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State Estimation for a Reactive Batch Distillation Column

Almıla Bahar*. Canan Özgen**

Department of Chemical Engineering, Middle East Technical University,
Ankara, 06531, Turkey
*e-mail: *abahar@metu.edu.tr, **cozgen@metu.edu.tr*

Abstract: An Artificial Neural Network (ANN) estimator is designed to predict the composition values of a reactive batch distillation system inferentially. The estimator for the reactive batch distillation system, which is recently a preferred industrial operation for specialty chemicals production, is designed using temperature measurements throughout the column. The reflux ratio of the batch distillation column is also used as input to the ANN as well as temperature values. The ANN used is an Elman network with two hidden layers; having 20 neurons in the first hidden layer, three neurons in the second hidden layer, and four neurons in the output layer. The performance of the designed network is tested in open-loop and it is found that, it is possible to predict the product compositions by using the designed ANN estimator which can be used in the control of the product compositions.

Keywords: Reactive Distillation, Batch Column, State Estimation, Artificial Neural Networks

1. INTRODUCTION

In reactive distillation, a high conversion is always expected with a satisfactory purity and this requires a high performance closed-loop control (Tade and Tian, 2000). Unfortunately, on-line measurement of compositions is a typical problem in industry as stated by many investigators (Mejdell and Skogestad, 1991; Quintero-Marmol and Luyben, 1992; Baratti et al., 1995; Kano et al., 2000; Bahar et al., 2004). On-line measurements of the product compositions can be possible with direct composition analyzers such as gas chromatographs and NIR (Near-Infra Red) analyzers. However, these are expensive, difficult to maintain, necessitate frequent calibrations and introduce undesirable time delays in the feedback control loop. An estimator that utilizes more than one temperature measurement can be used to infer the compositions.

Literature is full of studies on state estimation in continuous distillation columns whereas studies on the control of compositions in batch columns are rare. Batch distillation is complex, nonlinear and high-order process and it is intrinsically dynamic making the control a more challenging task. Composition profiles and operating conditions may change over a wide range of values during the entire operation and the state estimators must be designed to deal with the time-varying nature of the batch columns (Mujtaba and Macchietto, 1996; Oisiovici and Cruz, 2000). Also, batch distillation is an attractive choice in reactive distillation, when the reaction is slow and a large resident time is required to attain high conversion and when the reaction is so fast that a significant reaction may occur before the column reaches steady state (Wajge and Reklaitis, 1999).

The objective of this study is to design a state estimator for the esterification reaction of ethanol and acetic acid in a batch reactive distillation column by using ANN that estimates the product compositions which can be used in the control algorithm.

2. PROCESS DESCRIPTION

The process studied is an esterification reaction of ethanol with acetic acid to produce ethyl acetate and water in a batch distillation column. The working temperature of this endothermic, second order and reversible reaction is around 70^0C and atmospheric pressure is used. In this quaternary system, ethanol form azeotrope with water, ethyl acetate forms azeotropes with water (8.2 wt% water, boiling point 70.4^0C), and with ethanol (30.8 wt% ethanol, boiling point 71.8^0C). A ternary azeotrope between ethyl acetate-water-ethanol is also formed (7.8 wt% water, 9.0 wt% ethanol, boiling point 70.3^0C) (Ullmann, 1996). Besides many advantages like increase in overall reactant conversion, increase in energy efficiency and easier temperature control of reaction; reactive distillation also reacts away azeotropes and simplifies separation.

The operation of a batch column is divided into a number of stages as in the order of realization; start-up period, distillation at total-reflux, withdrawal of the lightest product, removal of a slop-cut, withdrawal of the next heaviest product, removal of a second slop-cut and so on. Fig. 1 shows the schematic of a multi-component batch distillation column system.

In this study, a previously developed dynamic simulation model is used. The column parameters are given in Table 1 and the details about the model can be found in Bahar (2007).

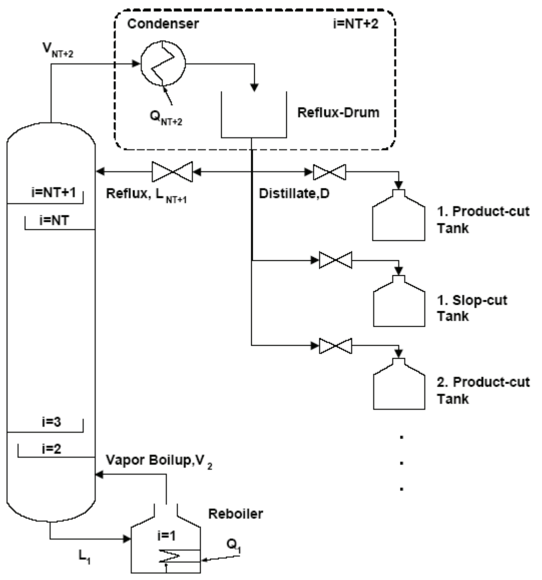

Fig. 1. The schematic of a multi-component batch distillation column.

Table 1. Column Parameters and Operating Conditions

No. of stages (including reboiler and total condenser)	10
Total fresh feed, mol	311.67
Feed composition (ethyl acetate, ethanol, water, acetic acid), mole fraction	0.0, 0.5, 0.0, 0.5
Column holdup, mol	
condenser+drum	30
internal plates	0.779
Reboiler heat duty, J/h	2.016×10^6
Column pressure, bar	1.013
Cooling water flow rate, lt/min	1.0

3. ANN STATE ESTIMATOR DESIGN

In this study, Artificial Neural Network (ANN) estimator to infer the product compositions from temperature measurements is developed which can provide a feedback control.

3.1 Observability Criteria and Selection of Measurement Points

The observability concept plays an important role in the design of control systems in state space. Although most physical systems are observable, corresponding mathematical models may not be observable. For this reason, it is necessary to know the conditions under which the system is observable. "A system is said to be observable at time t_0 if, with the system in state $X(t_0)$, it is possible to determine this state from the observation of the output over a finite time interval" (Ogata, 1997). Since the estimated compositions are used in the control of the column operation, the temperature measurements that are used as inputs to the estimator must be suitably selected in order to provide accurate estimation of the compositions because the measurement locations have significant effects on the performance.

Employing a degree-of-freedom concept, Yu *et al.* (1987) found that a distillation column is observable if the number of measurements is at least (*NC* - 1). The study of Quintero-Marmol *et al.* (1991) and Yıldız et al. (2005), dealing with the design of an Extended Luenberger Observer and Extended Kalman Filter, respectively, for multi-component batch distillation column, concluded that even though the linear observer in theory needs only (*NC* - 1) temperature measurements to be observable, to be effective at least (*NC*) thermocouples must be measured.

Furthermore, Yıldız et al. (2005) showed that, increasing the number of temperature measurements above NC does not result in better performance. Venkateswarlu and Kumar (2006) found in their study that the reboiler and the top tray are the most sensitive temperature measurement locations for a multi-component batch distillation column. Similarly, Yıldız et al. (2005) concluded that, the temperature measurement locations should be spread throughout the column homogeneously including the reboiler and the top tray. Considering these discussions, four temperature measurement location points, the reboiler, 2^{nd} tray, 5^{th} tray, and the top tray (8^{th} tray), are selected to be used in estimation.

3.2 Artificial Neural Networks (ANN) Estimator

The batch distillation system under study is highly nonlinear and it is observed that the composition profiles in the column changes significantly with different reflux ratio values. Thus, forming only one neural network and training it with input-output data obtained for various reflux ratio values is not reasonable. Therefore, a separate network is developed for each reflux ratio, R, and the value of the R is also given as input to the estimator. The output of the ANN estimator (distillate compositions) that corresponds to its inputs (temperatures and R) is found by interpolating the two networks, ANN_{i-1} and ANN_{i+1} between which the operating reflux ratio falls. As an example, if the value of R_i is between R_{i-1} and R_{i+1}, the output of the estimator is calculated from (1) and (2) where d_i represents the distance between R values.

$$\begin{aligned} d_1 &= \left| R_i - R_{i-1} \right| \\ d_2 &= \left| R_{i+1} - R_i \right| \end{aligned} \tag{1}$$

estimator output =

$$\frac{d_1}{d_1 + d_2} \times \text{output of} ANN_{i+1} + \frac{d_2}{d_1 + d_2} \times \text{output of } ANN_{i-1} \tag{2}$$

Each ANN is designed considering the network's architecture, normalization issue, and network performance with respect to verification and generalization tests.

ANN Architecture

In feed-forward networks, the output at any instant is dependent only on the inputs and the weights at that instant; therefore, these networks have no dynamic memory. In a recurrent network on the other hand, connections may be made between neurons in nonadjacent layers or within the same layer or feedback connections from a neuron in one layer to a neuron in a previous layer. Thus, signals can flow in both forward and backward directions and the output of that neuron becomes a function of both inputs from the previous layer at time t and its own output that existed at an earlier time. Because of this property, recurrent networks have a dynamic memory.

An Elman network, which is a recurrent network, is used in this study. In an Elman network, in addition to the input units, hidden units, and output units, there are also context units. The input and output units have an interaction with the outside environment, however the hidden and context units have not. The input units only pass the signals without changing them. The output units sum the signals fed to them. The context units are used only to memorize the previous activations of the hidden units. Thus, at a specific time, k, the previous activations of the hidden units (at time k-1) and the current inputs (at time k) are used as inputs to the network.

In the network structure, the number of input neurons corresponds to the number of input variables in the network. The number of output neurons is the same as the number of desired output variables, and since four composition values in the distillate are desired to be taken as outputs from the neural network, it must consist of four neurons in the output layer. The choice of the number of hidden layers and the neurons in the hidden layer(s) is not as straightforward as input and output layers, because it depends on the network application. However, they can be chosen by training the network with various configurations and selecting the configuration with the fewest number of layers and neurons which gives quickly and efficiently the minimum root-mean-squares (RMS) error. As Zilouchian and Jamshidi (2001) stated, adding a second hidden layer generally improves the network's prediction capability. However, adding an extra hidden layer commonly gives similar prediction capabilities with those of two hidden layer networks, but requires longer training times because of more complex structures. In this study; two hidden layers, with 20 neurons in the first hidden layer and 34 neurons in the second hidden layer, are used in the network structure. Because, increasing the number of hidden layers and the number of neurons in the hidden layers beyond these values did not decrease RMS error. The *tan-sigmoid* transfer functions are used for the hidden layers and *purelin* transfer function is used for the output layer.

Range of Variables

Neural networks cannot make accurate estimations if the operating input/output data are outside their training data range. The ANN in this study is trained with temperature and composition data generated by the help of simulation, utilizing unsteady state responses for different reflux ratio values. The reflux ratio (L/V) is changed between 0.5 and 1.0 for the constant reflux ratio period after the steady state is reached for total reflux. The lower values of the reflux ratio are found to be not suitable for separation in distillation.

The reflux ratio profiles, which are in the range of 20% of the optimal reflux profile, are also used in the training of the network. The optimal reflux ratio profile obtained for this system (Bahar, 2007) considering maximization of the Capacity Factor, CAP (Luyben 1988) is given in Table 2. The desired purities of the product-cuts are 0.52 for ethyl acetate product-cut tank, 0.50 for ethanol product-cut tank and 0.65 for water product-cut tank. The heaviest component in the system, acetic acid, is collected in the reboiler with a desired purity of 99%. The temperature profile throughout the column with the optimal reflux profile is shown in Fig. 2.

The 13 values of reflux ratio used in training are given in Table 3.

Table 2 Optimum Reflux Ratio Profile

Time Interval (hour)	Reflux Ratio, R
0 – 9.15	Total reflux
9.15 – 27.75	8.21
27.75 – 29.43	2.08
29.43 – 32.33	3.26
32.33 – 35.12	1.94
35.12 – 36.21	3.98
36.21 – 38.17	21.78

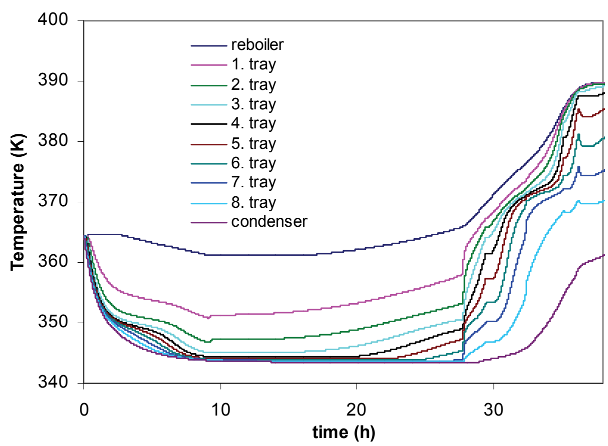

Fig. 2. Temperature profile throughout the column with the optimum reflux profile.

Table 3 Reflux Ratio Values Used in ANN Training

Reflux Ratio Trend After Total Reflux	Values of Reflux Ratio (L/V)
Constant	0.5, 0.6, 0.7, 0.8, 0.85, 0.9, 0.95, 1.0
	$R_{optimal}$
Variable with respect to a profile	$\pm$ 10% $R_{optimal}$
	$\pm$ 20% $R_{optimal}$

In the training of the ANN, back-propagation training algorithm is used which is simple, easy to apply and successful in application. The training of the ANN is done by using the dynamic data which are collected using the values of reflux ratios given in Table 3 utilizing the MATLAB simulation program.

Normalization

If the input and the output variables are not of the same order of magnitude, some variables may appear to have more significance than they actually do. Therefore, each input and output parameter, p, is normalized to the range [-1….1] before being used in the neural network and the network output is then converted back to its original values.

4. RESULTS AND DISCUSSION

For the prediction of the distillate compositions in the reactive batch distillation column under study, the temperature measurements throughout the column are used. The ANN estimator is designed considering the range of input variables, network's architecture, normalization issue, and network performance with respect to verification and generalization tests.

Estimator Performance

Checking the performance of a trained network must be done in two steps. In step one; how well the neural network recalls the output vector from data sets used to train the network (called the verification step) is tested; and in the second one how well the network predicts responses from data sets that were not used in the training phase (called the recall or generalization step) is tested.

Verification Tests

In Fig. 3 and Fig. 4, the responses of the distillate compositions for a reflux ratio (L/V) of 0.7 and for the optimum reflux ratio profile are shown respectively. It can be seen that, the network output will differ only slightly from the actual output data.

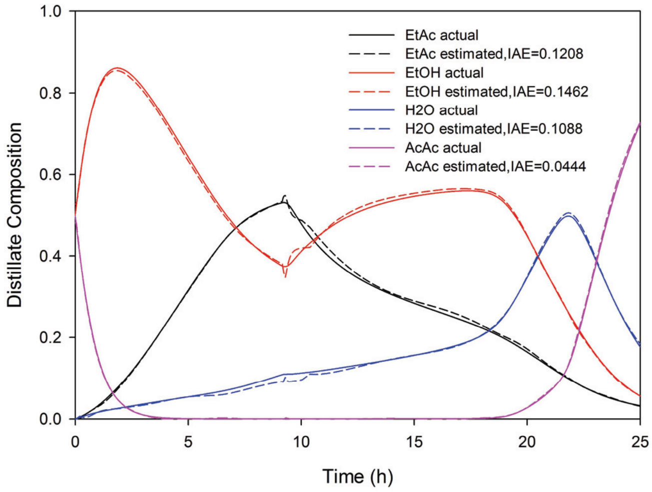

Fig. 3. Actual and estimated distillate compositions with total reflux followed by a reflux ratio of 0.7.

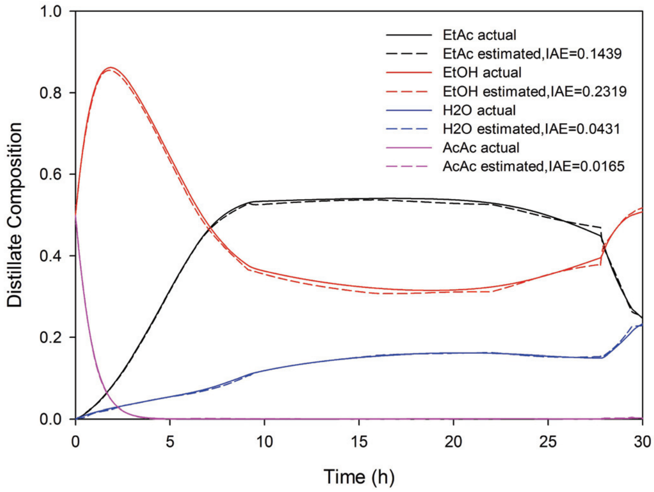

Fig. 4. Actual and estimated distillate compositions with optimal reflux profile.

Generalization Tests

The response of the column distillate compositions for a reflux ratio (L/V) of 0.75 is shown in Fig. 5. Furthermore, the responses of the column to a 10% increase in the optimal reflux ratio profile are given in Fig. 6.

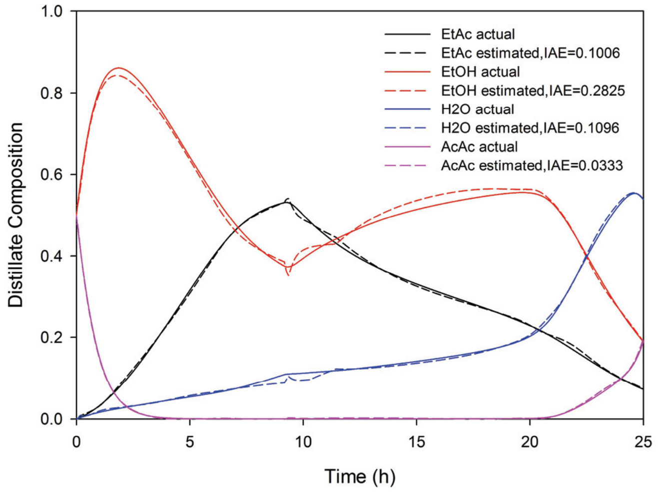

Fig. 5. Actual and estimated distillate compositions responses for total reflux period followed by reflux ratio of 0.75.

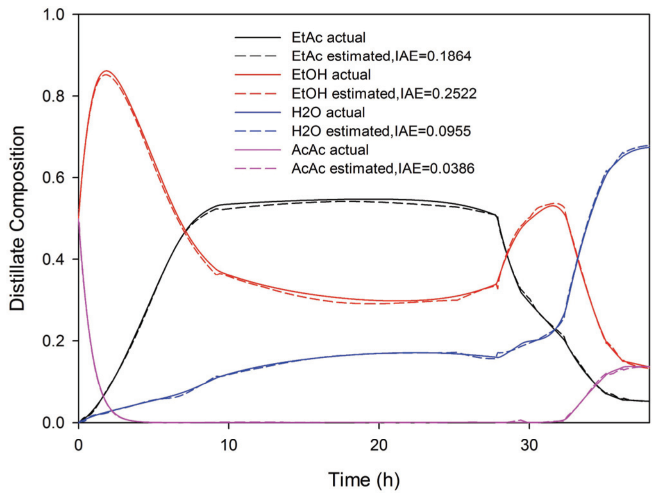

Fig. 6. Actual and estimated distillate compositions with 10% increase in optimal reflux profile.

It can be seen from the figures that, the network estimates the outputs by interpolation with a good accuracy.

5. CONCLUSIONS

In this work, the state estimator for a multi-component batch reactive distillation column is studied. The reaction studied is an esterification reaction where ethanol and acetic acid reacts to produce ethyl acetate and water.

The estimator designed is an ANN which utilizes an Elman network with two hidden layers having 20 neurons in the first hidden layer, three neurons in the second hidden layer and four neurons in the output layer. It is found that, using the designed ANN estimator it is possible to estimate the distillate composition values of the column from available four temperature measurements.

NOMENCLATURE

L	Liquid molar flow rate (mol/h)
R	Reflux ratio (L/D) or (L/V)
V	Vapor molar flow rate (mol/h)

Abbreviations:

AcAc	Acetic Acid
ANN	Artificial Neural Network
CAP	Capacity Factor
EtAc	Ethyl Acetate
EtOH	Ethanol
H2O	Water
IAE	Integral Absolute Error
NC	Number of components
NIR	Near-Infrared Spectroscopy
NN	Neural Network

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