# EKF AND ANFIS ESTIMATOR DESIGN IN MULTICOMPONENT BATCH DISTILLATION COLUMNS

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Abstract: In the control of batch distillation columns, one of the problems is the difficulty of monitoring the compositions. This problem can be handled by estimating the compositions from readily available online temperature measurements using a state estimator. In this study, an extended Kalman Filter (EKF) and an Adaptive Neuro-Fuzzy Inference System (ANFIS) state estimators that infer the product composition in a multicomponent batch distillation column (MBDC) from the temperature measurements are designed and tested using a batch column simulation. The designed EKF and ANFIS estimators are successfully used in the composition – feedback inferential control of MBDC operated under variable reflux-ratio policy with an acceptable deviation from the desired purity level of the products. 

Keywords: Batch Distillation, Simulation, State Observer, Kalman Filter, Adaptive Neuro-Fuzzy Inference System.

## 1. INTRODUCTION

"Batch distillation is generally used as a separation unit in the fine speciality chemicals, pharmaceuticals, biochemical and food industries. The demand and the uncertainty in specifications for these chemicals have increased recently, which increased the popularity of the use of batch distillation" (Barolo, M. and Cengio, P.D., 2001). Instead of using many continuous columns in series, multiple products can be obtained from a single batch distillation column during a single batch run. Moreover, batch distillation processes can easily handle variations both in the product specifications and in the feed compositions. This flexibility of batch distillation processes provides the ability to cope with a market characterized by short product life times and strict specification requirements.

In batch distillation, the operation of the column with optimized operation scenario; including reflux ratio policy, switching times, and method of recycling, is required to be realized in a convenient control system. However, in order to employ the operation scenario; the designed controller will require continuous information flow from the column, including the compositions throughout the column or temperatures reflecting the composition knowledge. The reason for this requirement is that, the value of reflux ratio and switching between product and slop cut distillations are optimized which are subject to the composition profile along the column and obtained as a function of it. Therefore, the need for knowledge of current composition in the column becomes obvious.

This composition knowledge can be generated by means of direct composition analyzers. Although there is a great development in the technology of online composition analyzers, such as gas chromatography, they bring large measurement delays and high investment and maintenance costs (Mejdell, T. and Skogestad, S., 1991; Venkateswarlu, C. and Avantika, S., 2001). The most popular alternative to the composition controllers utilizing analyzers is standard temperature feedback controllers. Although, temperature measurements are inexpensive and have negligible measurement delays, they are not accurate indicators of composition (Mejdell, T. and Skogestad, S., 1991). Another alternative is inferential control systems incorporating state estimators which use secondary temperature measurements.

State estimation can be defined as the process of extracting information from data which contain valuable information about a system and state estimator is the tool responsible for gathering valuable measurements to infer the desired information. Modern estimators also use known relationships in computing the desired information; taking into account the measurement errors, the effects of disturbances and control actions on the system, and prior knowledge about the system and measuring devices. While gathering these elements, they make use of some error criteria and try to minimize errors in some respect. The criteria and the method of minimization characterize the method of estimation and the use of minimization makes the estimate (extracted information) "optimal". If this optimality is realized statistically, the estimator type becomes stochastic; if deterministically it becomes deterministic. One of the estimators used in this work falls in the stochastic category and it is named as Kalman Filter.

However, if the sufficient input-output information is generated from the process, artificial intelligence methods that use this collected information can also be used to design a state estimator. ANFIS is one of the examples of these methods in which a fuzzy inference system is implemented in the framework of adaptive networks. It constructs an input-output mapping based both on human knowledge (in the form of fuzzy if-then rules) and on generated input output data pairs by using a hybrid algorithm that is the combination of the gradient descent and least square estimates (Jang 1993).

In this study, the aim is to design state estimators that infer the component concentrations of the multicomponent batch distillation column from the measured tray temperatures. The designed estimator is further tested using a rigorous column simulation to find its performance. The extended Kalman Filter (EKF) and the Adaptive Neuro-Fuzzy Inference System (ANFIS) are selected as the state estimators. Because it is based on the linear dynamic model of the process, the rigorous model used in the simulation is adapted to the EKF estimator algorithm mainly by simplifying the equilibrium model and by means of linearization. ANFIS estimator is designed using the data sets including temperature values and corresponding composition values obtained from the rigorous model. The performances of the developed estimators are tested by using the rigorous column simulation and discrete measurements of the top product compositions.

## 2. PROCESS DESCRIPTION

The case column for simulation is the one which was simulated by Mujtaba, I.M. and Macchietto, S., 1993 in their study on the subject of optimal operation of MBDC. The column is used to separate the mixture of cyclo-hexane, n-heptane and toluene.

The batch distillation column is under the perfect control of reflux-drum level and has two degrees-of-freedom for manipulation which are reboiler heat load, $Q_1$ and reflux-ratio, R. In this study, the reboiler heat load, $Q_1$ is kept at its maximum value given by design while the reflux-ratio, R is used as manipulated variable in order to realize the optimal operation policy recommended by Mujtaba, I.M. and Macchietto, S., 1993. This optimal operation policy is used to yield two product-cuts with the desired purity levels of 0.9 and 0.8 from the mixture of cyclo-hexane, n-heptane and toluene with the composition of (0.407, 0.394, 0.199). In the simulations, this optimal reflux ratio profile is employed.

There are many different rigorous models of batch distillation columns. They use the same basic strategy in the simulation model development which was used initially by the first studies on rigorous modelling of distillation columns. In batch column modelling, this common strategy was initiated by Meadows, E.L., 1963 and Distefano, G.P., 1968 which were followed by Stewart et al., 1973. The rigorous model used in this study is based on the study of Distefano, G.P., 1968 and its details are given by Yildiz (2002).

## 3. EKF ESTIMATOR

The Extended Kalman Filter (EKF) is defined as "optimal recursive data processing algorithm" (Maybeck, P.S., 1979), handling the estimation issues in the nonlinear system theory. EKF uses the nonlinear model of the system given by Eq.(1)

$$\underline{\dot{x}}(t) = f(\underline{x}(t), \underline{u}(t), t) + G(t)\underline{w}(t) \tag{1}$$

where f is the vector of the nonlinear system functions and the noise process, w(t) is modelled as white Gaussian noise with statistics

$$E\{\underline{w}(t)\} = 0 \tag{2}$$

$$E\{\underline{w}(t)\underline{w}(t')^T\} = \begin{cases} \underline{Q}(t), & t = t' \\ 0, & t \neq t' \end{cases} \tag{3}$$

and the nonlinear measurement model written as

$$\underline{z}(t_k) = h(\underline{x}(t_k), t_k) + \underline{v}(t_k) \tag{4}$$

where $h$ is the vector of the nonlinear measurement functions and noise process, $\underline{v}(t_k)$ is modelled as white Gaussian noise with statistics

$$E\{\underline{v}(t_k)\} = 0 \tag{5}$$

$$E\{\underline{v}(t_k)\,\underline{v}(t_l)^T\} = \begin{cases} \underline{R}(t)\ , t_k = t_l \\ 0 \quad , t_k \neq t_l \end{cases} \tag{6}$$

Moreover, EKF algorithm needs the linearized versions of these two models, specified by the Jacobian matrices and for the system it is given by Eq. (7) and for the measurement process by Eq. (8) .

$$\underline{F}(\hat{\underline{x}}(t), \underline{u}(t), t) = \left. \frac{df(\underline{x}(t), \underline{u}(t), t)}{d\,\underline{x}(t)} \right|_{\underline{x}=\hat{\underline{x}}} \tag{7}$$

$$\underline{H}(\hat{\underline{x}}^{-}(t_k), t_k) = \left. \frac{dh(\underline{x}(t_k), t_k)}{d\,\underline{x}(t_k)} \right|_{\underline{x}(t_k)=\hat{\underline{x}}^{-}(t_k)} \tag{8}$$

The extended Kalman Filter has a two-step recursive calculation algorithm. The first named as *the propagation stage* is responsible to calculate the prediction of the state at the current time using the best state estimate at the previous time step. The second is named as *the update stage* and updates the prediction found in the first stage using the measurements taken from the actual process and calculates the best state estimate. The propagation stage integrates the state and error covariance derivatives from the previous time step $t_{k-1}$ to the current time $t_k$ and uses the best state estimate $\hat{\underline{x}}^{+}(t_{k-1})$ and its error covariance $\underline{P}^{+}(t_{k-1})$ at the previous time step $t_{k-1}$, in order to calculate the prediction of the state, $\hat{\underline{x}}^{-}(t_k)$ and its error covariance $\underline{P}^{-}(t_k)$ at the current time step $t_k$. The update stage inovates the prediction of the state $\hat{\underline{x}}^{-}(t_k)$ and its error covariance $\underline{P}^{-}(t_k)$ at the current timestep $t_k$. In order to initiate the Kalman Filter algorithm, the initial conditions incorporating the initial state, $\hat{\underline{x}}(t_0) = \hat{\underline{x}}_0$ and its error covariance, $\underline{P}(t_0) = \underline{P}_0$ are required. At the initialization time step, when the first measurement is taken, requirements of the best state estimate, $\hat{\underline{x}}^{+}(t_{k-1}) = \hat{\underline{x}}^{+}(t_{-1})$ and it error covariance, $\underline{P}^{+}(t_{k-1}) = \underline{P}^{+}(t_{-1})$ at the time step $t_{-1}$ are supplied by replacing with the initial state $\hat{\underline{x}}_0$ and its error covariance $\underline{P}_0$.

The technique of EKF estimation will be applied to MBDC in order to infer the column compositions from the temperature measurements. At first, the observability of a multicomponent batch distillation column, which is a must to be able to estimate the system states, is to be analyzed. Employing a degree-of-freedom concept, Yu, c.C. and Luyben, W.L., 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, dealing with the design of an extended Luenberger Observer for MBDC, concluded that even though the linear observer in theory needs only (NC-1) temperature measurements to be observable, the nonlinear observer needed at least (NC) thermocouples to be effective. In addition, to improve the convergence without affecting the robustness, the use of (NC+2) measurements is recommended by Quintero-Marmol et al., 1991.

As a result, the nonlinear models for the system and for the temperature measurements are to be developed in the form required for EKF algorithm. However, the model developed for rigorous simulation of the batch column is not suitable for realistic situation in order to be implemented in EKF algorithm. The complexity of the simulation model requires high computational time and memory. Therefore, the rigorous column model for simulation is to be simplified and then the obtained nonlinear model is to be linearzed to achieve the Jacobian matrix both for the system and the measurement processes.

Some additional assumptions are needed for the simplification of the rigorous simulation model of MBDC. These assumptions are constant molar holdup on trays, neglecting the energy dynamics in the column, ideal trays, and use of Raoult's Law with Antoine's vapor pressure correlation for VLE description. As a result, the vapor flowrates throughout the column become equal as well as the liquid flowrates. The simplified model equations for MBDC are given by Yildiz (2002).

Lastly, the general forms of the linear system matrix

$$\underline{F}'(\underline{x}(t), \underline{u}(t), t) = \frac{d\,f(\underline{x}(t), \underline{u}(t), t)}{d\,\underline{x}(t)} \tag{9}$$

and the linear measurement matrix

$$\underline{H}'(\underline{x}(t_k), t_k) = \frac{d\,\underline{h}(\underline{x}(t_k), t_k)}{d\,\underline{x}(t_k)} \tag{10}$$

are evaluated analytically. Their expanded forms and the details of the derivation are given by Yildiz (2002).

Consequently, all the information required for EKF estimator has been obtained. This information incorporates nonlinear and linearized models for the system of MBDC and the measurement process given respectively by $\underline{f}, \underline{h}, \underline{F}', \underline{H}'$.

## 4. ANFIS ESTIMATOR

In ANFIS, Takagi-Sugeno (TS) fuzzy model is used. A simple example of ANFIS with two TS type fuzzy rules is given in Figure 1. The output of each rule can be a linear combination of input variables plus a constant term or can be only a constant term. The final output is the weighted average of each rule's output.

Rule1: If x is $A_1$ and y is $B_1$, then $f_1 = p_1x + q_1y + r_1$

Rule2: If x is $A_2$ and y is $B_2$, then $f_2 = p_2x + q_2y + r_2$

The node functions in the same layer are the same as described below:

Layer 1: Every node $i$ in this layer is an adaptive node with a node function as:

$$0_{1,i} = \mu_{A_i}(x), \ for \ \ i = 1,2$$
$$0_{1,i} = \mu_{B_i - 2}(y), \ for \ \ i = 3,4 \qquad (11)$$

where x is the input to node $i$, and $A_i$ (or $B_{i-2}$ ) is a membership function (MF) associated with this node. Parameters in this layer are the MF's parameters.

Layer 2: Every node in this layer is a fixed node labeled as Π, whose output is the product of all incoming signals:

$$0_{2,i} = w_i = \mu_{A_i}(x)\mu_{B_i}(y), \quad i = 1,2 \qquad (12)$$

Each node output represents the *firing strength* of a fuzzy rule.

Layer 3: Every node in this layer is a fixed node labeled N. The $i$th node calculates the ratio of the rule's firing strength to the sum of all rules' firing strengths:

$$0_{3,i} = w_i = w_i/(w_1 + w_2), \quad i = 1,2 \qquad (13)$$

Outputs of this layer are called "normalized firing strengths".

Layer 4: Every node $i$ in this layer is an adaptive node with a node function as:

$$0_{4,i} = \overline{w_i} f_i = \overline{w_i}(p_i x + q_i y + r_i) \qquad (14)$$

where $\overline{w_i}$ is a normalized firing strength from layer 3 and $\{p_i, q_i, r_i\}$ is the parameter set of this node.

Layer 5: The single node in this layer is a fixed node labeled Σ that computes the overall output as the summation of all incoming signals:

$$0_{5,i} = overall \ \ output = \sum_i \overline{w_i} f_i = \frac{\sum_i w_i f}{\sum_i w_i} \qquad (15)$$

The computation of parameters is facilitated by a gradient vector, which provides a measure of how well the ANFIS is modeling the input output data for a given parameter set. Once the gradient vector is obtained, backpropagation or hybrid learning algorithm, combination of the gradient descent and least square estimates, can be applied in order to adjust the parameters (Jang 1993). Detailed design procedure for the ANFIS estimator can be found in the study of Güner (2003).

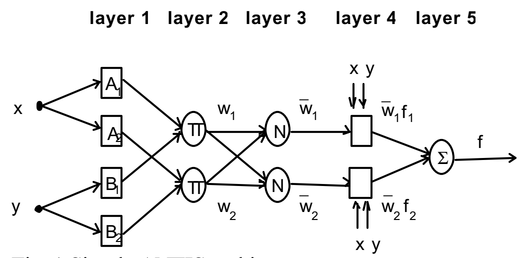


Fig. 1 Simple ANFIS architecture

## 5. RESULTS AND DISCUSSION

The EKF estimator implementation is performed in three phases. First, an extended Kalman Filter for the estimation of product compositions for a MBDC from temperature measurements is designed. Then the designed EKF is implemented on the case MBDC to check the performance of the EKF. In the third phase the designed EKF is utilized for control purposes in the MBDC.

After designing the EKF state estimator, several simulation test runs are done to obtain the optimum values of the tuning parameters by selecting the integral absolute error (IAE) as the performance criteria reflecting the fitness of the EKF design parameters. The tuning parameters for EKF are the diagonal terms of process noise covariance matrix, q, and the diagonal terms of measurement model noise covariance matrix, r. Also, the effect of number of measurement points and measurement period, $\Delta t_m$ have been considered.

The optimum value of the diagonal terms of process noise covariance matrix, q and the diagonal terms of measurement model noise covariance matrix, r are searched in the range where the EKF estimator is stable. Performing some trial runs, the stability region of the estimator is found where the value of q and r are in the range of 50 - $1x10^{-7}$ and 0.5 - $5x10^{8}$, respectively. The best result (i.e. one having the lowest IAE sum) is obtained for the diagonal terms of process noise covariance matrix, q=5000 and for the diagonal terms of measurement model noise covariance matrix, r=0.00001. The best result is obtained for three measurement points and for the measurement location set with reboiler, 4th and top trays. The effect of measurement period, $\Delta t_m$ on IAE scores is also investigated. Although, the measurement period selected in this simulation study is the integration time step (i.e. the minimum possible value), in real-time estimation problems, the value of $\Delta t_m$ is to be chosen considering the limits of the computational power. The measurement periods of 3 min. even 5 min. can satisfactorily be used without much change in EKF performance. Given this optimum set of the tuning parameters, the actual and estimated reflux-drum composition profiles are shown in Figure 2 for the case column under the open-loop control actions.

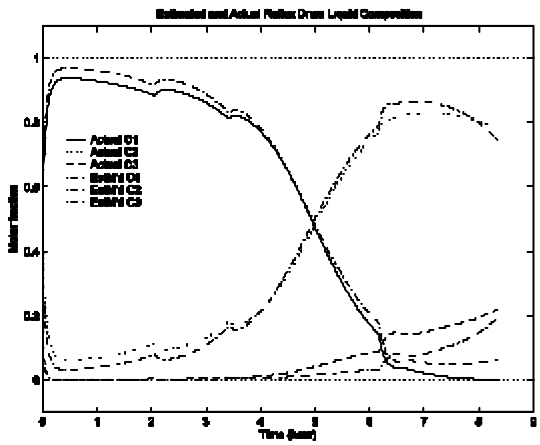

Fig.2. Actual and estimated reflux-drum composition profiles for the optimum values of the tuning parameters under open-loop control.

In last phase of the study, it is aimed to analyze the performance of the EKF estimator for a MBDC system in a composition-feedback inferential control structure which realizes an actual scheduling policy explained previously. In the simulation of this control structure, the compositions can be obtained directly from the process simulation or from the EKF estimator. Firstly, to create a reference point, a simulation is done, taking the composition knowledge directly from the column as the feedback information to the controller. The response of this reference run in terms of the liquid compositions, both in the reflux-drum and the reboiler are given in Fig.3.

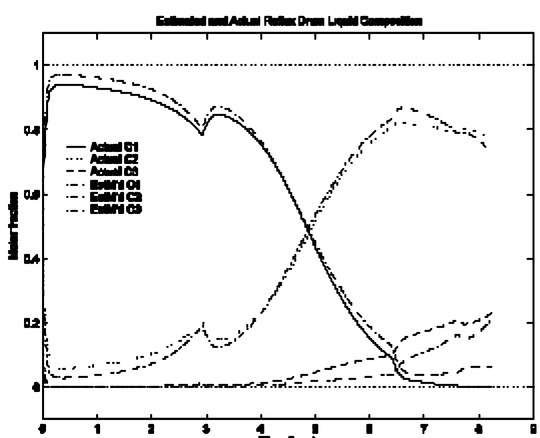

Fig.3. Actual and estimated reflux-drum composition profiles for the optimum values of the tuning parameters under open-loop control.

To see the performance of EKF, secondly the same simulation is realized using the estimated compositions as the feedback to the controller. For the design parameters of the EKF estimator, previously obtained optimum values are used. Actual and estimated compositions of the reflux-drum are shown in Fig.4. Thus, this batch distillation column can be controlled satisfactorily for variable reflux ratio policy by the use of EKF estimator utilizing a simplified model.

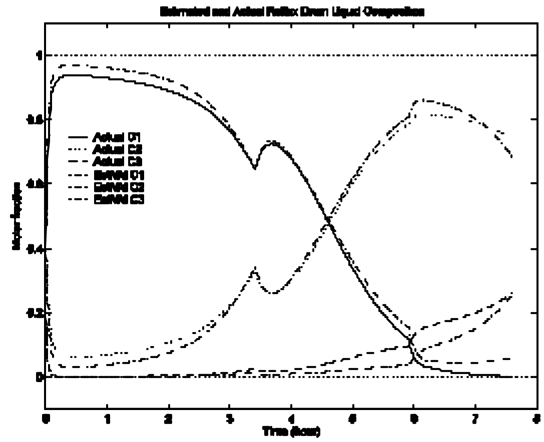

Fig.4. Actual and estimated reflux-drum composition profiles for the optimum values of the tuning parameters under closed-loop control.

The ANFIS estimator design is performed in three phases. First, input process variables which are in operational range are changed and output variables are obtained from rigorus model simulations. Then, training data sets are generated using these input-output data and different ANFIS architectures are trained with these data sets. Finally, trained architectures are implemented on the case MBDC to check the performance of the estimators. The structure that gives the minimum IAE score after the simulations is selected as an ANFIS estimator. Fig5 shows the performance of the selected ANFIS state estimator. It can be seen from the Fig. 5 that ANFIS estimator performance is very good. It can also be seen from the Fig.6. that performance of the ANFIS estimator is better than the EKF state estimator.

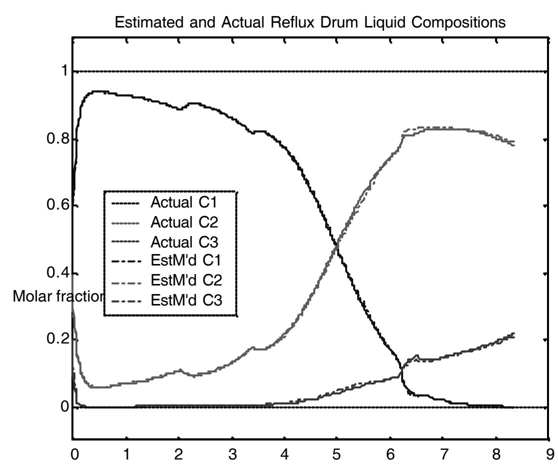


Fig.5. Actual and estimated reflux-drum composition profiles for the selected ANFIS estimator under open-loop control

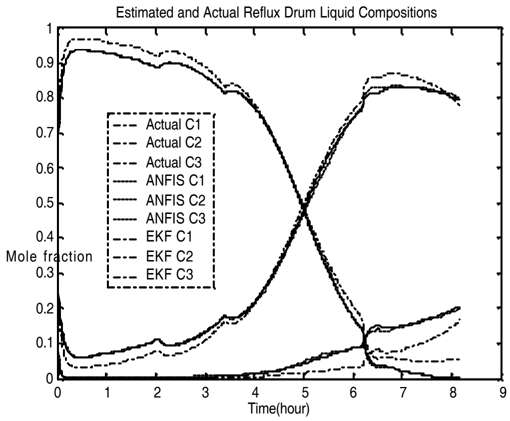


Fig.6. Comparison of the selected ANFIS estimator and EKF estimator under open-loop control

## 6. CONCLUSION

The study is aimed to estimate the compositions in the multicomponent batch distillation column from temperature measurements using EKF and ANFIS estimators, separately. It is found that, the most important part of the modelling affecting the performance of the EKF estimator is the selection of the VLE formulation. EKF parameters of the diagonal terms of process noise covariance matrix and the diagonal terms of measurement model noise covariance matrix are selected basing on the least sum of individual IAE scores for the reflux-drum and the reboiler composition estimates. From the input-output data of the rigorous plant simulation ANFIS estimator is trained and from several simulation runs for different architectures of ANFIS estimator the estimator performance is optimized. The designed EKF and ANFIS estimators are implemented in the open-loop control of the MBDC. It is seen that ANFIS estimator performs more accurate estimations of the reflux-drum compositions than the EKF does. The superior performance of the ANFIS is due to having the information directly taken from the input-output data of the simulated plant. However, the EKF estimator incorporates the simplified model and its linearized version of the plant causing plant-model mismatches.

## REFERENCES


Barolo, M. and Cengio, P.D. (2001). Closed-loop Optimal Operation of Batch Distillation Columns. *Computers and Chemical Engineering*, **25**, 561-569.

Distefano, G.P. (1968). Mathematical Modelling and Numerical Integration of Multicomponent Batch Distillation Equations. *AIChE J.*, **14**, 190-199.

Furlonge, H.I., Pantelides, C.C., Sorensen, E. (1999). Optimal Operation of Multivessel Batch Distillation Columns. *AIChE J.*, **45**, 781-801.

Güner, E. (2003). Adaptive Neuro-Fuzzy Inference Applications in Chemical Processes, *M.Sc. Thesis*, Middle East Technical University, Ankara.

Jacobs, O.L.R. (1974). *Introduction to Control Theory*, Clarendon Press.

Jang, R.J. (1993). ANFIS: Adaptive-Network-Based Fuzzy Inference System. *IEEE Transections on Man, and Cybernetics*, **23**, No. 3, 665-683.

Luyben, W.L. (1988). Multicomponent Batch Distillation. 1. Ternary Systems with Slop Recycle. *Ind. Eng. Chem. Res.*, **27**, 642-647.

Maybeck, P.S. (1979), *Stochastic Models, Estimation, and Control*, Academic Press Inc.

Meadows, E.L. (1963). *Chem. Eng. Progr. Symp. Ser. 46*, **59**, 48.

Mejdell, T. and Skogestad, S. (1991). Estimation of Distillation Compositions from Multiple Temperature Measurements Using Partial-Least-Squares Regression. *Ind. Eng. Chem. Res.*, **30**, 2543-2555.

Mujtaba, I.M. and Macchietto, S. (1993). Optimal Operation of Multicomponent Batch Distillation---Multiperiod Formulation and Solution. *Computers chem. Engng.*, **17**, 1191-1207.

Perry, R.H., Green, D.W., Maloney, J.O. (1999). *Perry's Chemical Engineer's Handbook*. McGraw -Hill.

Quintero-Marmol, E., Luyben, W.L. and Georgakis, C. (1991). Application of an Extended Luenberger Observer to the Control of Multicomponent Batch Distillation. *Ind. Chem Eng. Res.*, **30**, 1870-1880.

Stewart, R.R., Weisman, E., Goodwin, B.M., Speight, C.E. (1973). Effect of Design Parameters in Multicomponent Batch Distillation. *Ind. Eng. Chem. Process Des. Develop.*, **12**, 130-136.

Venkateswarlu, C. and Avantika, S. (2001). Optimal State Estimation of Multicomponent Batch Distillation. *Chemical Engineering Science*, **56**, 5771-5786.

Yildiz U. (2002). Multicomponent Batch Distillation Column Simulation and State Observer Design. *M.Sc. Thesis*, Middle East Technical University, Ankara.

Young, S.C. and Luyben, W.L. (1987). Rigorous Dynamic Models of Distillation Columns. *Ind. Eng Chem. Res.*, **26**, 2158-2161.

Yu, c.C. and Luyben, W.L. (1987). Control of Multicomponent Distillation Columns Using Rigorous Composition Estimators, Distillation and Absorption. *Institute of Chemical Engineering of Symposium Series*, **104**, A29-A69.