ADAPTIVE NEURO-FUZZY INFERENCE SYSTEMS (ANFIS) MODELING OF REACTIVE DISTILLATION PROCESS

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ABSTRACT

This work has been carried out to develop ANFIS models for the reactive distillation process used for the production of isopropyl alcohol from the hydration reaction of propylene. The data used for the development of the models were generated from the Aspen HYSYS system of the process that comprised two feed streams - the upper feed stream from where the less volatile feed, water, was fed and the lower feed stream from where the more volatile feed, propylene, was fed into the column. The hydration reaction of the process was a reversible type occurring in liquid phase in the reaction sections of the column. The ANFIS models were trained, tested and simulated with the aid of MATLAB. The inputs of the models were the reflux ratio and the reboiler duty while the outputs were the top segment and the bottom segment temperatures. The high fit values and the low means of absolute errors obtained respectively from the training and the testing of the ANFIS models developed for the top segment and the bottom segment of the reactive distillation column used for the production of isopropyl alcohol have revealed that the developed ANFIS models represented the reactive distillation process in a very good manner.

Keywords: ANFIS, reactive distillation, Aspen HYSYS, modeling, simulation.

1. INTRODUCTION

Reactive distillation is a process that combines both separation and chemical reaction in a single unit. It is sometimes an excellent alternative to conventional flow sheets with separate reaction and separation sections [1-3]. It combines the benefits of equilibrium reaction with distillation to enhance conversion provided that the product of interest has the highest or the lowest boiling point [3, 4]. It has a lot of advantages, especially for those reactions occurring at temperatures and pressures suitable for the distillation of the resulting components [3, 5], which include: (a) shift of chemical equilibrium and an increase of reaction conversion by simultaneous reaction and separation of products, (b) suppression of side reactions, and (c) utilization of heat of reaction for mass transfer operation. These synergistic effects normally result in significant economic benefits of reactive distillation compared to a conventional design. These economic benefits include: (a) lower capital investment, (b) lower energy cost and, (c) higher product yields [6, 7]. Reactive distillation is a very advantageous process, but, due to its complexity as a result of combined reaction and separation [3], its modeling is still a challenge to Process Engineers.

It has been discovered that, with the aid of adaptive techniques like Adaptive Neuro-Fuzzy Inference Systems (ANFIS), Fuzzy Logic can be used to model nonlinear functions of arbitrary complexity by creating a fuzzy system to match any set of input-output data.

Adaptive Neuro-Fuzzy Inference System (ANFIS) is a kind of neural network that is based on Takagi-Sugeno Fuzzy Inference System. Since it integrates both neural networks and fuzzy logic principles, it has the potential to capture the benefits of both in a single framework. Its inference system corresponds to a set of fuzzy IF-THEN rules that have learning capability to approximate nonlinear functions [8]. Hence, ANFIS is considered to be a universal approximator [9].

Actually, different methods have been used to model reactive distillation. For instance, Giwa and Karacan [4] used three different types of delayed neural network (Nonlinear Auto Regressive (NAR), Nonlinear Auto Regressive with eXogenous inputs (NARX) and Nonlinear Input-Output (IO)) models to represent a reactive distillation column, used for the production of ethyl acetate, in predicting the temperatures of the top and the bottom sections of the column and they were able to obtain very good results from both NAR and NARX models while the results given by IO models were found unsatisfactory. Also, Giwa and Karacan [7] developed two nonlinear black-box (tree partition and sigmoid network NARX) models for a 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 tree partition NARX model in representing the reactive distillation process studied in their work. Khazraee *et al.*, [10] applied Adaptive Neuro-Fuzzy Inference System (ANFIS) instead of a highly nonlinear model to optimize a reactive batch distillation column used for producing ethyl acetate and their results showed that ANFIS was able to properly create a robust model of the reactive batch distillation apart from the fact that the CPU use was reduced to 1/18,000 of that of a real mathematical model. Besides, using the obtained optimization policy they estimated using the developed ANFIS model, they were able to obtain highest yield and mole fraction of ethyl acetate. Khazraee and Jahanmiri [11] employed an inferential state estimation scheme based on Adaptive Neuro-Fuzzy Inference System (ANFIS) for composition estimation by using temperature measurements in multicomponent reactive batch distillation and the simulation results they obtained show that ANFIS estimator was able to provide reliable and accurate estimations for component concentrations in reactive batch distillation.

In this work, it is aimed to use Adaptive Neuro-Fuzzy Inference System (ANFIS) to develop models for a reactive distillation process used for the production of isopropyl alcohol taking the reflux ratio and the reboiler duty of the column as the input variables and its top segment and bottom segment temperatures as the output variables.

2. PROCEDURES

The modeling of the process used for the production of isopropyl alcohol (IPA) via the hydration of propylene in a reactive distillation column, studied in this work, was accomplished using the methods described in the subsections below.

2.1. Data acquisition

The input-output data used for the development of the models were acquired from the reactive distillation system developed with the aid of Aspen HYSYS [12]. The column (shown in Figure-1) had two feed streams. The feeds (reactants) involved were water and propylene. Water, being less volatile than propylene, was passed into the column via the upper feed segment while propylene was fed from the lower feed segment of the column. The main reaction occurring in the reaction sections (the middle section and the reboiler) of the column was between the fed reactants (water and propylene) to produce isopropyl alcohol and it is as given in Equation (1) below.

$$H_2O + C_3H_6 \xleftrightarrow{K_{eq}} C_3H_8O \quad (1)$$

As a by-product (from a side reaction), di-isopropyl ether (DIPE), was also produced in the reaction sections of the column according to the reaction given in Equation (2).

$$C_3H_8O + C_3H_8O \xleftrightarrow{K_{eq}} C_6H_{14}O + H_2O \quad (2)$$

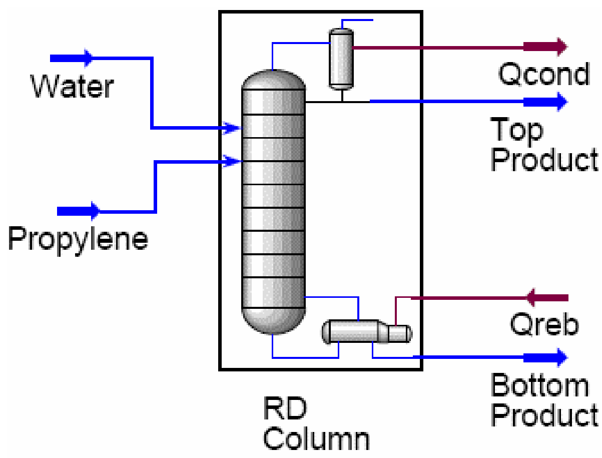

Figure-1. Process flowsheet of reactive distillation process for the production of isopropyl alcohol.

Given in Table-1 below are the data used for the development of the reactive distillation system used for the production of isopropyl alcohol in Aspen HYSYS environment.

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Table-1. Isopropyl alcohol reactive distillation Aspen HYSYS system development data.

Parameter	**Value**
Upper Feed	
Temperature (K)	298.15
Pressure (kPa)	110
Flow rate (m^3/hr)	0.0018
Composition (Mole fraction)	
Water (H_2O)	1.0000
Propylene (C_3H_6)	0.0000
2-Propanol (C_3H_8O)	0.0000
Di-i-P-Ether ($C_6H_{14}O$)	0.0000
Lower Feed	
Temperature (K)	298.15
Pressure (kPa)	1250
Flow rate (m^3/hr)	0.0018
Composition (Mole fraction)	
Water (H_2O)	0.0000
Propylene (C_3H_6)	1.0000
2-Propanol (C_3H_8O)	0.0000
Di-i-P-Ether ($C_6H_{14}O$)	0.0000
Fluid Package	General NRTL
Column	
Type	Packed
Packing type	Custom (Void Fraction = 0.8, Specific Surface Area = 100 m^2/m^3, Robins Factor = 70)
No. of segment	15
Upper feed segment	6
Lower feed segment	10
Stage packing height (m)	0.1
Stage diameter (m)	0.1
Reaction	
Type	Equilibrium
Segment	6 - 10 and reboiler
K_{eq} source	Gibbs Free Energy
Basis	Molar concentration
Phase	Liquid

2.2. Modeling and simulation

The development of the ANFIS model of the reactive distillation process considered in this study was carried out with the aid of MATLAB [13] using Fuzzy Logic Toolbox. In the process development, as mentioned earlier, the top segment and the bottom segment temperatures were selected as the output variables while the reflux ratio and the reboiler duty of the column were chosen as the input variables. Considering these variables, random data set values of the input variables generated using the Parametric Utility of Aspen HYSYS were used to run the system and the corresponding output variables

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(top segment temperature and bottom segment temperature) as well as the corresponding generated random input variables were recorded. Two data sets were generated from the Aspen HYSYS system of the reactive distillation process. 90% and 10% of one of the data sets were respectively used for training and checking the Adaptive Neuro-Fuzzy Inference Systems network model while the other one was used for testing the developed model. Since there were two output variables, two different models were developed; one between the inputs (reflux ratio and reboiler duty) and the top segment temperature and the other between the inputs (reflux ratio and reboiler duty) and the bottom segment temperature of the reactive distillation system. The parameters used for the formulations of each of the models of the process are given in Table-2 below.

Table 2. ANFIS model formulation parameters.

Parameter	Value
Number of inputs	2
Number of outputs	1
Training epoch number	100
Training error goal	0.001
Initial step size	0.01
Step size decrease rate	1.0
Step size increase rate	1.0
Membership function types	[gauss2mf gaussmf]
Membership function numbers	[7 5]

Moreover, the structure of the developed ANFIS model having two inputs and one output is shown in Figure-2 below.

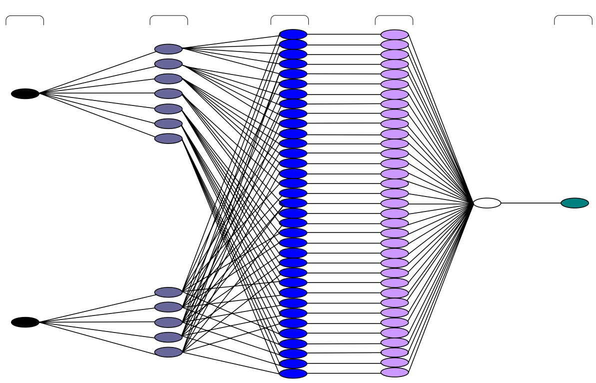

Figure-2. ANFIS model structure of the process.

After the development of the models, their simulations were carried out with the aid of MATLAB using both the training and the testing input data sets and the performances of the models were determined for both the training and the testing simulations using fit value and mean of absolute error criteria respectively. The fit value performance criterion was used to determine the percentage of the data accounted for by the developed model while the mean of absolute error criterion revealed the average of the differences between the recorded temperatures from the system and the predicted ones from the model.

3. RESULTS AND DISCUSSIONS

The data obtained from the simulations of the Aspen HYSYS system developed for the reactive distillation used for the production of isopropyl alcohol are as shown in Figures 3-6.

Figure-3 shows the responses obtained from the system in form of top segment temperatures towards the randomly generated inputs (reflux ratio and reboiler duty) shown as subplots below the plot of top segment temperatures in Figure-3.

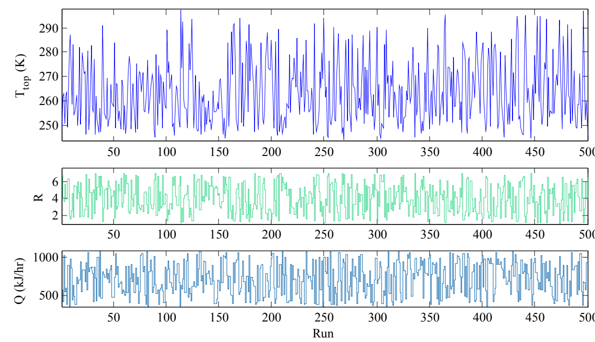

Figure-3. Training and checking input-output top segment data set.

In Figure-4, the plot of the bottom segment temperatures recorded when the system was run with the same randomly generated input values used for the generation of the data shown above in Figure-3 is given.

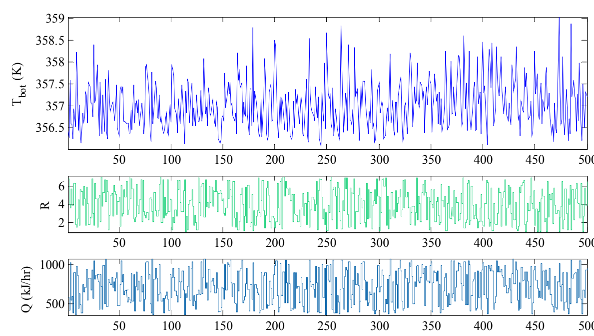

Figure-4. Training and checking input-output bottom segment data set.

The data given in Figures 3 and 4 above were acquired from the Aspen HYSYS system of the reactive distillation process and they were used for the training and the checking of the ANFIS model of the process.

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Given in Figures 5 and 6 are the top segment and the bottom segment temperatures together with the randomly generated input values used to obtain them from another separate simulation of the reactive distillation system developed using Aspen HYSYS. These data (Figures 5 and 6) were generated for the testing of the model. As can be seen from the figures, the ranges of the input values used for the generation of the testing data were different from the ones used to generate the data used for training and checking the model; however, the lower and the upper limits were within those of the ones used for generating the training and checking data. This was made so in order to ascertain the robustness of the developed model to the data not used for the training of the model.

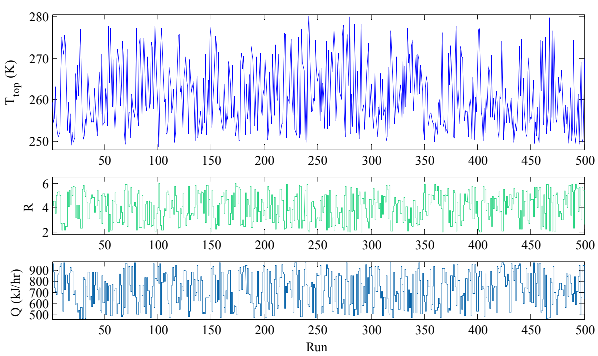

Figure 5. Testing input-output top segment data set.

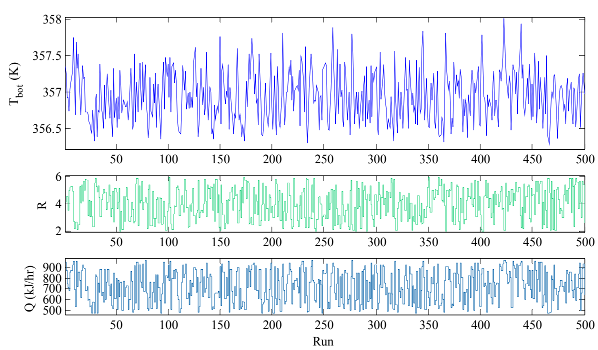

Figure-6. Testing input-output bottom segment data set.

As can be noticed from the results shown in Figures 3-6, when the generated input (reflux ratio and reboiler duty) values were used to run the system, there were significant responses seen to occur in the output variables (top segment and bottom segment temperatures). In other words, the selected output variables were found to respond to changes in the input variables and, thus, discovered to be functions of the input variables used. That is, the top segment temperature and the bottom segment temperature of the reactive distillation process studied in this work were found to be functions of both the reflux ratio and the reboiler duty.

Using the generated data for model training and checking given in Figures 3 and 4 respectively for the top segment and the bottom segment temperatures to develop two Adaptive Neuro-Fuzzy Inference Systems (ANFIS) models each for the top segment and the bottom segment of the reactive distillation system, even though the models could not be physically obtained and written in form of equations, their performances known as "fit values" that showed the percentage of the training data accounted for by the developed models were estimated and found to be 91.11% for the developed top segment model and 88.07% for the model developed for the bottom segment. The fit values obtained were found to be satisfactory enough for the models representing this complex reactive distillation process.

After the ANFIS models of the system were developed by training and checking, they were simulated using the training inputs values. The simulated top segment and bottom segment temperatures were compared to the recorded values obtained from the Aspen HYSYS model of the system as shown in Figures 7 and 8.

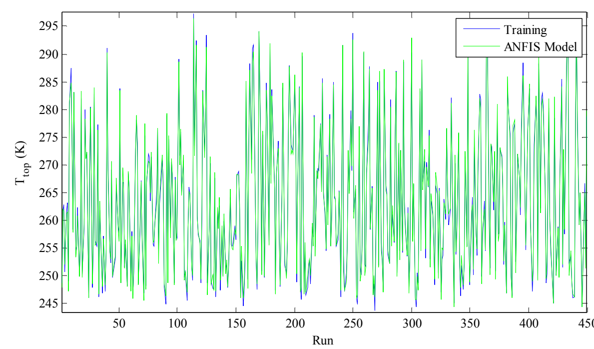

Figure-7. Training simulation and measured top segment temperature profiles.

Figure-7 shows the comparisons between the developed ANFIS model simulated top segment temperatures and those recorded from Aspen HYSYS system of the process. From the figure, it was observed that there were good comparisons between the two (simulated top segment temperature and recorded top segment temperature) profiles given.

Given in Figure-8 is the comparison between the bottom segment temperatures obtained from the simulation of the developed ANFIS model and the recorded ones obtained from the Aspen HYSYS system of the process using the input data generated and used for the training of the model. The good comparisons obtained from the profiles of the top segment temperatures were also discovered to exist in this case of the bottom segment temperatures of the reactive distillation system.

Considering the good fit values of the models and the comparisons made between the top segment and the bottom segment temperatures based on the model training carried out, it was observed that the developed models for the top segment and the bottom segment temperatures have been trained well.

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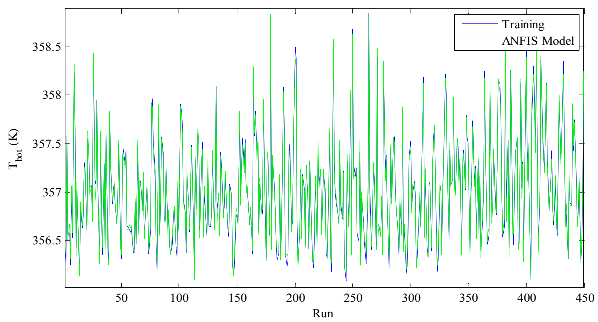

Figure-8. Training simulation and measured bottom segment temperature profiles.

Furthermore, the developed models were simulated using the input values recorded, specifically for model testing, from the developed Aspen HYSYS system of the reactive distillation process used for the production of isopropyl alcohol from the hydration of propylene. The results of the testing simulations are as shown in Figures 9 and 10 respectively for the top segment and the bottom segment temperatures. It was discovered from the figures that the agreements between the recorded temperatures obtained from the Aspen HYSYS system and those given by the simulations of the developed ANFIS models of the process were good enough to say that the developed models for the top and the bottom segments of the reactive distillation column were good representations of the process, even in the model testing.

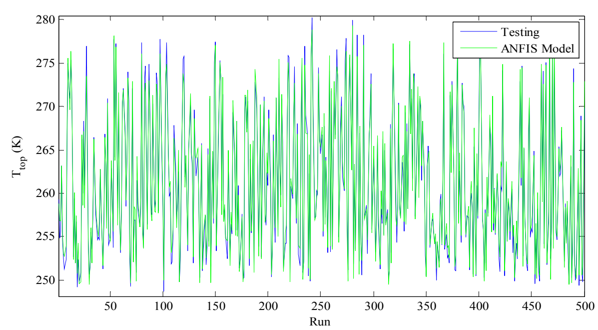

Figure-9. Testing simulation and measured top segment temperature profiles.

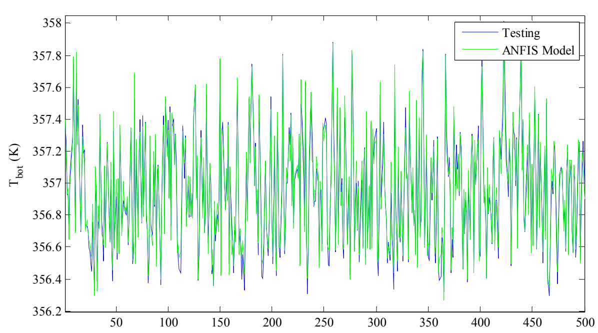

Figure 10. Testing simulation and measured bottom segment temperature profiles.

In order to numerically determine how good the performances of the models were in the testing simulations of the developed ANFIS models for the top and the bottom segments of the reactive distillation system, their means of absolute errors were calculated. The values obtained for the top and the bottom segment models which were estimated to be 0.9683 and 0.05623 respectively were found to be low enough for good models developed for a complex process like the reactive distillation process considered in this work.

4. CONCLUSIONS

The high fit values and the low means of absolute errors obtained respectively from the training and the testing of the ANFIS models developed for the top segment and the bottom segment of the reactive distillation system for the production of isopropyl alcohol from the hydration reaction involving propylene, studied in this work, have revealed that the developed ANFIS models represented the reactive distillation process very well.

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Nomenclature

ANFIS	Adaptive Neuro-Fuzzy Inference Systems
Di-i-P-Ether	di-isopropyl ether (DIPE)
K_{eq}	Equilibrium constant
NRTL	Non-Random Two-Liquid
Qcond	Condenser duty (kJ/hr)
Qreb	Reboiler duty (kJ/hr)
T_{bot}	Bottom segment temperature (K)
T_{top}	Top segment temperature (K)

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