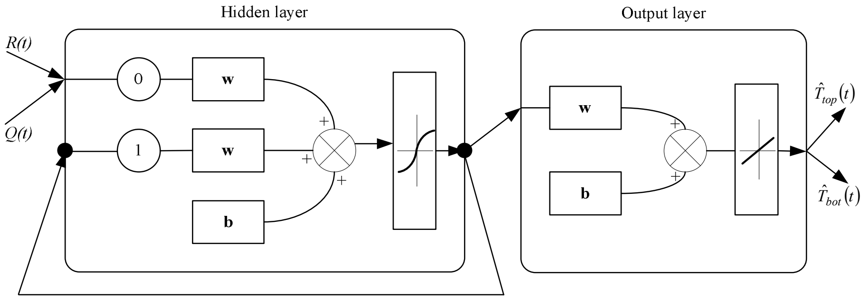

Fig. 2. Layer-Recurrent Neural Network of metathesis RD process

In order to determine the validities of the developed models, they were simulated and their performance values were calculated. The performance criteria used were fit values (indicating the percentage of the data accounted for by the developed models), means of absolute errors and sums of squared errors.

3. Results and Discussions

The acquired measured data sets of the input and the output variables used for training and testing the neural network models are given in Figures 3 and 4 respectively for the top segment and the bottom segment temperatures.

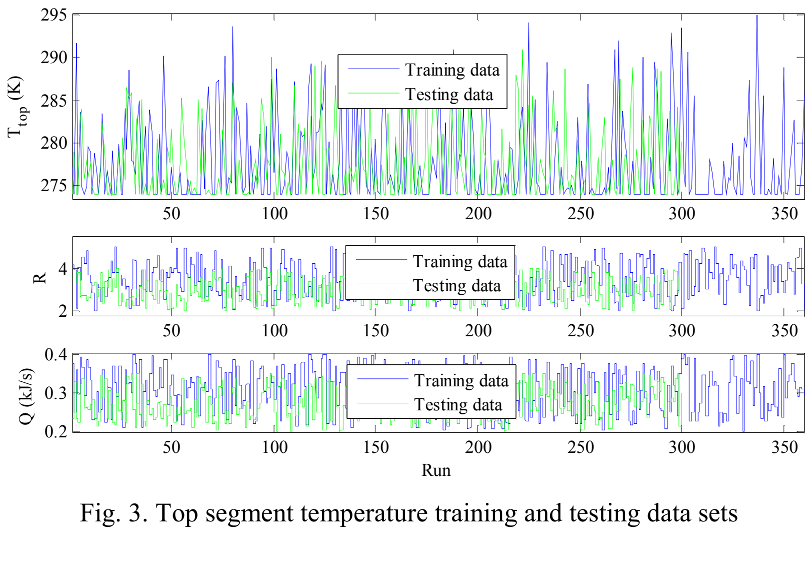

Fig. 3. Top segment temperature training and testing data sets

As can be seen from Figures 3 and 4, there were corresponding changes in the responses of the two segment temperatures as a result of the changes in the input variables. Also noticed from the results shown in Figures 3 and 4 was that the lengths of the training and the testing data for both segment temperatures were not the same but the overall limits of the testing manipulated variables used were within the ones used for the generation of the training data. The different data length was made so in order to test the robustness of the developed neural network model to another data with length different from that of the one used for its training.

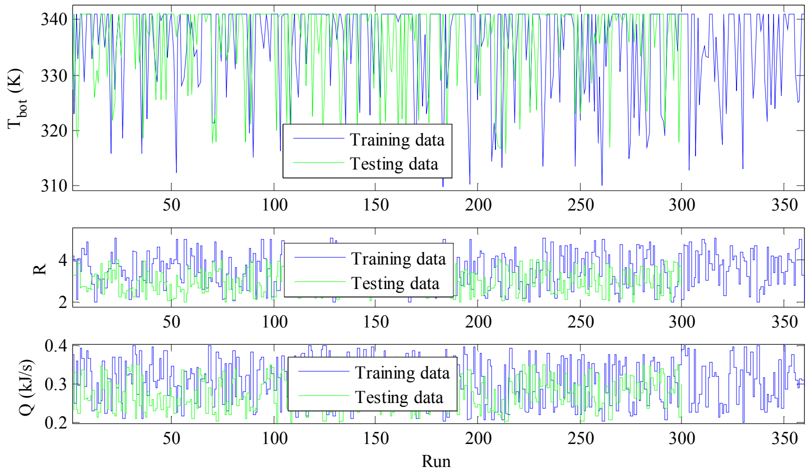

Fig. 4. Bottom segment temperature training and testing data sets

After training the Layer-Recurrent Network Models of the process, even though the models could not be obtained as physical ones, they were simulated using the manipulated variable values used for the training and the performance values of the models obtained from the training simulation are as shown in Table 3. It was observed from the table that the fit values of the models were appropriately very high and the means of absolute errors and the sums of squared errors were low enough to say that the models were well trained. Further considering the fit values of the training simulations, it was discovered that the developed neural network models could account for approximately 99% of the data used for developing them.

Table 3. Performance values of network training simulation

Performance criterion	**Performance value**	
	$\mathbf{T_{top}}$	$\mathbf{T_{bot}}$
Fit value	99.08	99.27
Mean of absolute errors	0.04	0.04
Sum of squared errors	0.80	1.33

In addition, the top and the bottom segment temperatures obtained from the training simulations of the developed neural network models were plotted together with the measured ones and their graphs are as shown in Figures 5 and 6 respectively for the top segment temperature and the bottom segment temperature profiles. From Figure 5, it was observed that there was a good relationship between the measured and the simulated top segment temperature profiles because, as seen from the graph, the trends of the two plots were found to follow each other very well. Also, as noticed from Figure 6, good relationship was found to exist between the profiles of the bottom segment temperatures measured and those estimated with the developed model. The good relationships between the plots contained in Figures 5 and 6 have been discovered to be in support of the excellent performance values of the models (see Table 3).

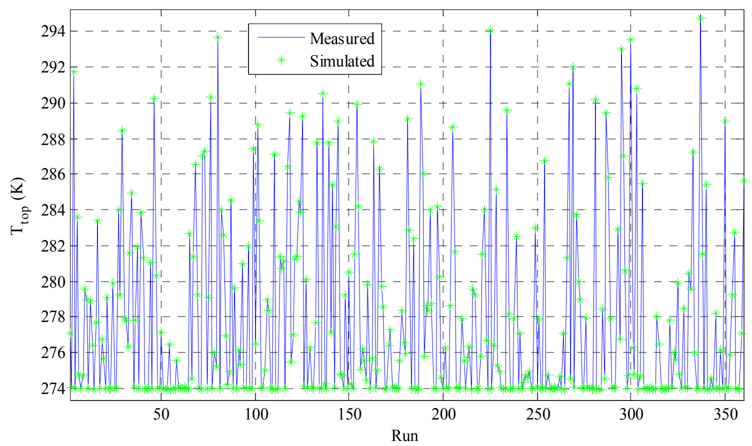

Fig. 5. Measured and simulated top segment temperatures

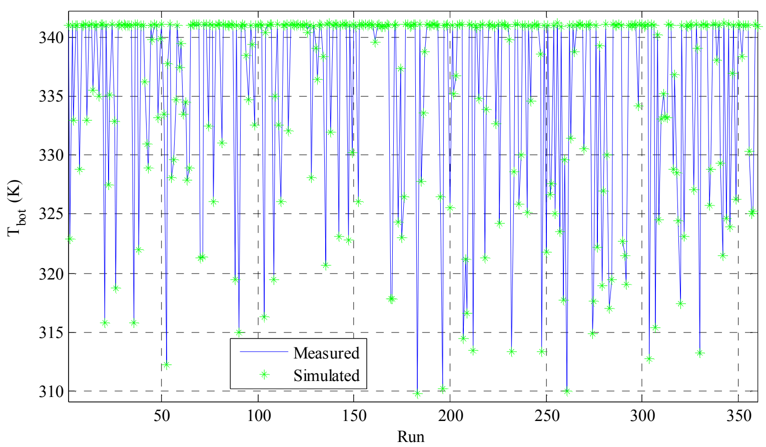

Fig. 6. Measured and simulated bottom segment temperatures

Apart from simulating the developed models with the manipulated (input) variables used for the training, testing data set generated for the purpose of model testing, and which was not used for the training of the models, was also used to simulate the developed models and the performance values obtained from the testing simulations are as given in Table 4. As can be seen from the table, in the testing simulation also, the fit values were found to be very high. In addition, the means of absolute errors and the sums of squared errors for both the top and the bottom segment temperatures were obtained to be very low and appropriate enough for good models.

Table 4. Performance values of network testing simulation

Performance criterion	**Performance value**	
	T_{top}	**T_{bot}**
Fit value	98.74	98.63
Mean of absolute errors	0.05	0.07
Sum of squared errors	0.95	3.15

In addition, the representations of the Reactive Distillation Process of this work by the developed neural network models were as well investigated by plotting the testing simulation results of both the top and the bottom segment temperatures against the measured ones as shown in Figures 7 and 8, respectively.

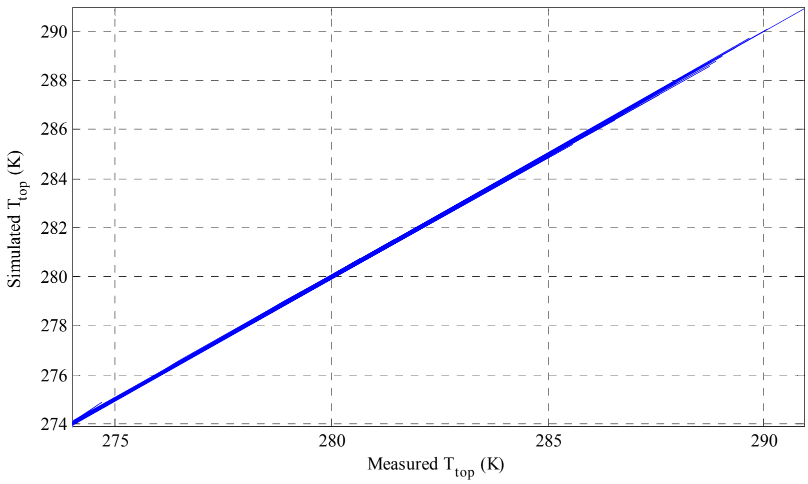

Fig. 7. Top segment simulation results of neural network testing

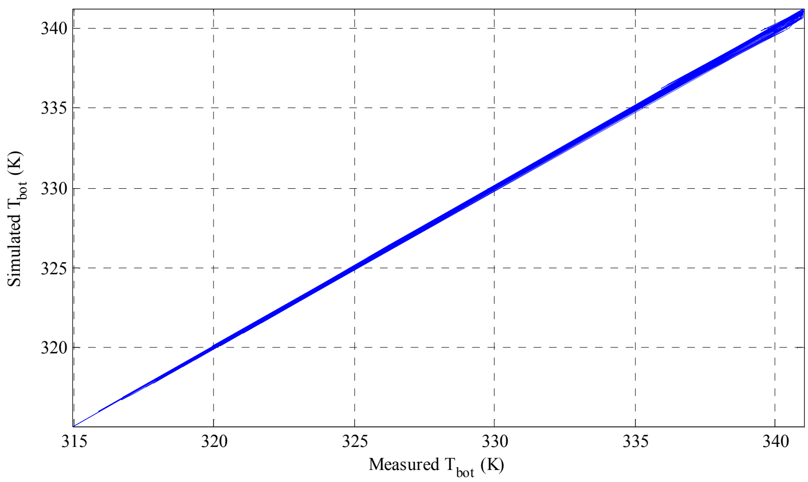

Fig. 8. Bottom segment simulation results of neural network testing

According to the results shown in Figures 7 and 8, the 45 degree lines given by the plots of the testing simulations of the top and the bottom segment temperatures against the measured ones were found to be other indications of the good representations of the Reactive Distillation Process by the developed neural network models.

It has thus been seen that the developed neural network models for the top and the bottom segment temperatures of the reactive distillation column have been found to perform very well both in the training and in the testing simulations. The good performances obtained from the developed models have demonstrated the versatility of neural network in representing complex processes very well.

4. Conclusions

The very high fit values, the low means of absolute errors and the low sums of squared errors obtained from the training and the testing simulations of the Layer-Recurrent Neural Network models developed for the olefin metathesis Reactive Distillation Process, used for the production of trans-2-butene and trans-2-hexene from trans-2-pentene, have confirmed the validities of the developed models for the top and the bottom segment temperatures of the column in which the process was accomplished. Therefore, Layer-Recurrent Neural Network model has been revealed to be an excellent tool in representing the complex Reactive Distillation Process.

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