

Adaptive Neuro Fuzzy Inference System In Distillation Column

Thesis submitted in partial fulfillment
of the requirement for the award of degree of

Master of Engineering

in

Electronics Instrumentation and Control Engineering



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June 2009

CERTIFICATE

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ABSTRACT

Neuro-Fuzzy systems are incorporated in this thesis for learning the system under consideration. Adaptive Neuro-Fuzzy inference system (ANFIS) is one of the Neuro Fuzzy systems in which a fuzzy system is implemented in the framework of adaptive networks. ANFIS constructs an input-output mapping based both on human knowledge (in the form of fuzzy rules) and on generated input-output data pairs after certain trainings to the similar situations arising from different conditions within the system.

Effective control for distillation systems in the chemical industries is considered in my work. Composition measurement is not feasible, since, these analyzers, like gas chromatographs, involve large measurement delays. As an alternative, compositions can be estimated from temperature measurements. Thus, an online estimator that utilizes temperature measurements can be used to infer the produced compositions. In this study, ANFIS estimators are designed to infer the top and bottom product compositions in a continuous distillation column and to infer the reflux drum compositions in a batch distillation column from the measurable tray temperatures. Designed estimator performances are further compared with the other types of estimators such as NN.

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LIST OF ABBREVIATIONS

ANFIS	Adaptive Neuro Fuzzy Inference System
ANN	Artificial Neural Network
FAM	Fuzzy Associative Memory
FLC	Fuzzy Logic Controller
FNN	Fuzzy Neural Network
IAE	Integral of the Absolute Error
NC	Number of Components
NF	Neuro-Fuzzy
NFC	Neuro Fuzzy Control
NN	Neural Network
RNN	Recurrent Neural Networks

CHAPTER 1

INTRODUCTION

An intelligence system is a system that is able to make decisions like humans. Intelligence systems adapt themselves to the situations and they take correct decisions automatically for future similar situations. Neural networks (NNs), Fuzzy systems, and Neuro-Fuzzy systems are the examples of the artificial intelligence systems.

Fuzzy systems provide a unified framework for taking into account the gradual or flexible nature of variables, and representation of incomplete information. This is an alternative to classical approach and is based on the observations that, humans think using linguistic terms such as “small” or “large” and others rather than numbers. The concept is described in a natural language, by Zadeh using fuzzy sets introduced by him in 1965. The essence of fuzzy systems is conditional if-then rules, which use fuzzy sets as linguistic terms in antecedent and conclusion parts. A collection of these fuzzy if-then rules can be determined from human experts or alternatively can be generated from observed data (examples). The main advantage of such fuzzy systems is the easiness to interpret knowledge in the rule base.

NNs are the systems that get inspiration from biological neuron systems and mathematical theories for learning. They are characterized by their learning ability with a parallel-distributed structure and also can be considered as black box modeling. They are useful empirical modeling tools that have been used for process estimation and control since 1950’s.

In most fuzzy systems, fuzzy if-then rules were obtained from a human expert. However, this method of knowledge acquisition has great disadvantages; not every expert can and/or wants to share his/her knowledge. For this reason, NNs were incorporated into fuzzy systems, which can acquire knowledge automatically by learning algorithms of NNs. These systems are called Neuro- Fuzzy systems and have advantages over fuzzy systems, i.e., acquired knowledge is easy to understand. Like in NNs, knowledge is saved in connection weights, but can also be easily interpreted as fuzzy if then rules. The Neuro- Fuzzy systems can be viewed as a mixture of local experts (rules operate dominantly in each fuzzy region) and their parameters are updated using gradient and least squares optimization methods. Adaptive network based fuzzy inference system or adaptive Neuro-Fuzzy inference system (ANFIS), first proposed by Jang is one of the

examples of Neuro Fuzzy systems in which a fuzzy inference system is implemented in the framework of adaptive networks. ANFIS 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. ANFIS is not a black box model and works well with optimization techniques, which is computationally efficient and is also well suited to mathematical analysis. Therefore, it can be used in modeling and controlling studies, and also for estimation purposes.

In batch and continuous distillation processes, composition control is very important. Especially, in order to meet the purity specifications, a batch column has to be operated as precisely as possible. If the current compositions are known, they can form a basis for improving the process performance through an operator decision making for the development of a closed loop control scheme. An effective feedback control systems for continuous distillation columns can also be easily designed with the known composition values. Online measurements of the compositions can be done using direct composition analyzers. However, online composition measurement is not feasible, since, these analyzers, like gas chromatographs, involve large measurement delays as well as high investment and maintenance costs. As an alternative, compositions can be estimated from temperature measurements. Thus, an online estimator that utilizes temperature measurements can be used to infer the produced compositions. In this study, ANFIS estimators are designed to infer the top and bottom product compositions in a continuous distillation column and to infer the reflux drum compositions in a batch distillation column. Designed estimator performances are further compared with the other types of estimators such as NN.

CHAPTER 2

LITERATURE SURVEY

In this chapter, the literature survey on Neural Network (NN), Fuzzy Logic (FL) and Neuro-Fuzzy (NF) systems are given. In the first section, studies on NNs, in the second section cases in which fuzzy systems were applied are presented. In the last section, studies on NF systems development and implementation are given. At the end of each section, summary of the studies are also presented in tables.

2.1 NEURAL NETWORKS

A neural network is a data processing system consisting of a large number of simple, highly interconnected processing elements (artificial neurons) in an architecture inspired by the structure of the cerebral cortex of the brain. The formal realization that the brain in some way performs information processing tasks was first spelt out by McCulloch and Pitts (1943). They represented the activity of individual neurons using simple threshold logic elements, and showed how networks made out of many of these units interconnected could perform the logical operations. Rosenblat (1959) developed the concept of perceptron, a generalization of the McCulloch and Pitt's concept of the functioning of the brain, by adding learning (Lisboa 1992). These studies were the initiations of NNs.

In chemical engineering, since NNs provide good empirical models of complex nonlinear processes, they have been frequently used in complex modeling problems. They have also used in control schemes as aid or controller. Fault detection, prediction of polymer quality and data rectification are some other examples of NN applications in chemical engineering (Himmelblau 2000).

Yamamura et. al. (1988) proposed three different methods; general learning, specialized learning and combination of them to train the NN controller to act as the inverse of the plant. Since using general learning can be very difficult to provide adequate performance in practical control applications, method of error propagation backwards through the plant is introduced to train the network exactly on the operational range of the plant. Also, combination of generalized and

specialized training was proposed to use their advantages and to avoid their potential disadvantages

Bhat and McAvoy (1990) discussed the use of backpropagation, the most widely used NN, for non-linear dynamic modeling and model-based control of chemical process systems. In their paper, after a review of the backpropagation algorithm, a comparison between NN dynamic modeling and traditional modeling are presented. The backpropagation technique was shown to be able to pick up more of the non-linear characteristics of the CSTR than the traditional modeling. Then two approaches that use NNs for model-based control were discussed.

Himmelblau and MacMurray (1995) implemented a NN for MPC in a packed distillation column. Their column had the interesting feature of multiple changes in the sign of the process gain as the operating conditions change. They used an External Recurrent Network to model the process over a significant part of the state space and compared the model performance with a simplified principles model. Although both models gave similar performance, in some instances the NN model was better. They concluded that, when the process is too complex to be modeled by a first principles model, or takes too long to model.

Wang et. al. (1998) proposed a nonlinear predictive control framework, in which nonlinear processes are modeled using NNs. In this framework, a predictive controller, based on the NN model, calculates the optimal manipulated variable; while at the same time the available measured output (controlled variable) is used to modify the output predicted by the NN model.

Hussain (1999) provided an extensive review of the various applications utilizing NNs for chemical process control, both in simulation and also in online implementation. He categorized the review under three major control schemes; inverse model based control, predictive control and adaptive control methods. The review shows that using NNs in chemical process control is widespread and multilayered feedforward NN is the most popular network for such process control applications. However, it is emphasized that there is lack of actual successful online applications.

Jutan and Krishnapura (2000) proposed an adaptive NN controller for the control of nonlinear dynamical systems. The NN controller was adaptive in structure and used no explicit model of

the process in the design. Contrasting traditional NNs, which have many connection weights, the proposed controller network had a few weights.

2.2 FUZZY LOGIC SYSTEM

“As the complexity of a system increases, our ability to make precision and yet significant statements about the behavior diminishes until a threshold is reached beyond which precise and significance become almost mutually exclusive characteristics.” (Zadeh 1971)

The concept of fuzziness was first proposed by Zadeh (1965). He aimed to describe complex and complicated systems using fuzzy approximation and introduced fuzzy sets. “Generally, fuzzy logic can be considered as a logical system that provides a model for modes of human reasoning that are approximations rather than exact” (Rutkowska 2002).

Fuzzy logic systems had found successful applications in wide variety of fields such as: automatic control, pattern recognition, signal processing, expert systems, communication, system identification and time series prediction (Czogala and Leski 2000). In chemical engineering systems, they have been generally used in control studies. Since Fuzzy Logic Control (FLC) does not require a model and the control is based on expertise human reasoning, they have been applied in many control schemes. Also, they are used extensively in modeling.

Kim and Kim (1995) combined the fuzzy control and predictive control and applied it to the binary distillation column. They compared its performance by simulation and experimentation. They used a combined technique in which a switching scheme was implemented. When error or change of error between the controlled variable and the set point of the variable was larger than a certain value, the fuzzy control was used in control computation. It was concluded that combined method improved the control performance for set point tracking and disturbance rejection. Considering the IAE scores it was found that combined control technique improved the control performance by 9%.

A fuzzy classifier that can be used as an adequate and reliable expert system to perform quality qualifications in chemical engineering system was proposed by Bafas et. al.(2002). The method builds a fuzzy logic model, which infers the quality variables from other accurately measured system parameters. It was applied to two chemical engineering problems; the wine distillate

maturation and the tissue making process and compared with a feedforward NN methodology and a fuzzy identification method. It was confirmed that classifications of proposed fuzzy logic model were more accurate.

2.3 NEURO-FUZZY SYSTEM

In most fuzzy systems, fuzzy rules were obtained from the human expert. However, every expert does not want to share his knowledge and there is no standard method that exists to utilize expert knowledge. As a result, ANNs were incorporated into fuzzy systems to be able to acquire knowledge automatically by learning algorithms. The learning capability of the NNs was used for automatic fuzzy if then rules generation (Czogala and Leski 2000).

The connection of fuzzy systems with an ANN is called neuro-fuzzy, NF, systems. Like in NNs where knowledge is saved in connection weights, it is interpreted as fuzzy if then rules in NF systems. The most frequently used NN in NF systems is radial basis function neural network, RBFNN in which each node has radial basis function such as Gaussian and Ellipsoidal. Their popularity is due to the simplicity of structure, well-established theoretical basis and faster learning than in other types of NNs. Also, there are many developed fuzzy neural networks (FNN) as NF algorithms in literature. Adaptive network based fuzzy inference system, ANFIS, is one of them.

Jang (1992) proposed to use the ANFIS architecture to improve the performance of the fuzzy controllers. The performance of the fuzzy controller relies on two important factors: knowledge acquisition and the availability of human experts. For the first problem, Jang proposed the ANFIS to solve the automatic elicitation of the knowledge in the form of fuzzy if then rules. For the second problem, that is how the fuzzy controller is constructed without using human experts; a learning method based on a special form of gradient descent (backpropagation) was used. The proposed architecture identified the near optimal membership functions and the other parameters of a controller rule base for achieving a desired input-output mapping. The backpropagation type gradient descent method was applied to propagate the error signals through different time stages to control the plant trajectory. The inverted pendulum system was employed to show the effectiveness and robustness of the proposed controller.

In 1992, Uchikawa et. al. presented a fuzzy modeling method using fuzzy neural networks, FNNs, with the backpropagation algorithms. They proposed three types of NN structures of which the connections weights have particular meanings for getting fuzzy inference rules for tuning membership functions. These structures are categorized into FNNs and these different types FNNs realize three different types of reasoning.

In another paper, Uchikawa et. al. (1995) presented a new design method of adaptive fuzzy controller using linguistic rules of fuzzy models of the controlled objects. FNNs identify fuzzy models of nonlinear systems automatically with the backpropagation algorithm in this method. Authors also presented a rule-to-rule mapping method for describing the behavior of fuzzy dynamical systems. Using this methodology, first, the control rules are modified by considering rule-to-rule transitions. After that, designed controller was implemented with another FNN. The adaptive tuning of the control rules was done using the fuzzy model of the controlled object by utilizing the derivative value from the fuzzy model. A second order system was simulated to show the feasibility of the proposed design method.

A methodology for batch process automation using reinforcement learning was presented Martinez and Wilson (1997). In this study, an autonomous controller continuously learned to implement control actions that can drive the process state very close to desired one with near optimal performance. This methodology was exemplified using a batch process involving simultaneous reaction and distillation.

Peng and Chen (1999) developed an intelligent control system for the direct adaptive control of chemical processes in the presence of unknown dynamics, nonlinearities and uncertainties. They constructed a Neuro-Fuzzy Controller (NFC) with an equivalent four-layer connectionist network. With a derived learning algorithm, fuzzy rules and membership functions were updated adaptively by observing the process output error. A shape tunable NN with backpropagation algorithm was also suggested as the estimator in order to provide a reference signal to the controller.

Belarbi et. al. (2000) proposed a FNN that learns rules of inference for a fuzzy system through classical backpropagation. The network was trained off-line in a closed loop simulation to design Fuzzy Logic Controller (FLC). Another network was used as a design model in order to

backpropagate the error signal. Controller rules were extracted from the trained network to build the rule base of the FLC. The framework was applied to the estimation and control of a batch pulp digester. The Kappa number, the controlled variable, which cannot be measured online was estimated with same type of FNN through the measurements of the batch temperature and concentration of the alkali. Although the FLC was quite simple with nine rules, simulation results showed good degree of robustness in the face of parameter variations and changes in operating conditions.

Leiviska et. al. (2001) used linguistic equations (fuzzy models) and NN models in prediction of Kappa number in the continuous digester. Actual prediction data was collected from a continuous digester house. It included the extraction flow measurements and reactive index, temperature in the extraction flow, and the measurement of Kappa number from an online device after digester. Then the data was divided into training and testing data. ANFIS was used as one of the fuzzy model and gave the best performance in other fuzzy models.

Castillo and Melin (2001) used an ANFIS methodology in electrochemical process. The problem in battery manufacturing was to find how much the current could be increased without causing battery to explode due to the increase in temperature and at the same time minimizing the time of loading. Since ANFIS can be used to adapt the membership functions and consequents of the rule base according to the historical data of the problem, ANFIS was used as fuzzy controller in this research. Fuzzy logic toolbox of MATLAB was used with 5 membership functions and first orders Sugeno function in the consequents. ANFIS controller input and output were temperature and electrical current, respectively. They found that, the ANFIS methodology gave better results than manual, conventional and fuzzy control methods.

CHAPTER 3

STRUCTURES OF ARTIFICIAL INTELLIGENCE SYSTEMS

In this chapter, the theoretical background and structures for artificial intelligence systems will be given. Characteristics of NNs and the theory of fuzzy logic will be presented. Also, the structure of ANFIS will be explained in detail.

3.1 NEURAL NETWORKS (NN)

Basic characteristics of NNs will be summarized in this section. First, a neuron model and architecture of NN will be described. After that, learning in NNs will be explained. Also, adaptive network will be given as an example of NN with backpropagation and hybrid learning algorithms.

3.1.1 Models of Neuron

A neuron is a special nervous cell in organisms, which have electric activity. These cells are mainly intended for the operation of the organism. The biological neuron is shown schematically in Figure 3.1 . A neuron consists of a cell body, which is surrounded by a membrane. The neuron has dendrites and axons, which are its inputs and outputs of neuron. Axons of neurons join to dendrites of other neurons by forming synaptic contacts (synapses).

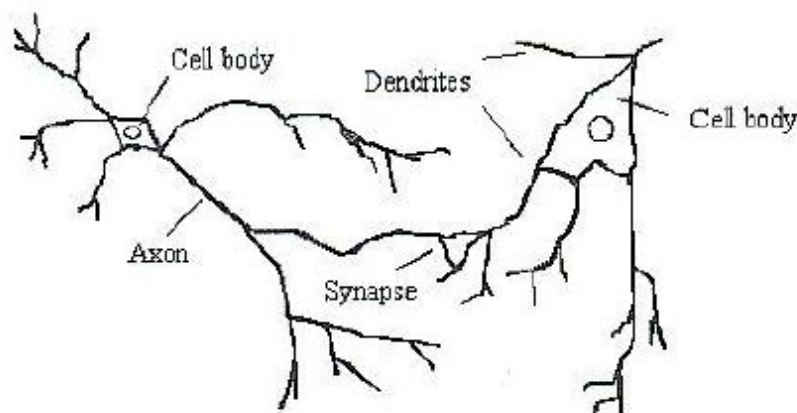


Fig 3.1 Biological neuron

Input signals of the dendrite tree are weighted and added in the cell body and formed in the axon, where the output signal is generated. The signal's intensity, consequently, is a function of a weighted sum of the input signal. The output is passed through the branches of the axon and reaches the synapses. Through the synapses the signal is transformed into a new input signal for neighbor neurons. The input signal can be either positive or negative (exciting or inhibiting), depending on the synapses.

In accordance with the biological model, different mathematical models were suggested. The mathematical model of the neuron, which is usually utilized under the simulation of NN, can be shown in Figure 3.2. The neuron receives a set of input signals x_1, x_2, \dots, x_n (vector X) which are usually the output signals of other neurons. Each input signal is multiplied to a corresponding connection weight, w , and analogue of the synapse's efficiency. Weighted input signals come to the summation module corresponding to cell body, where their algebraic summation is executed and the excitement level of neuron is determined:

$$I = \sum_{i=1}^n x_i w_i \tag{3.1}$$

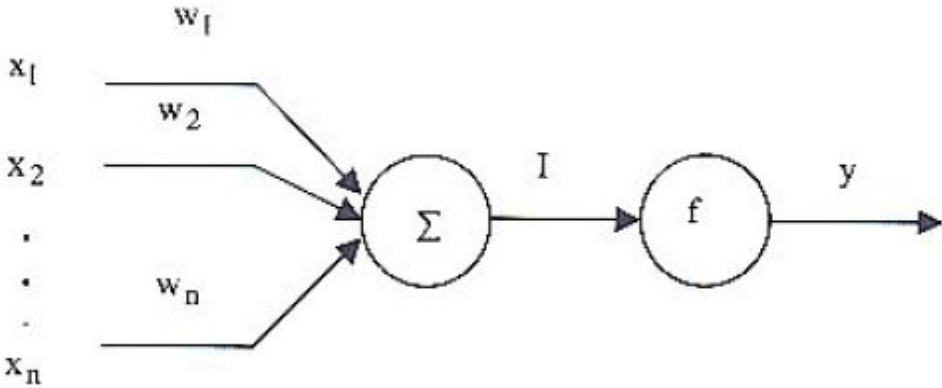


Fig3.2 Mathematical Neuron

The output signal of a neuron is determined by conducting the excitement level through the function f , called activation function as in Equation 3.2.

$$y = f(I) \tag{3.2}$$

The following activation functions can be utilized as function f:

Linear function

$$y = k.I, k = \text{constant} \quad 3.3$$

Binary (Threshold function)

$$y = \begin{cases} 1, & \text{if } I \geq \theta \\ 0, & \text{if } I < \theta \end{cases} \quad 3.4$$

Sigmoid function

$$y = \frac{1}{1 + (e)^{-I}} \quad 3.5$$

3.1.2 Architectures of Neural Networks

The totality of the neurons, connected with each other and with the environment, forms the NN. Figure 3.3 shows the basic structure of the neural network. The input vector comes to the network by activating the input neurons. A set of input signals of a network's neurons is called the vector of input activeness. Connection weights of neurons are represented in form of matrix W, element w_{ij} of which is the connection weight between i-th and j-th neurons. During the network functioning process, the input vector is transformed into output one, i.e. some information processing is performed. The computational power of the network, thus, solves problems with its connections. Connections link inputs of one neuron with output of others. The connection strengths are given by weight coefficients. NN can also consist a bias term, which acts on a neuron like an offset. The function of the bias is to provide a threshold for the activation of neurons. The bias can be connected all neurons in network.

NNs can be divided into two types of architectures: feedforward networks and recurrent NNs.

Feedforward networks have no feedback connections. In this type of network, neurons of the j-th layer receive signals from environment (when j=1) or the neurons of previous the (j-1)-th layer

when $(j>1)$ and pass their outputs to neurons of the next $(j+1)$ -th layer to the environment (when j is the last layer). Feedforward networks can be single-layer or multi-layer. Multilayer NNs

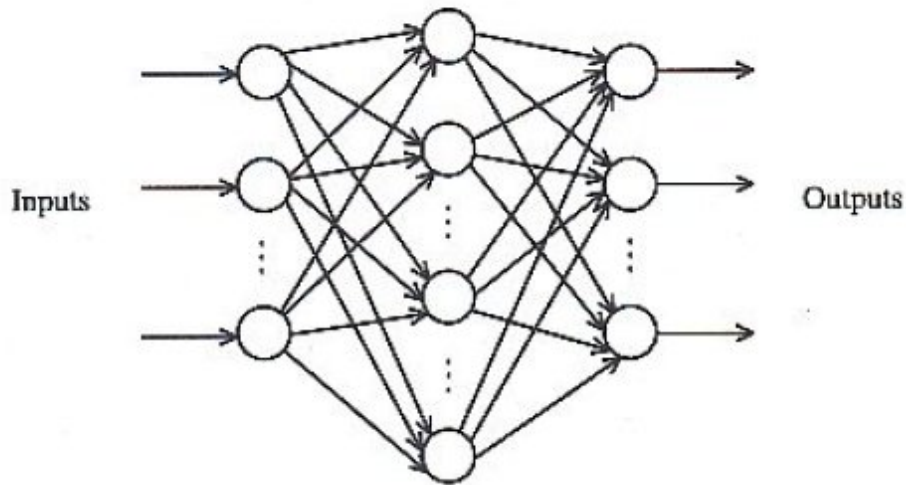


Fig 3.3 Basic structure of Neural Network

consist of input, output and hidden layer. The use of hidden layers allows an increase in the computational power of the network. Choosing the optimal structure of a network provides an increase in reliability and computational power, and a decreased processing.

Recurrent neural networks have structures similar to standard feedforward NN with layers of nodes connected via weighted feed-forward connections, but also include time delayed feedback or recurrent connections in the architecture. The important advantage of the RNN is the ability to approximate a continuous or discrete nonlinear dynamic system by neural dynamics defined by a system of nonlinear differential equations. This offers the opportunities for applications to adaptive control problems.

3.1.3 Learning in Neural Networks

Generally, learning is the process by which the NN adapts itself to a stimulus, and eventually it produces a desired response. It is also a continuous classification process of input stimuli: when a stimulus appears at the network, the network either recognizes it or it develops a new classification. Actually, during the process of learning, the network adjusts its parameters, the

synaptic weights, in response to an input stimulus so that its actual output response converges to the desired output response. When the actual output response is the same as the desired one, the network has completed the learning phase. Learning rules for networks are described by mathematical expressions called learning equations. The neurons in NNs may be interconnected in different ways; however, the learning process is not same for the all. It is known that, different learning methodologies suit different people. Like this, different learning techniques suit different NNs. There are two general categories of learning in NNs, supervised and unsupervised learning.

In supervised learning, both the input and the actual response and the desired response are available and are used to formulate a cost (error) measure. If the actual response differs from the target response, the NN generates an error signal, which is then used to calculate the adjustment that should be made to the network's weights so that actual output matches the target output .

Unlike supervised learning, there is no target output in unsupervised learning. During the training period, the network receives at its input many different input patterns and it arbitrarily organizes the pattern into categories. When a stimulus is later applied, the network provides an output response indicating the class to which the stimulus belongs. If a class cannot be found for the stimulus, a new class is generated. This type of learning sometimes referred to as self-organizing learning.

3.1.4 Adaptive networks

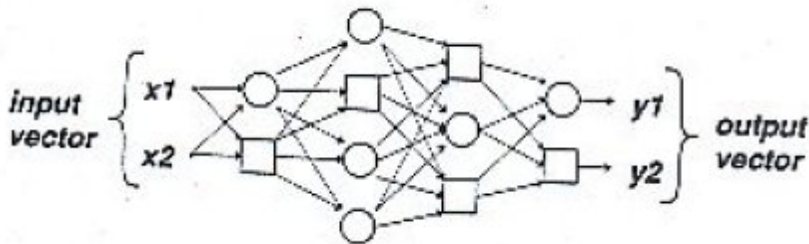


Fig 3.4 Adaptive Network

An adaptive network (Figure 3.4) is an example of multilayer feedforward NN in which each node performs a particular function (node function) on incoming signals as well as a set of parameters pertaining to this node. The formulas for the node functions may vary from node to

node, and the choice of each node function depends on the overall input-output function, which the adaptive network is required to carry out. The links in an adaptive network only show the flow direction signals between nodes. No weights are associated with the links .

The basic learning rule of adaptive networks is the backpropagation learning rule. However, since it is slow and tends to become trapped in local minima, a hybrid learning rule algorithm was proposed to speed up the learning algorithm.

3.2 FUZZY LOGIC SYSTEMS

This section presents general information about the theory of fuzzy logic. Definition of a fuzzy set and linguistic variable conception are presented. The meaning of a fuzzy rule is explained and some rule examples are given. Fuzzy reasoning mechanism and fuzzy inference systems are also presented.

3.2 .1 Fuzzy set

A “fuzzy set” is a simple extension of the definition of a classical set in which the characteristic function is permitted to have any values between 0 and 1 (Castillo and Melin 2000). A “fuzzy set” A in X can be defined as a set of ordered pairs:

$$A = \{(x, \mu_A(x)|x \in X\} \quad 3.14$$

where $\mu_A(x)$ is called membership function for the fuzzy set A . It maps each x to a membership grade between 0 and 1. Examples of membership functions (Triangular, Trapezoidal and Gaussian) can be seen in Figure 3.5 and described with the following formulas:

Triangular MFs (3.15):

$$triangle(x; a, b, c) = \begin{cases} 0, & x \leq a \\ (x - a)/(b - a), & a \leq x \leq b \\ (c - x)/(c - b), & b \leq x \leq c \\ 0, & c \leq x \end{cases}$$

Trapezoidal MFs (3.16):

$$\text{trapezoidal}(x; a, b, c, d) = \begin{cases} 0, & x \leq a \\ (x-a)/(b-a), & a \leq x \leq b \\ 1, & b \leq x \leq c \\ (d-x)/(d-c), & c \leq x \leq d \\ 0, & d \leq x \end{cases}$$

Gaussian MFs (3.17):

$$\text{gaussian}(x; c, \sigma) = e^{\frac{-(x-c)^2}{2\sigma}}$$

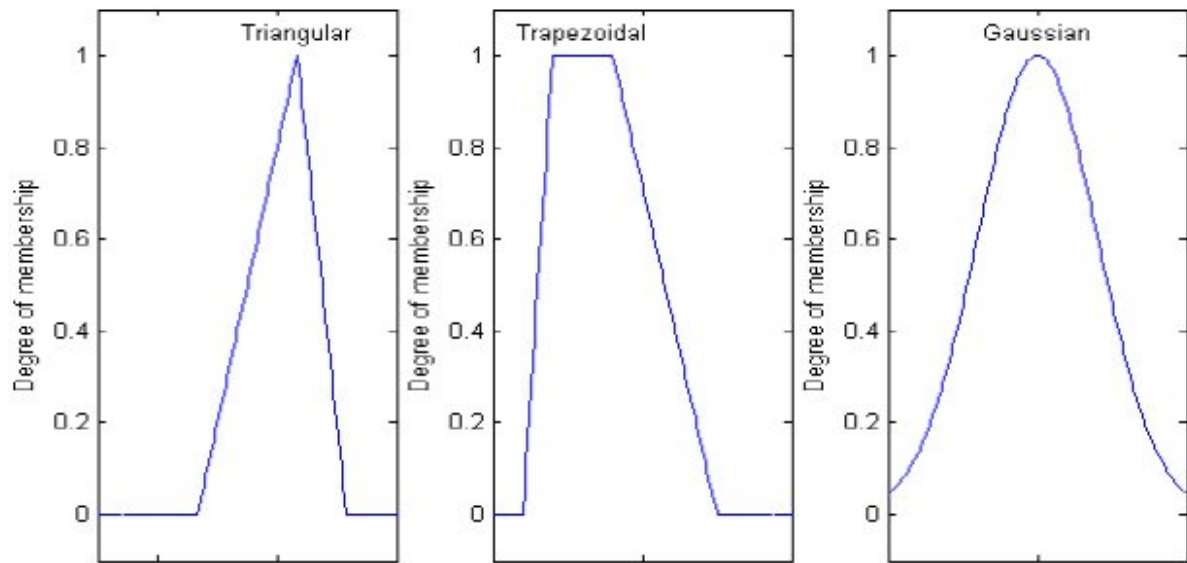


Fig 3.5 Examples of membership functions

3.2 .2 Linguistic Variables

The concept of linguistic variables was introduced by Zadeh (1973) to provide a basis for approximate reasoning. A linguistic variable was defined as a variable whose values are words or sentences. For instance, Age can be linguistic variable if its values are linguistic rather than numerical, i.e., young, very young, old, very old, etc., rather than 20, 21, 23, 45.... Figure 3.6 illustrates the term set Age expressed by the Gaussian MFs.

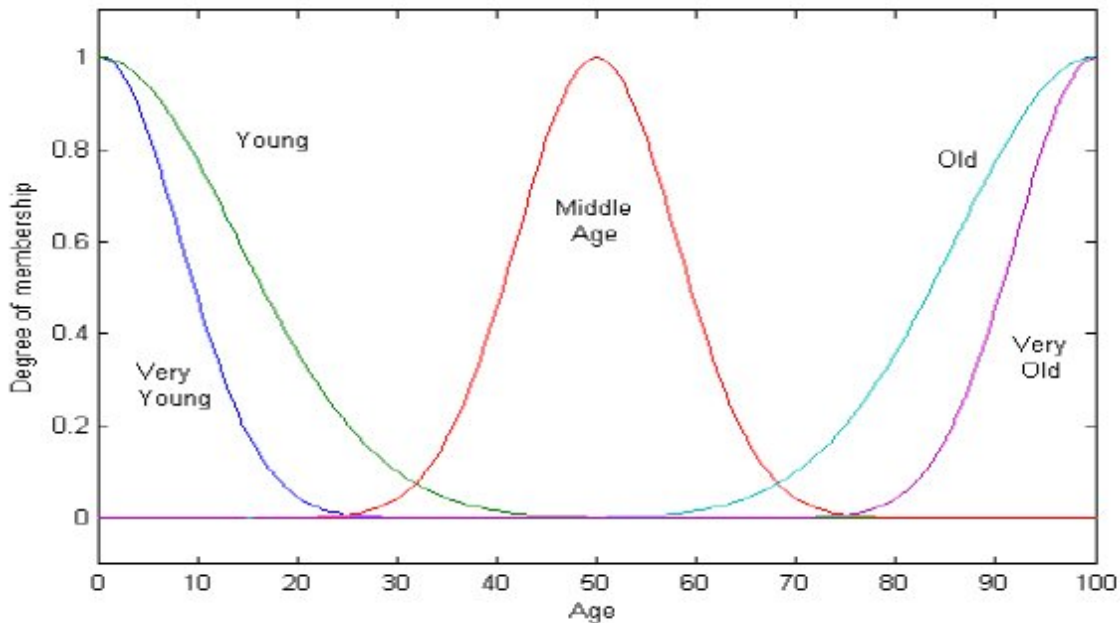


Fig 3.6 Membership functions of the term set Age

3.2 .3 Fuzzy if then Rules

A fuzzy if-then rule (fuzzy rule, fuzzy implication, or fuzzy conditional statement) is expressed as follow:

If x is A then y is B

where A and B linguistic values defined by fuzzy sets. “x is A” is called “antecedent” or “premise”, while “y is B” is called the “consequence” or “conclusion”.

Some of the if-then rule examples can be given below:

- If pressure high, then volume is small.
- If the speed is low AND the distance is small, then the force on brake should be small.

3.2.4 Fuzzy Systems

Fuzzy systems are made of a knowledge base and reasoning mechanism called fuzzy inference engine. The structure of fuzzy inference engine is shown in Figure 3.7. A fuzzy inference engine combines fuzzy if-then rules into a mapping from the inputs of the system into its outputs, using fuzzy reasoning methods. That is, fuzzy systems represents nonlinear mapping accompanied by fuzzy if-then rules from the rule base. Each of these rules describes the local mappings. The rule base can be constructed either from human expert or automatic generation that is extraction of rules using numerical input-output data.

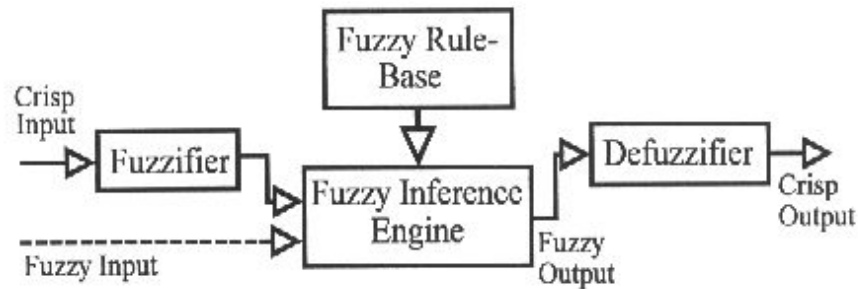


Fig 3.7 Fuzzy Inference Engine

Mamdani and Takagi-Sugeno fuzzy systems are the examples of fuzzy inference systems. Mamdani fuzzy inference system was first used to control a steam engine and boiler combination by a set of linguistic rules obtained from human operators. Figure 3.8 illustrates how a two rule Mamdani fuzzy inference system derives the overall output z when subjected to two numeric inputs x and y . Takagi-Sugeno fuzzy inference system was first introduced by Takagi and Sugeno. The difference of Takagi- Sugeno model is that each rule has a crisp output, and the overall output is determined as weighted average of single rules output. This type of fuzzy inference system is shown in Figure 3.8

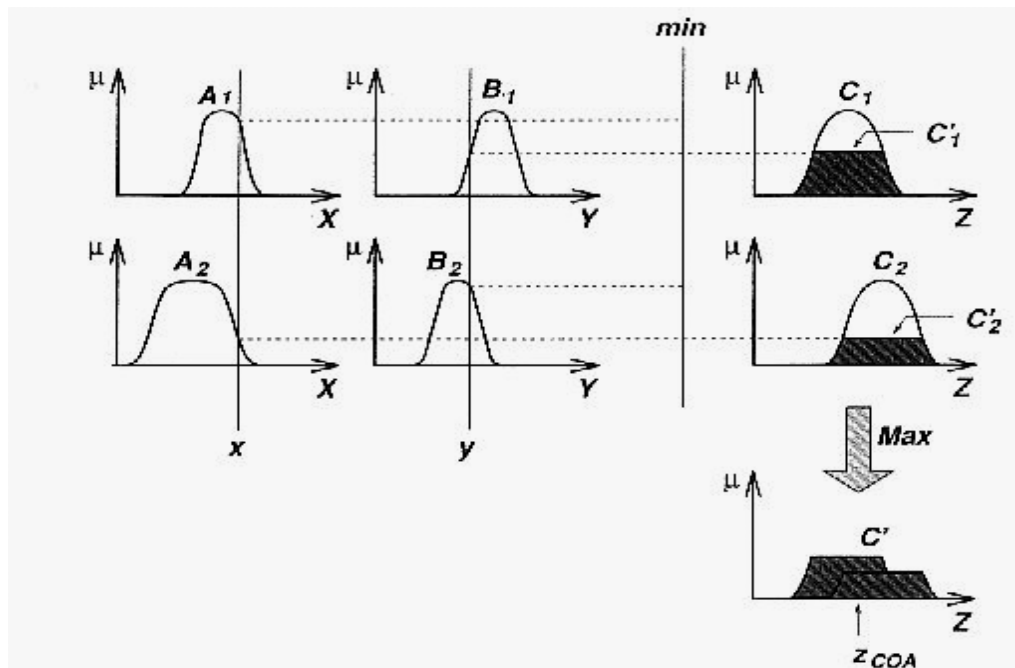


Fig 3.8 Mamdani Fuzzy Inference System

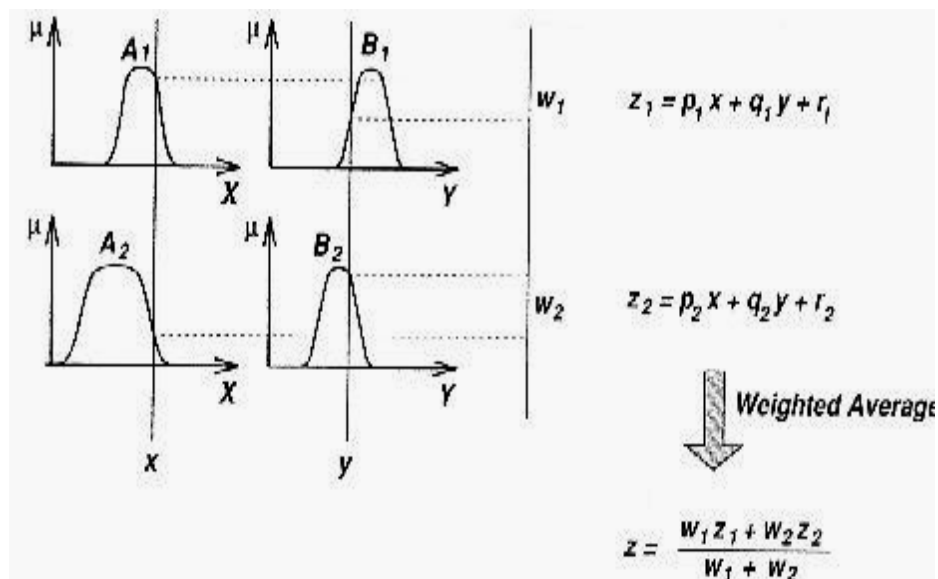


Fig 3.9 Takagi-Sugeno Fuzzy Inference System

3.3 ANFIS

As previously stated, ANFIS is an adaptive network that is functionally equivalent to fuzzy inference system, and referred in literature as “adaptive network based fuzzy inference system” or “adaptive Neuro fuzzy inference system”.

3.3.1 ANFIS architecture

In ANFIS, Takagi-Sugeno type fuzzy inference system is used. 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. Basic ANFIS architecture that has two inputs x and y and one output z is shown in Figure 3.10. The rule base contains two Takagi-Sugeno if then rules as follows:

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 $f_2 = p_2x + q_2y + r_2$

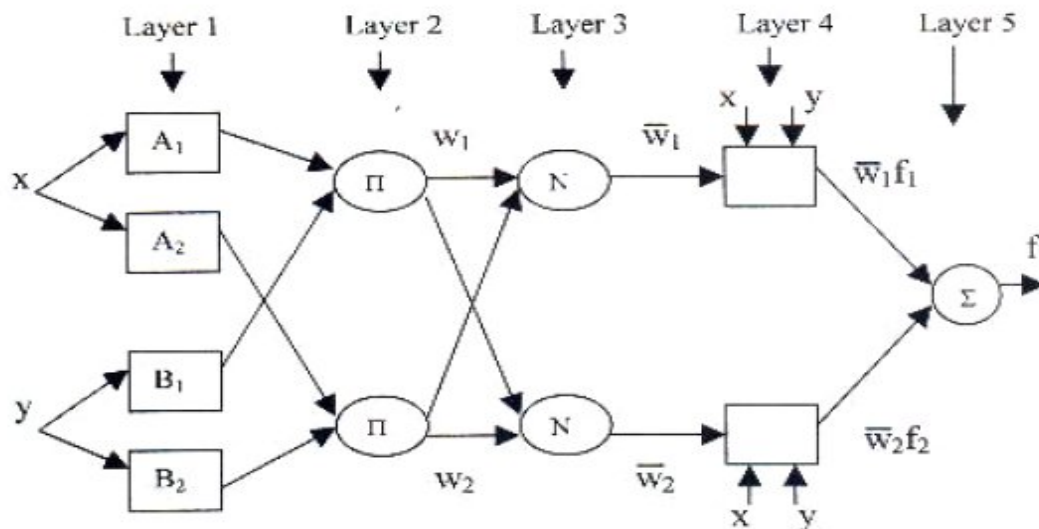


Fig 3.10 Basic structure of ANFIS

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

Layer 1: Every node i in this layer is a square node with a node function as (3.18):

$$\begin{aligned} O_{1,i} &= \mu_{A_i}(x), \quad \text{for } i=1,2 \\ O_{1,i} &= \mu_{B_{i-2}}(y), \quad \text{for } i=1,2 \end{aligned}$$

where x is the input to node i , and $i A$ (or $i-2 B$) is a linguistic label (such as “small” or “large”) associated with this node. In other words, $O_{1,i}$ is the membership grade of a fuzzy set A and it specifies the degree to which the given input x satisfies the quantifier A . The membership function for A can be any appropriate membership function, such as the Triangular or Gaussian. When the parameters of membership function changes, chosen membership function varies accordingly, thus exhibiting various forms of membership functions for a fuzzy set A . Parameters in this layer are referred to as “premise parameters”.

Layer 2: Every node in this layer is a fixed node labeled as Π , whose output is the product of all incoming signals (3.19):

$$O_{2,i} = w_i = \mu_{A_i}(x)\mu_{B_i}(y), \quad i=1,2$$

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 (3.20):

$$O_{3,i} = w_i = w_i / (w_1 + w_2), \quad i=1,2$$

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 (3.21):

$$O_{4,i} = \overline{w}_i f_i = \overline{w}_i (p_i x + q_i y + r_i)$$

where w_i is a normalized firing strength from layer 3 and $\{p_i, q_i, r_i\}$ is the parameter set of this node. Parameters in this layer are referred to as “consequent parameters”.

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 (3.22)

$$\text{overall output} = o_{5,i} = \sum_i \bar{w}_i f_i = \frac{\sum_i w_i f_i}{\sum_i w_i}$$

Thus an adaptive network, which is functionally equivalent to the Takagi- Sugeno type fuzzy inference system, has been constructed. Other example of ANFIS with nine rules can be shown in Figure 3.11. Three membership functions are associated with each input, so the input space partitioned into nine fuzzy subspaces. The premise part of a rule describes a fuzzy subspace, while the consequent part specifies the output within this fuzzy subspace.

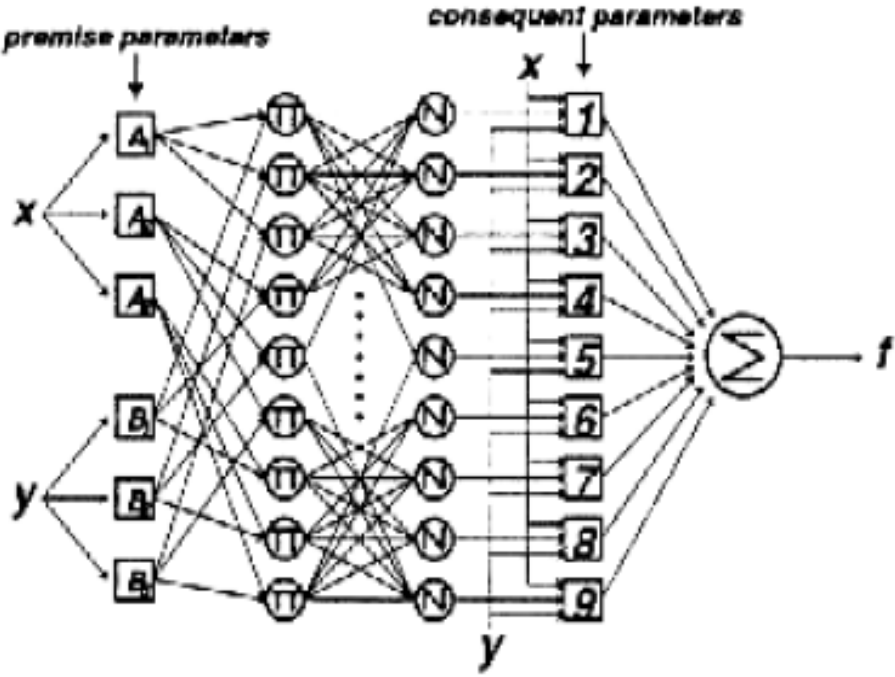


Fig 3.11 ANFIS Architecture with nine rule

CHAPTER 4

ANFIS DESIGN AND CASE STUDIES

In this study, as a continuation of previous studies done by Bahar (2003), and Yildiz (2003), the aim is to use the ANFIS methodology, a hybrid structure, in the estimation of compositions using tray temperatures in continuous and batch distillation columns. The performance of the ANFIS estimator is compared with the performance of the NN and Extended Kalman Filter (EKF) estimators. In this chapter, the design of ANFIS architecture for the estimation and control purposes will be explained. Also, the case studies used for the applications will be presented.

4.1 DESIGN OF ANFIS

The basic idea behind the neuro-adaptive learning techniques is very simple. These techniques provide a method for the fuzzy modeling procedure to learn information about data set, in order to compute the membership function parameters that best allow the associated fuzzy inference system to track the given input-output data. ANFIS constructs an input-output mapping based on both human knowledge (in the form of fuzzy if-then rules) and simulated input output data pairs. It serves as a basis for building the set of fuzzy if-then rules with appropriate membership functions to generate the input output pairs.

The parameters associated with the membership functions are open to change through the learning process. The computation of these parameters (or their adjustment) 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, described in the previous chapter, can be applied in order to adjust the parameters.

As stated previously, ANFIS can be used in modeling, estimating and controlling studies in chemical engineering processes similar to other artificial intelligence methods such as NNs and Fuzzy Logic (FL). In this work, the designed ANFIS is utilized as an estimator. Estimation is done for compositions from the temperature measurements in continuous and batch distillation columns.

4.1.1 ANFIS as an Estimator

ANFIS can be used for the estimation of some dependent variables in chemical process. The designed ANFIS estimator is used to infer the compositions from measurable tray temperatures in batch and continuous distillation columns. Estimation scheme is shown in Figure 4.1. In estimator design process, different ANFISs are constructed and trained to find the architecture that gives the best performance as an estimator.

In order to design an estimator, first, training data sets should be generated to train the estimator networks. These data sets consist of estimator inputs and desired output values. They are produced from the process input output data. Since, ANFIS is a data processing method, it is important that the input-output data must be within the sufficient operational range including the maximum and minimum values for both input and output variables of the system. If this is not provided, estimator performance cannot be guaranteed and thus the designed estimator will not be accurate. Having generated the training data, estimators that have different architectures are trained with the obtained data sets.

Performances of the trained estimators are evaluated with model simulations and best estimator architecture is obtained. These simulations are made to verify and to generalize the ANFIS structures. Verification is done to show how good the estimator structure learned the given training data. This is carried out by simulating the column models with specific initial process inputs used in obtaining training data sets. Generalization capabilities of the estimators are found with other simulations in which input process variables are in operational range but not used in training data formation.

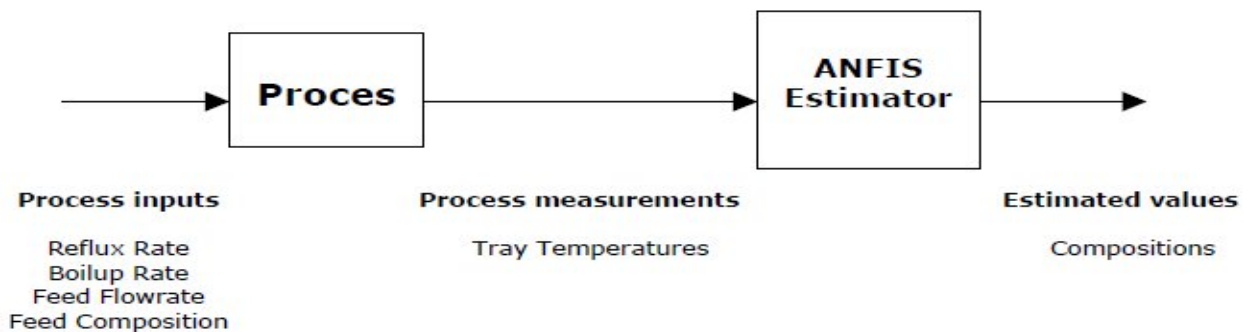


Fig 4.1 Estimation using ANFIS estimator

ANFIS estimator design consists of two parts: constructing and training. In constructing part, structure parameters are determined. These are type and number of input Membership Functions (MFs), and type of output MF. Any of several MFs such as Triangular, Trapezoidal and Gaussian can be used as an input MF. Frequently used MFs in literature are the Triangular and Gaussian. For this reason, they are chosen as input MF type in this study. Number of MFs on each input can be chosen as 3, 5, and 7 to define the linguistic labels significantly. Effective partition of the input space is important and it can decrease the rule number and thus increase the speed in both learning and application phase. Output MFs can be either a constant or in linear form. Both of these two forms are used for the output MF in this study. Having described the number and type of input MFs, the estimator rule base is constituted. Since, there is no standard method to utilize the expert knowledge; automatic rule generation (grid partition) method is usually preferred. According to this method, for instance, an ANFIS model with two inputs and three MFs on each input would result in $3^2=9$ Takagi-Sugeno fuzzy if-then rules automatically. Although this method can require much computational knowledge especially in systems that have to be defined with many inputs, it is used in this study due to advantage of MATLAB software. Therefore, rule bases of the estimators are formed automatically with the number of inputs and number of MFs. After the ANFIS structure is constructed, learning algorithm and training parameters are chosen. As mentioned in the previous chapter, backpropagation or hybrid learning can be used as a learning algorithm. The hybrid learning algorithm is used in this study. Parameters in the algorithm are epoch size (presentation of the entire data set), error tolerance, initial step size, step size decrease rate, and step size increase rate. Since there is no exact method in literature to find the optimum of these parameters a trial and error procedure is used. In all trainings, they are taken as 10, 1×10^{-5} , 0.01, 0.9, and 1.1, respectively as default constant value as proposed in MATLAB.

MATLAB fuzzy logic toolbox is used to design ANFIS estimators' structures. The toolbox constructs an ANFIS structure using either a backpropagation algorithm alone, or in combination with least squares type of method (hybrid algorithm). ANFIS model can be generated either from the command line, or through the ANFIS GUI. In this study, ANFIS is used to generate the ANFIS models with the chosen design parameters in construction phase.

4.2 CASE STUDIES

In this section, the cases in which ANFIS methodologies are implemented will be given. In the first part, the multicomponent industrial continuous distillation column will be described. The case of batch distillation column will be given in the second part.

4.2.1 Industrial Continuous Distillation Column

The industrial continuous distillation column used in this study is C3-C4 Splitter column. presents the sketch of the column. A mixture of propane, i-butane, n-butane, and i-pentane enters the column from the 22nd tray and propane and n-butane are separated as a top and bottom product, respectively. Top product composition purity is controlled by manipulating the reflux flow rate. The bottom product purity is controlled by measuring the temperature of the bottoms and manipulating the steam flow rate to the reboiler. Liquid heights in the column bottom and receiver drum are controlled by adjusting the bottoms and liquid distillate flow rates, respectively. The pressure in the column is controlled by manipulating the overhead vapor flow rate to the receiver drum. Design parameters and the operating data of the column are given in Table 4.1.

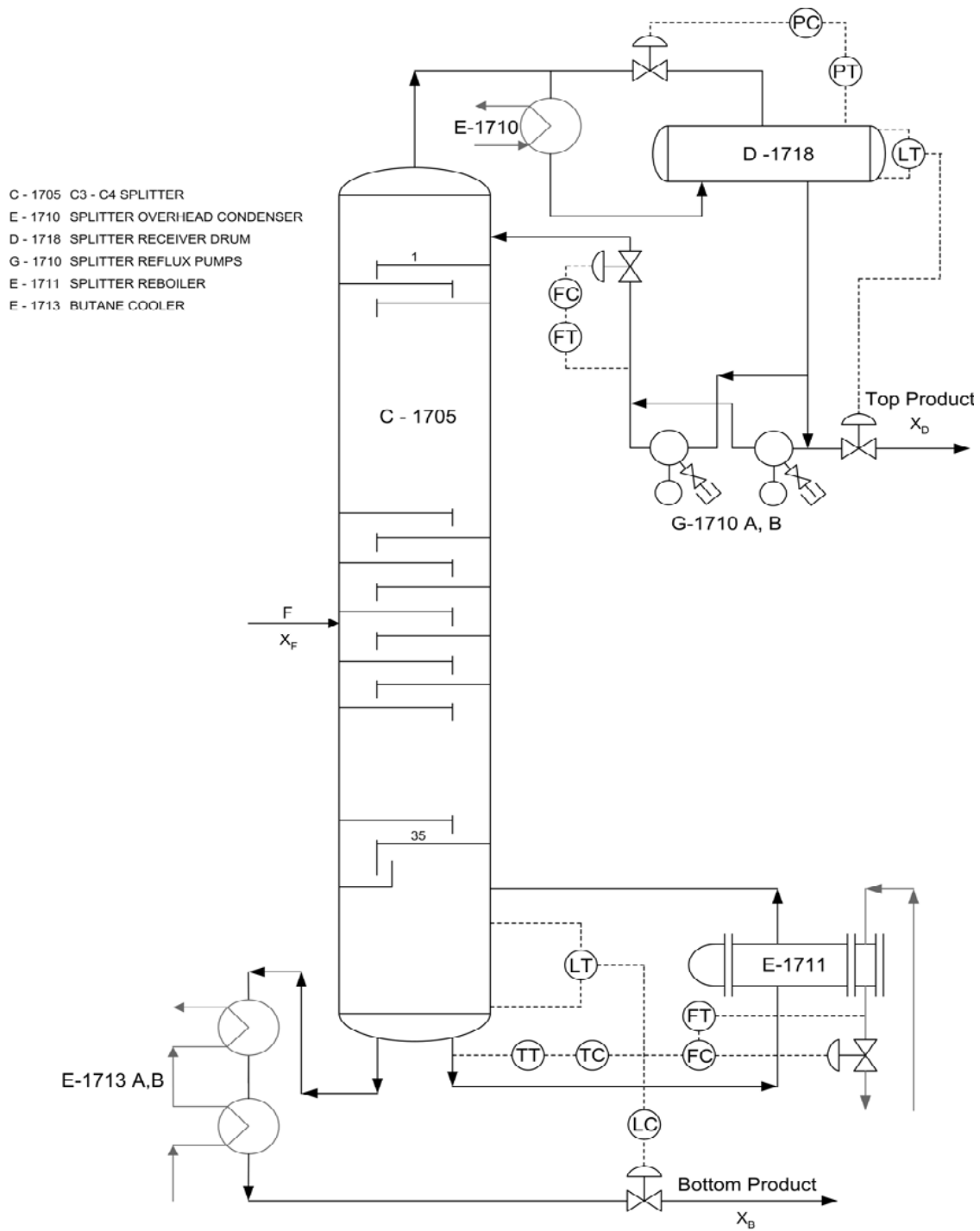


Fig 4.2 splitter column

Table 4.1 Plant Data

Column Specifications

Number of Trays	35
Column Inside Diameter	1000 mm
Tray Spacing	600 mm
Weir Length	880 mm
Weir Height	50 mm
Maximum Capacity (% of nominal design)	110 %
Minimum Capacity (% of nominal design)	50 %

Feed Condition

Feed Rate	118.53 kmol/hr
Feed Pressure	18.04 bar
Feed Temperature	84 °C
Feed Composition (mole fraction)	
Propane	0.3933

i-Butane	0.2384
n-Butane	0.3678
i-Pentane	0.0005

Operational Values (Design)

Maximum Pressure Drop for One Tray	5 mm Hg
Top Tray Pressure	16.18 bar
Bottom Tray Pressure	16.67 bar
Top Tray Temperature	48 °C
Bottom Tray Temperature	98 °C
Reflux Rate	161.51 kmol/hr
Distillate Rate	32.76 kmol/hr
Bottoms Rate	85.77 kmol/hr
Reboiler Duty	1930 MW

4.2.2 Batch Distillation Column

The batch distillation column simulated is used in the second study. Figure 4.6 illustrates the sketch of the batch column. This column separates a mixture of cyclo-hexane, n-heptane and toluene. Design parameters for the case column is given in Table 4.2. The column is under the perfect control of reflux drum level and reflux ratio (R) is used as the manipulated variable in order to realize the optimal operation policy recommended. In this policy, a switching time between R and shortcuts was optimized according to the minimization of the capacity factor.

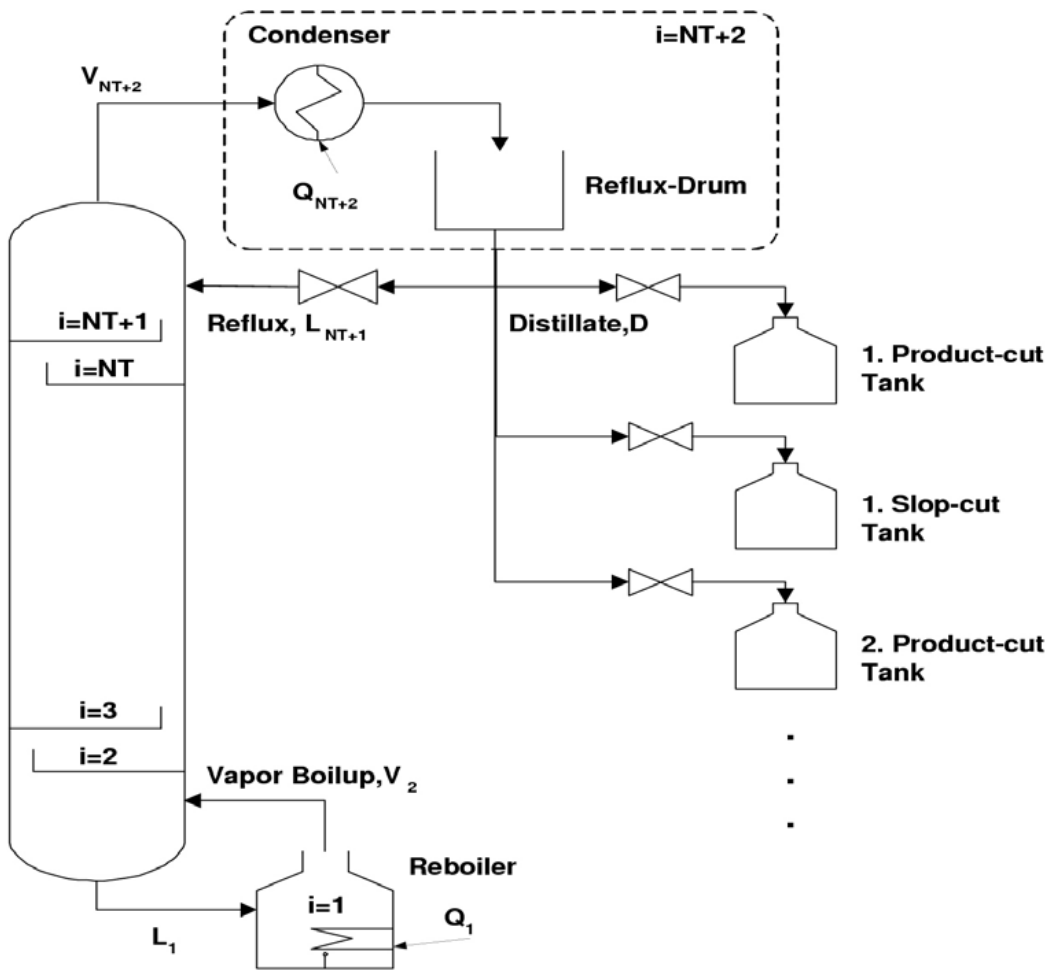


Fig 4.2 Batch Distillation Column

Table 4.2 Design parameters for the batch distillation column

Number of trays	8
Condenser-Reflux-Drum Holdup	0.02 kmol
Trays Holdup	0.01 kmol
Maximum Boil-up rate	2.75 kmol/h

Table 4.3 Optimal reflux ratio policy parameters

Amount of fresh feed	2.93 kmol
Feed composition:	
<i>cyclo-hexane</i>	0.407
<i>n-heptane</i>	0.394
<i>toluene</i>	0.199
Desired purity of comp. 1 in Product-cut 1	0.9
Desired purity of comp. 2 in Product-cut 2	0.8
Optimum Reflux Profile	
<i>Time Interval (hour) Reflux Ratio</i>	
0-2.04	0.875

2.04-3.4	0.911
3.4-6.17	0.933
6.17-6.51	0.831
6.51-8.35	0.876

CHAPTER 5

RESULTS AND DISCUSSIONS

In this study, the aim is to design ANFIS architectures for chemical processes in estimation problems and to see their performances. For this purpose, ANFIS architecture is applied to batch and continuous distillation columns to estimate the compositions from measured tray temperatures.

In this chapter, simulation results will be given and be discussed in detail. Design and implementations of ANFIS estimators will be demonstrated

5.1 ESTIMATION IN CONTINUOUS DISTILLATION COLUMN

In the continuous distillation column for estimation purposes, two parallel ANFIS estimators are designed to estimate the top (propane) and bottom (butane) product compositions from tray temperatures. Static mapping of the compositions from the temperatures are achieved using the ANFIS estimators. This is performed in four phases. In the first phase, estimators' inputs are selected. Then, in the second phase, training data sets are generated. Estimator structures are trained in the third phase. And, in the last phase, simulations are done to obtain the results for performance evaluations.

5.1.1 Selection of Estimator Inputs

In estimators, estimation accuracy can be easily affected from the inputs behavior. Also estimator performance depends strongly on the number of inputs. For these reasons, selection of the inputs is a critical issue in estimator design process.

Bahar (2003) designed NN estimator for the continuous distillation column under study to estimate the bottom and top compositions from temperatures and past composition values. According to this temperature measurements are needed for the composition estimation. Hence, three trays from top and three from bottom were found to estimate the top (propane) and bottom (butane) compositions. These are 31st, 32nd, and 33rd trays for the top, and 10th, 11th, and 12th trays for the bottom.

In this study, it is aimed to estimate the compositions only from temperature measurements. However, since ANFIS has a single output, only one of the product compositions can be estimated using the temperature values. There is no need to use past composition values as estimator inputs as NN needs. Also, as the number of measurements is increased as system inputs, structure complexity is increased which affects the convergence of the problem. Therefore, it is decided to use three-tray measurement for estimation process. Thus, by referring to the Bahar's study, 31st, 32nd, and 33rd trays are selected to estimate the top product (propane) composition and 10th, 11th, and 12th trays are selected to estimate the bottom product (butane) composition in the column. The estimation scheme for continuous distillation column is shown in Figure 5.1.

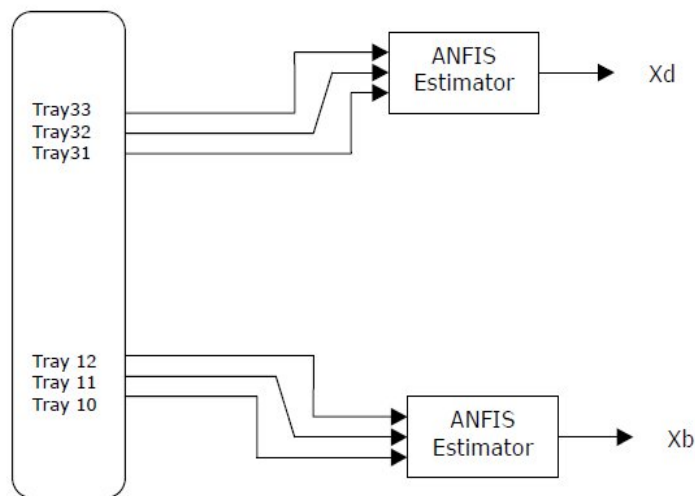


Fig 5.1 Estimation scheme for continuous distillation column

5.1.2 Generation of Training Data

If the operating input-output data are outside their training data range, estimator will not operate accurately. As a result, the training data set should possess sufficient operational range including the maximum and minimum values for input-output variables. The data set should include data for each process variable, evenly distributed throughout the range for which estimation is desired.

The maximum and minimum values of reflux and boil up rates in the column were determined by Bahar (2003) by looking at the closed-loop responses of the system without the estimator obtained by Dokucu (2002) to 10% increase in feed flow rate. This corresponds to approximately

maximum +7% change in the reflux rate, and maximum +5% change in the boil up rate. These are considered to be their maximum changes in operation. The percent changes for each process variable used in training data generation are shown in Table 5.1. Thus, model simulations are done to obtain the input-output data by using these values. Then, tray temperature values and corresponding top and bottom product compositions are collected. In training data sets (matrix of 4 columns), first three columns correspond to tray temperature values and the last column corresponds to composition values.

Table 5.1 Range of Process Variables

Process Variable	% changes
Reflux Rate, R	+1, +4, +7
Boilup Rate, Q	+1, +3, +5
Feed Flowrate, F	+1, +5, +10
Feed Composition, z_F	-1, -5, -10

5.1.3 Training of ANFIS estimators

Estimator structure design and training are realized as explained in the previous chapter using MATLAB software. First, generated training data is loaded using the GUI Editor. Then, with chosen design parameters, initial estimator structure is constructed. For example, if three triangular MFs are used for each input and constant output MF is chosen, GUI Editor determines the initial parameters of triangular MFs automatically using loaded data and constructs the initial Tri3con (three triangular MFs for each input and constant output MF)ANFIS structure. Trainings of the structures are done by running the written code in MATLAB. This code is given in Appendix B.1. All structures are trained in the same way only by changing the training data. In the design of top product estimator, training data set corresponded to 31st, 32nd, and 33rd trays

temperatures and actual top product composition. In the bottom product estimator design, data set that includes 10th, 11th, and 12th trays' temperatures and actual bottom product composition.

5.1.4 Simulations results

After the training of the ANFIS structures, performances of estimators are investigated through the model for both the verification and generalization tests. These tests are made by utilizing the different estimator structures. The responses of the compositions to a 4% increase in reflux rate and a 5% increase in feed rate are obtained by simulations to verify the estimator's learning performances. Also, reflux rate and feed rate are increased by 5% and 7% respectively to see the generalization capabilities of the estimators. In all simulations, the Integral of the Absolute Error (IAE) scores for the error between the actual and estimated compositions are calculated as the performance criteria. Simulation results are given in Tables 5.2-5.5. Verification capabilities of the estimators can be followed considering the IAE scores giving how well these different estimator structures can generalize what they have learned.

Table 5.2 Verification: 5% increase in Feed Flowrate

Input MF	Number of input MF	Output MF	IAE score Top product Xd	IAE score Bottom product xb
Triangular	3	Constant	0	0
Triangular	3	Linear	0	0
Triangular	5	Constant	0	0
Triangular	5	Linear	0	0

Triangular	7	Constant	0	0
Triangular	7	Linear	0	0
Gaussian	3	Constant	0	0
Gaussian	3	Linear	0	0
Gaussian	5	Constant	0	0
Gaussian	5	Linear	0	0
Gaussian	7	constant	0	0
Gaussian	7	linear	0	0

Table 5.3 Verification: 4% increase in Reflux Rate

Input MF	Number of input MF	Output MF	IAE score Top product Xd	IAE score Bottom product xb
Triangular	3	Constant	0.00049	0.0038
Triangular	3	Linear	0.00017	0.0011
Triangular	5	Constant	0.00026	0.0035
Triangular	5	Linear	0.00015	0.0007

Triangular	7	Constant	0.00025	0.0032
Triangular	7	Linear	0.00019	0.0008
Gaussian	3	Constant	0.00172	0.0038
Gaussian	3	Linear	0.00014	0.0014
Gaussian	5	Constant	0.00037	0.0026
Gaussian	5	Linear	0.00012	0.0006
Gaussian	7	constant	0.00027	0.0021
Gaussian	7	linear	0.00048	0.0023

Table 5.4 Verification: 7% increase in feed flow Rate

Input MF	Number of input MF	Output MF	IAE score Top product Xd	IAE score Bottom product xb
Triangular	3	Constant	0	0
Triangular	3	Linear	0	0
Triangular	5	Constant	0	0
Triangular	5	Linear	0	0

Triangular	7	Constant	0	0
Triangular	7	Linear	0	0
Gaussian	3	Constant	0	0
Gaussian	3	Linear	0	0
Gaussian	5	Constant	0	0
Gaussian	5	Linear	0	0
Gaussian	7	constant	0	0
Gaussian	7	linear	0	0

Table 5.5 Generalization: 5% increase in Reflux rate

Input MF	Number of input M F	Output MF	IAE score Top product Xd	IAE score Bottom product xb
Triangular	3	Constant	0.0003	0.0124
Triangular	3	Linear	0.0001	0.0075
Triangular	5	Constant	0.0030	0.0290

Triangular	5	Linear	0.0004	0.0083
Triangular	7	Constant	0.0003	0.0054
Triangular	7	Linear	0.0004	0.0219
Gaussian	3	Constant	0.0018	0.0312
Gaussian	3	Linear	0.0013	0.0420
Gaussian	5	Constant	0.0036	0.0376
Gaussian	5	Linear	0.0014	0.0364
Gaussian	7	constant	0.0086	0.0543
Gaussian	7	linear	0.0032	0.0528

When investigating the generalization capabilities, it is seen from Table 5.4 that all structures give actual composition values when the system is disturbed by feed flow rate changes. Their performances are also very good in estimating the top product composition as reflux ratio changes. However, it is observed that predictions of Triangular structures are better considering the IAE scores than that of Gaussian structures for bottom product composition in reflux ratio changes. Table 5.5 shows that minimum IAE score for top product composition is achieved from the Tri3lin structure. For bottom product, although Tri7con, Tri5lin, and Tri3lin structures show almost similar performance, Tri7con structure has the minimum IAE score. Thus, Tri3lin structure can be selected as the estimator architecture for top product composition. Figure 5.2 illustrates the Tri3lin structure performance in terms of top and bottom product compositions

responses to 5% increase in reflux ratio. Performances of Tri7con and Tri5lin can be seen in Figure 5.3 and 5.4.

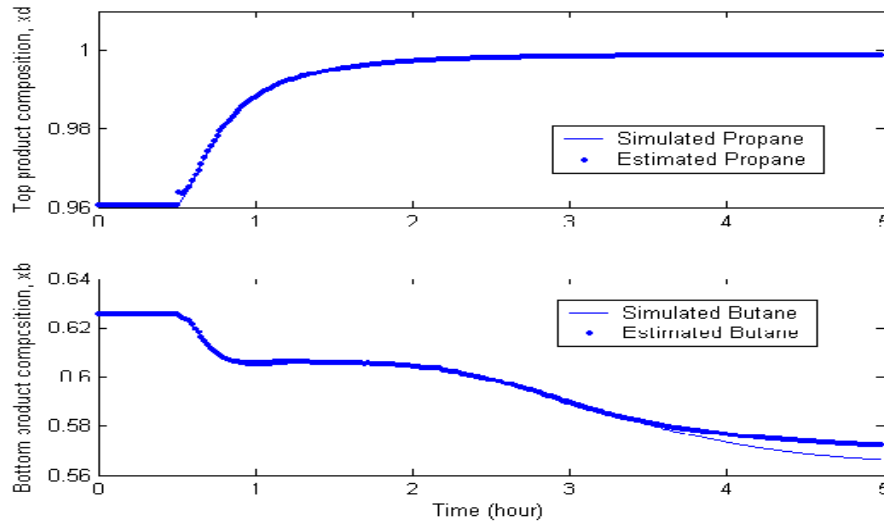


Fig 5.2 Tri3lin structure performance to 5% increase in reflux rate with the IAE scores 0.00014 and 0.0074 for top and bottom product

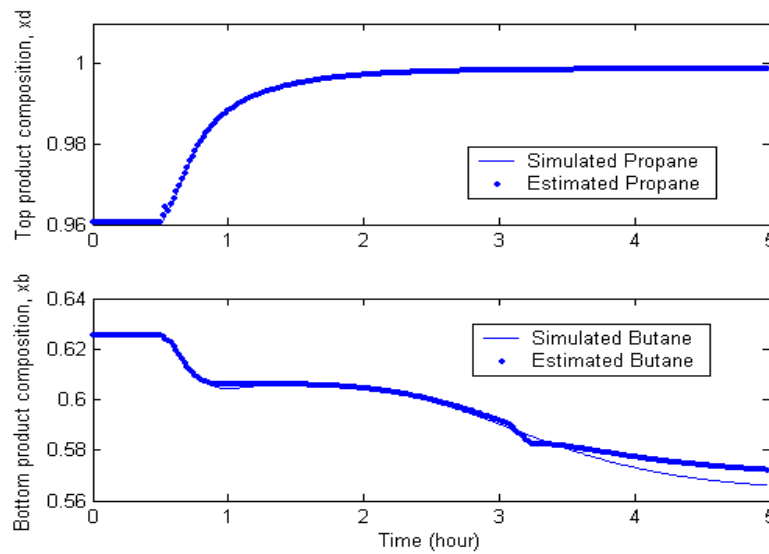


Fig 5.3 Tri5lin structure performance to 5% increase in reflux rate with the IAE scores 0.00044 and 0.0088 for top and bottom product

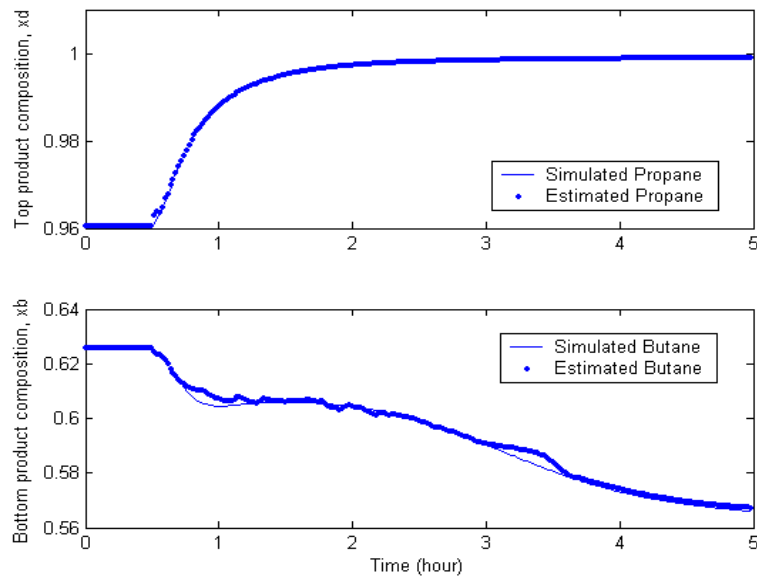


Fig 5.4 Tri7con structure performance to 5% increase in reflux rate with the IAE scores 0.00034 and 0.0054 for top and bottom product

It can be seen from the Figure 5.2 and 5.3 that structures with linear output show excellent performance up to 3.5 hours of response time. Tri3lin structure is somewhat better than Tri5lin structure. It is also found that defining of the inputs with many MFs do not improve performances of the structures that have linear output. However, in Figure 5.4, it is seen that that structure with seven MFs in input and with constant output results in good estimates for the steady state value with slight deviations from the actual values in short response time.

Therefore, in order to determine the estimator structures, another generalization simulation is made. The reflux ratio is increased by 3% and 6%, and then Tri3lin and Tri7con estimator performances are investigated. Figures 5.5-5.9 illustrate the performances of Tri3lin and Tri7con structures, respectively.

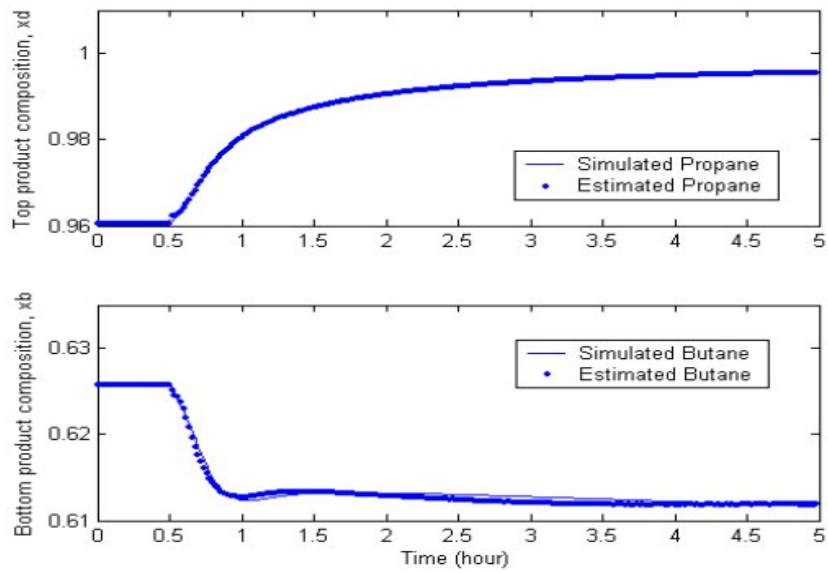


Fig 5.5 Tri3lin structure performance to 3% increase in reflux rate with IAE scores 0.0002 and 0.0018, for top and bottom product

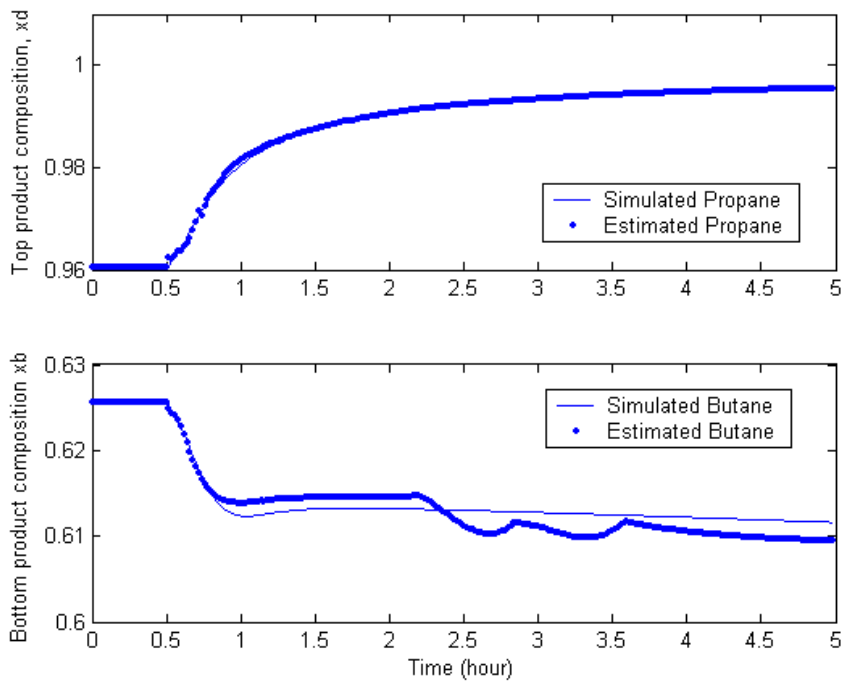


Fig 5.6 Tri7con structure performance to 3% increase in reflux rate with IAE scores 0.0008 and 0.0151, for top and bottom product

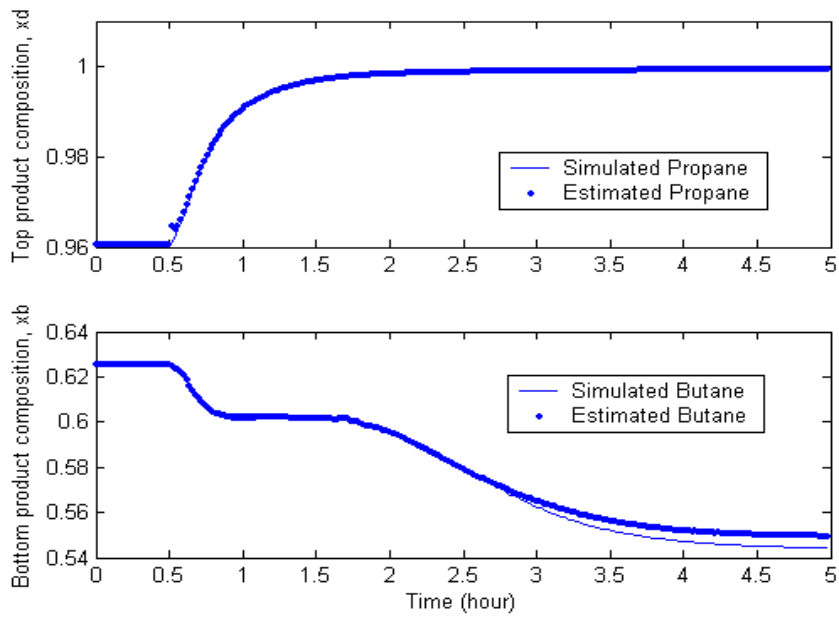


Fig 5.7 Tri3lin structure performance to 6% increase in reflux rate with IAE scores 0.00014 and 0.0108, for top and bottom product

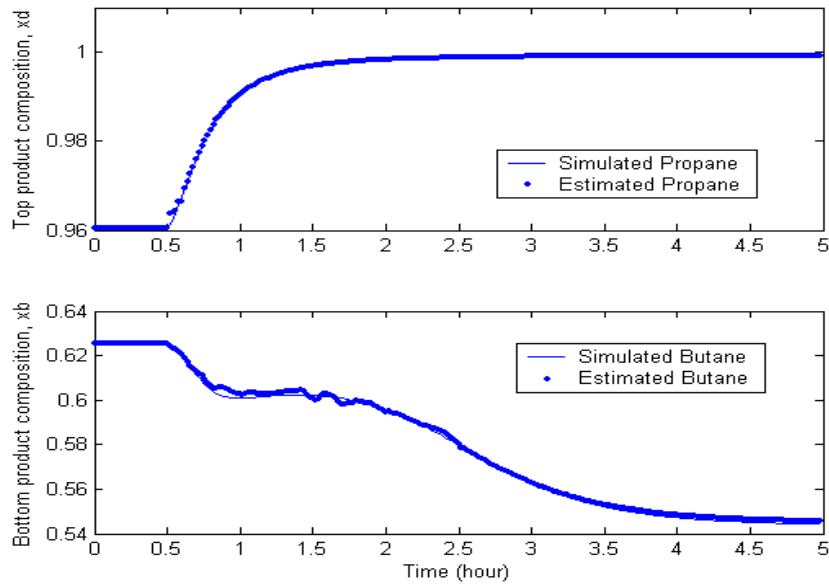


Fig 5.8 Tri7con structure performance to 6% increase in reflux rate with IAE scores 0.00032 and 0.00487, for top and bottom product

As can be seen from the Figures 5.5-5.9 and IAE scores, the Tri3lin structure performance is better to estimate the top product composition and is selected as the top product estimator. However, when the results are evaluated for bottom product composition Tri3lin and Tri7con structure's performances are similar. Although IAE scores of Tri7con structure are smaller in total, Tri3lin structure performance is very good up to 3 hours of response time. The Tri7con structure performance becomes also weak especially in small increase in reflux ratio. This can be seen in Figure 5.6 as the reflux ratio is increased by 3%.

In this study, Tri3lin and Tri7con structure performance are also evaluated for the other compositions in the column. It is seen from the Figures 5.9 and 5.10 that Tri3lin structure performance is very good for other compositions in the top of the column. Figures 5.11 to 5.14 show the structure's performances for the compositions in bottom. It can also be seen from the Figures 5.12 and 5.14 that Tri3lin structure performance is better than Tri7con structure for the i-butane composition in bottom. If the many training data are collected from the part of simulations after 3 hours, better learning of the Tri3lin structure can be achieved and thus estimator performance can be developed.

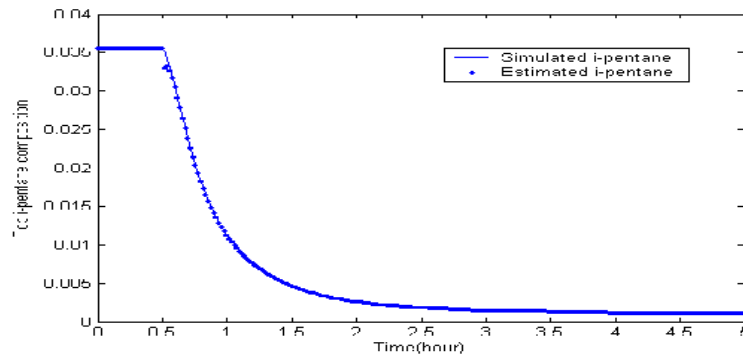


Fig 5.9 Tri3lin structure performance to 5% increase in reflux rate for the i-pentane composition in top with IAE score, 0.00012

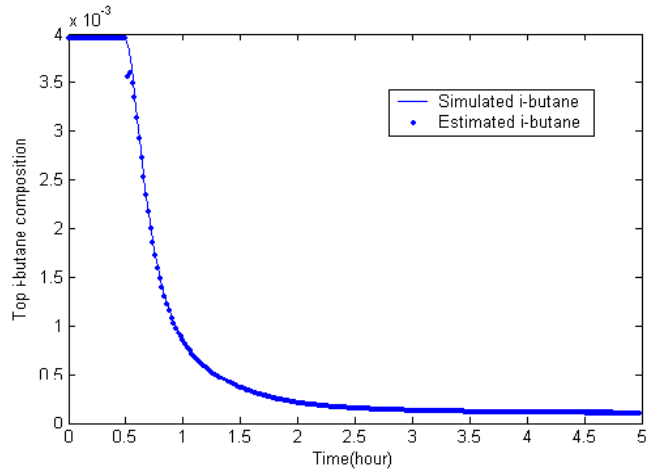


Fig 5.10 Tri3lin structure performance to 5% increase in reflux rate for the i-butane composition in top with IAE score, 0.00047

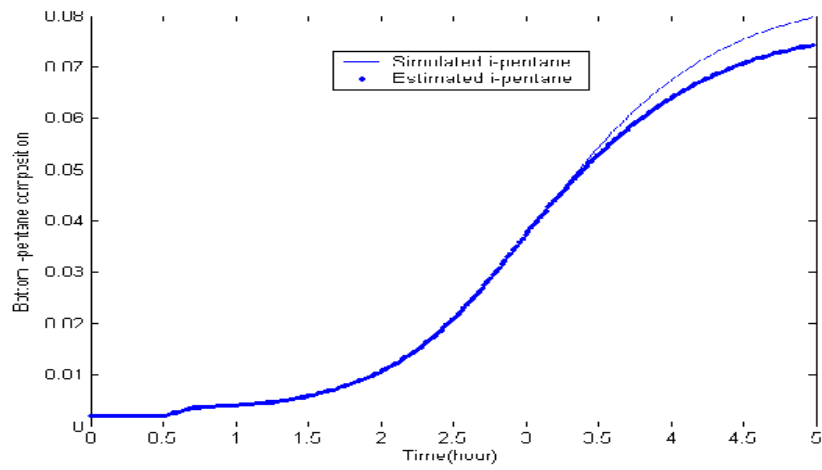


Fig 5.11 Tri3lin structure performance to 5% increase in reflux rate for the i-pentane composition in bottom with IAE score, 0.0065

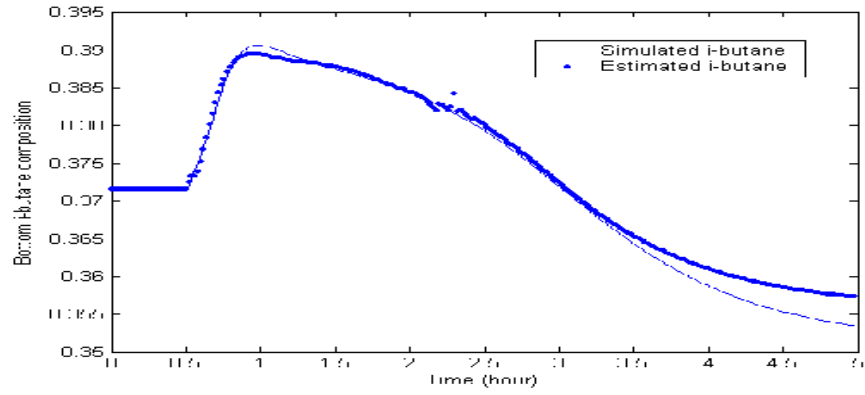


Fig 5.12 Tri3lin structure performance to 5% increase in reflux rate for the i-butane composition in bottom with IAE score, 0.0056

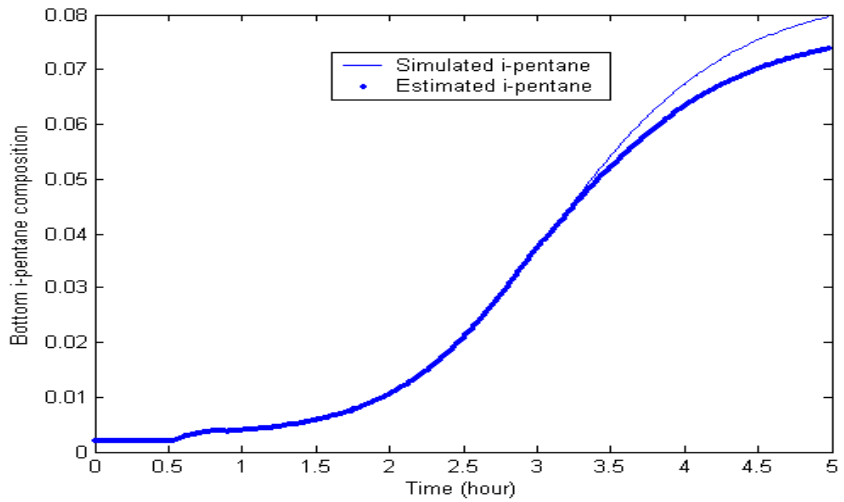


Fig 5.13 Tri7con structure performance to 5% increase in reflux rate for the i-pentane composition in bottom with IAE score 0.0075

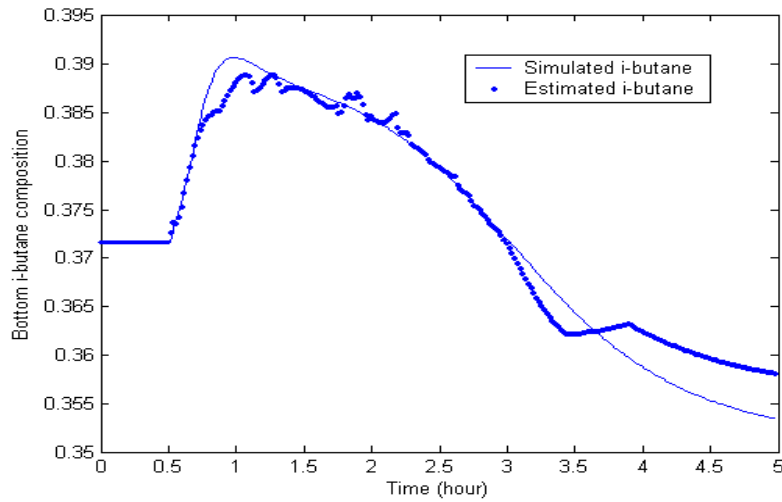


Fig 5.14 Tri7con structure performance to 5% increase in reflux rate for the i-butane composition in bottom with IAE score, 0.0096

Therefore, evaluating all the obtained simulation results; Tri3lin structure can be used as ANFIS estimator to predict the top and bottom product compositions, and the other compositions, in the continuous distillation column under study. It can be implemented to the real plant and online estimation of the compositions from temperatures can be achieved.

Designed ANFIS estimators are also compared with NN estimator developed by Bahar (2003). This NN estimator was designed to be used in MPC framework for the control of product compositions of the column. Estimator's performances for the 5% increase in reflux rate for top and bottom product compositions are shown in Figures 5.7 and 5.8, respectively. It is seen that ANFIS estimator is very good compared to the NN estimator.

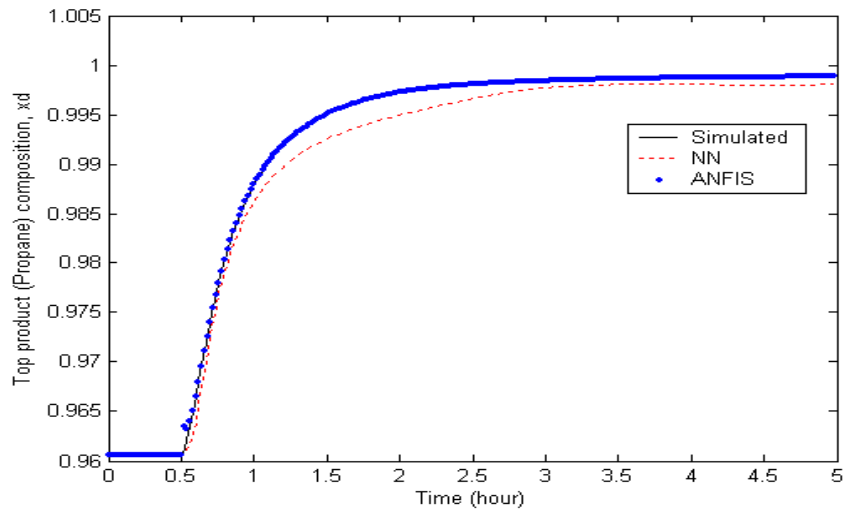


Fig 5.15 Comparison of the ANFIS and NN estimators for top product compositions for a 5% increase in reflux rate with the IAE scores, 0.00014 0.0059, respectively

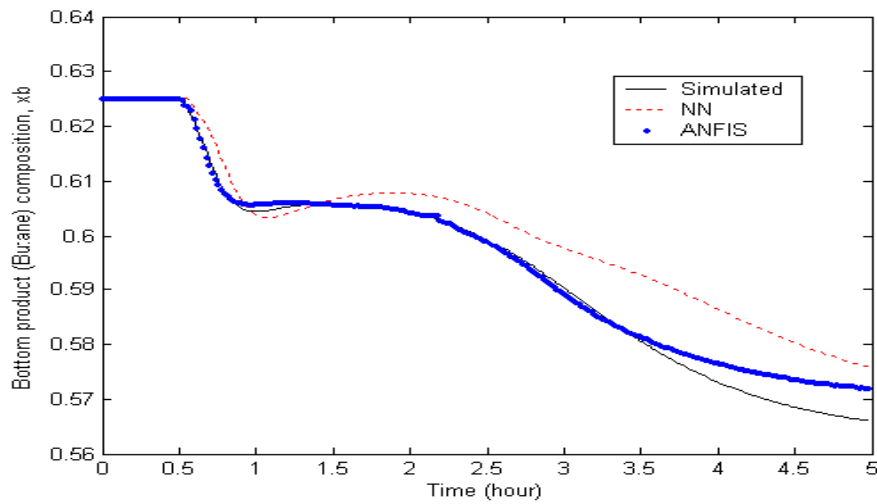


Fig 5.16 Comparison of the ANFIS and NN estimators for bottom product compositions for a 5% increase in reflux rate with the IAE scores, 0.0074 0.0308, respectively

In the designed NN estimator in Bahar’s study which predicts the top and bottom compositions, input vector also considers the past composition values. The past composition values are also the outputs of the estimator. Therefore, the estimator, which can produce inaccurate composition values in the past, is used for the estimator at next time steps. This brings errors to the system and it reduces the system performance. In NN estimator, many input output data pairs are needed for

training and normalization process. If the input and output variables are not of the same order of magnitude, some variables may appear to have more significance than they actually do. Thus, training data and network inputs and outputs are needed to be normalized to values between 0 and 1. Besides, system with many inputs and parameters can require additional computational power, especially in online applications. As a result, although different estimators should be designed for each composition, it can be said that, ANFIS can be utilized for a better estimation in distillation columns instead of NNs.

5.2 ESTIMATION IN BATCH DISTILLATION COLUMN

In this part of the study, it is aimed to investigate the ANFIS structure performances in batch distillation column. For this purpose, three parallel ANFIS estimators are developed to predict the reflux drum compositions; cyclo-hexane (C_1), n-heptane (C_2) and toluene (C_3) from tray temperatures by applying the same procedure as implemented in the case of continuous distillation column.

5.2.1 Selection of Estimator Inputs

In continuous distillation column, since four components were separated, three tray temperatures were used as the estimator's input. It was also seen from the results that three tray temperature measurements were sufficient to estimate the compositions. In batch distillation column, since three components are separated, two tray temperature measurements should be selected and used for estimation in batch distillation column.

In the case study of continuous distillation column, number of trays on which the temperature can be measured is 37. However, batch distillation column under study has 8 trays. Besides, batch distillation process has much complex characteristics than continuous distillation columns. Therefore in order to reflect the column dynamic well, instead of two trays, three trays are used in batch distillation column without analysis. Thus, 2nd, 5th and 9th trays, one from bottom, one from middle and one from top of the column, are selected and used for the composition estimation.

5.2.2 Generation of training data

As stated in the previous chapter, the column is worked under optimal reflux ratio policy. Optimal reflux ratio policy and column design parameters can be seen in Table 4.2 and 4.3. Rigorous model for column developed by Yıldız (2003) is used with these column parameters. Different simulations are done with this model by changing the initial composition of the feed charge to the column to generate the training data for estimators. Initial fractions for feed used in simulations are given in Table 5.6. C_1 , C_2 and C_3 are the compositions of cyclo-hexane, n-heptane and toluene, respectively. Having collected the input output data, three different training data sets are formed and used in training.

Table 5.6 Initial feed compositions

RUN NO	C_{1init}	C_{2init}	C_{3init}
1	0.20	0.20	0.60
2	0.25	0.50	0.25
3	0.30	0.15	0.55
4	0.35	0.40	0.25
5	0.40	0.30	0.30
6	0.50	0.25	0.25
7	0.60	0.35	0.05
8	0.22	0.60	0.18

5.2.3 Training of ANFIS structures

Estimations based on simulations for continuous column indicated that, Triangular structures are better than Gaussian structures both in verification and generalization. Therefore, only Triangular

structure's performances are used in batch distillation studies. These structures are trained with generated training data sets. Thus, number of trainings and test simulations are decreased.

5.2.4 Simulations results

After trained the structures, estimators' verification and generalization capabilities are tested using the rigorous model of the column as a real plant. Verification test is done using Run No 6 from the Table 5.6 as the initial feed compositions. This can also be seen from the IAE scores given in Table 5.7. Therefore, it is decided to use only constant output structures in generalization tests.

First generalization test is done with the initial fractions of Cinit [0.407; 0.394; 0.199]. Results are shown in Figures 5.17, 5.18 and 5.19. Tri3con and Tri5con performance are nearly same but Tri7con structure performance is not good as the others. Therefore, another generalization test is done to make better decision.

Table 5.7 Verification test results with the initial fractions of [0.5; 0.25; 0.25]

INPUT MF	NO OF INPUT MF	OUTPUT MF	IAE SCORE OF C1	IAE SCORE OF C2	IAE SCORE OF C3	TOTAL IAE SCORE
Triangular	3	Constant	0.04211	0.0972	0.0644	0.20374
Triangular	3	Linear	0.0783	0.1845	0.1036	0.3664
Triangular	5	Constant	0.0521	0.1073	0.0627	0.2200
Triangular	5	Linear	0.1173	0.3009	0.17918	0.5975
Triangular	7	Constant	0.079	0.1594	0.0873	0.3258
Triangular	7	Linear	0.123	0.2761	0.1652	0.5644

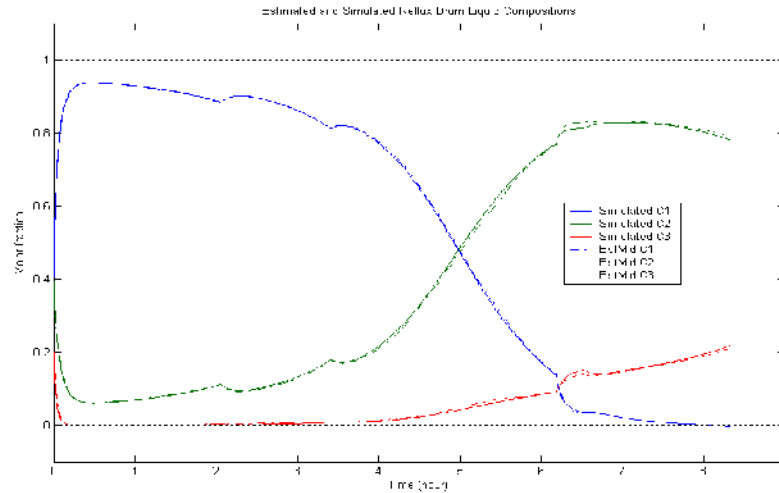


Fig 5.17 Generalization of Tri3con structure; C_{init} [0.407; 0.394; 0.199] with the IAE scores 0.0213, 0.0428 and 0.0251, respectively

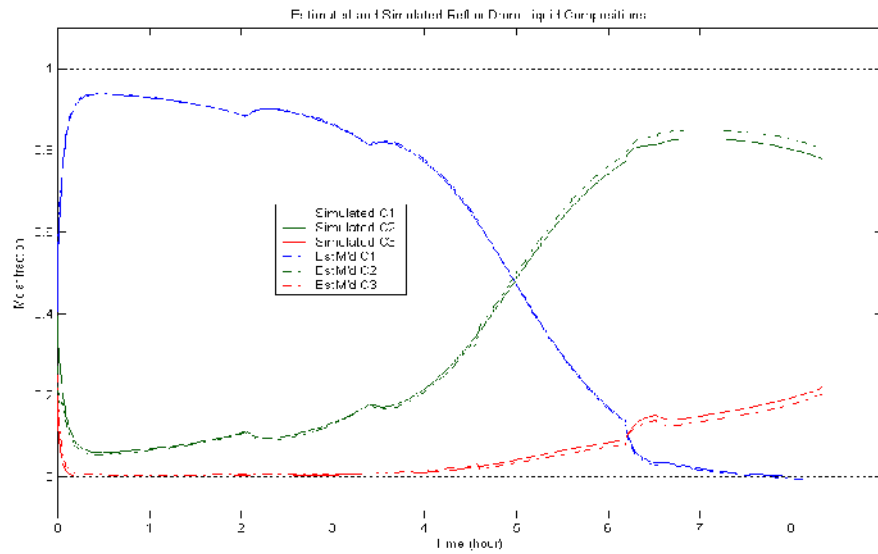


Fig 5.18 Generalization of Tri5con structure; C_{init} [0.407; 0.394; 0.199] with the IAE scores 0.0285, 0.1002 and 0.0645, respectively

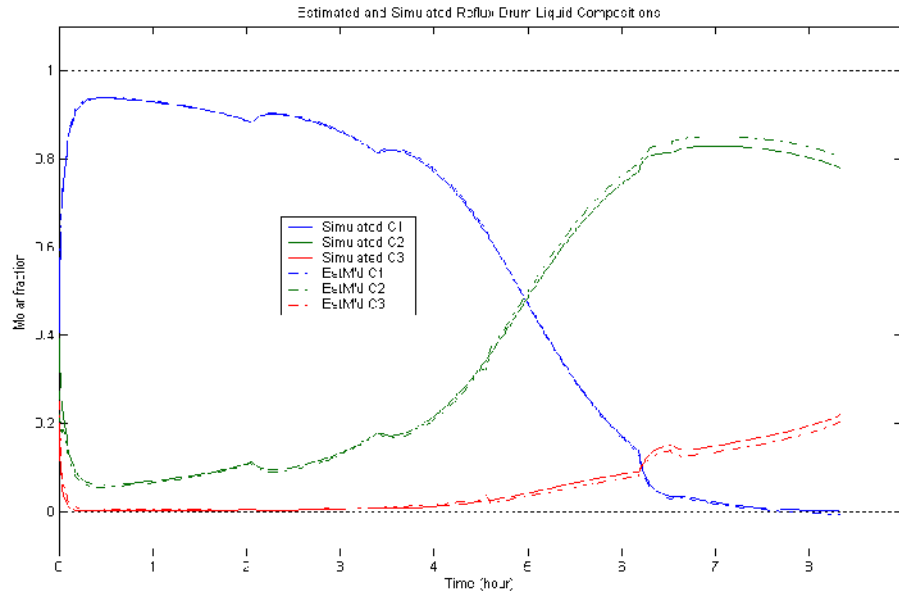


Fig 5.19 Generalization of Tri7con structure; C_{init} [0.407; 0.394; 0.199] with the IAE scores 0.0609, 0.2114 and 0.1335, respectively

The Second generalization test is done with the initial fractions of C_{init} [0.25; 0.35; 0.40]. Figure 5.20, 5.21 and 5.22 shows the estimator performances. It can be seen that Tri3con shows the best performance among the constant output structures.

Moreover, additional generalization simulations are done and Tri3con structure performance is investigated in detail with the different initial feed fractions. It can be seen from Figures 5.23 to 5.25 and from IAE scores that Tri3con structure performance is very good. This structure can be used as ANFIS estimator to predict the reflux drum compositions from the 2nd, 5th and 9th trays temperatures in batch distillation column under study.

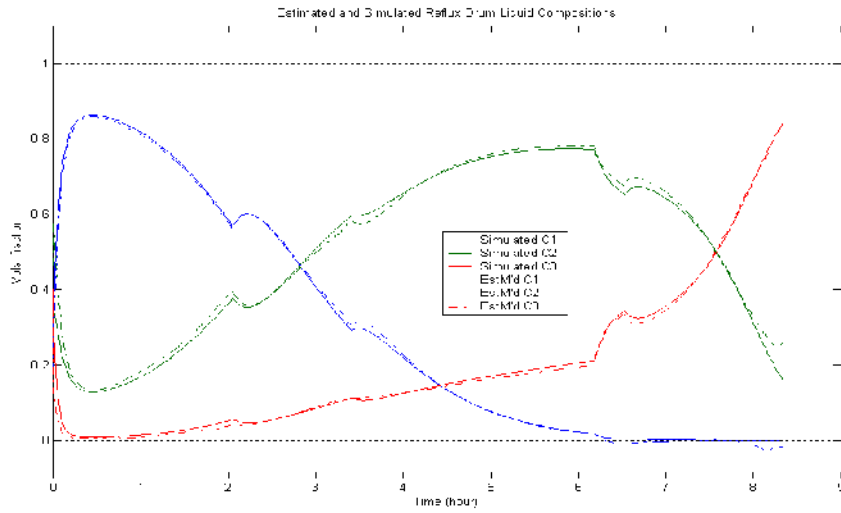


Fig 5.20 Generalization of Tri3con structure; C_{init} [0.25; 0.35; 0.40] with the IAE scores 0.0552, 0.1126 and 0.0626, respectively

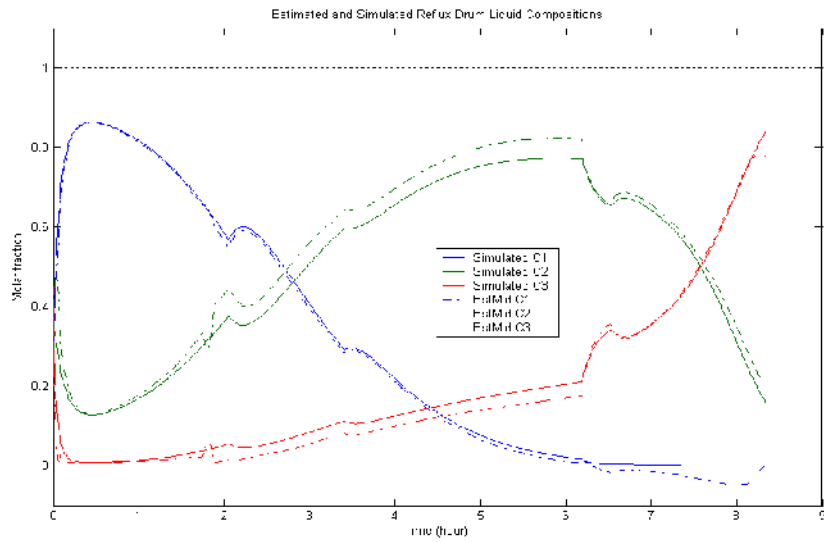


Fig 5.21 Generalization of Tri5con structure; C_{init} [0.25; 0.35; 0.40] with the IAE scores 0.1088, 0.2849 and 0.1605, respectively

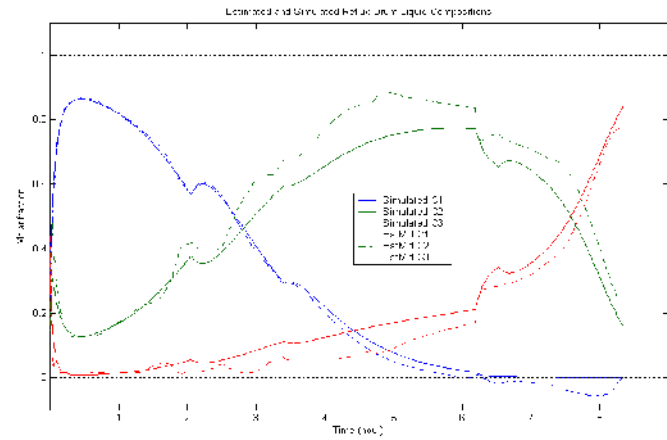


Fig 5.22 Generalization of Tri7con structure; C_{init} [0.25; 0.35; 0.40] with the IAE scores 0.1459, 0.5813 and 0.3378, respectively

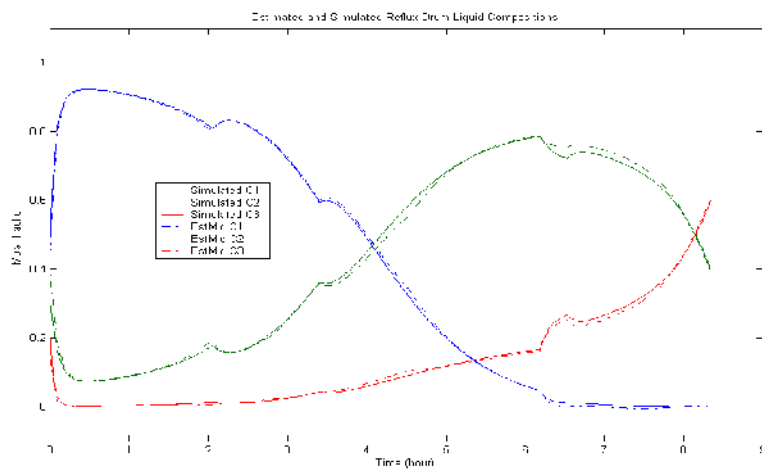


Fig 5.23 Generalization of Tri3con structure; C_{init} [0.34; 0.33; 0.33] with the IAE scores 0.0456, 0.0826 and 0.0451, respectively

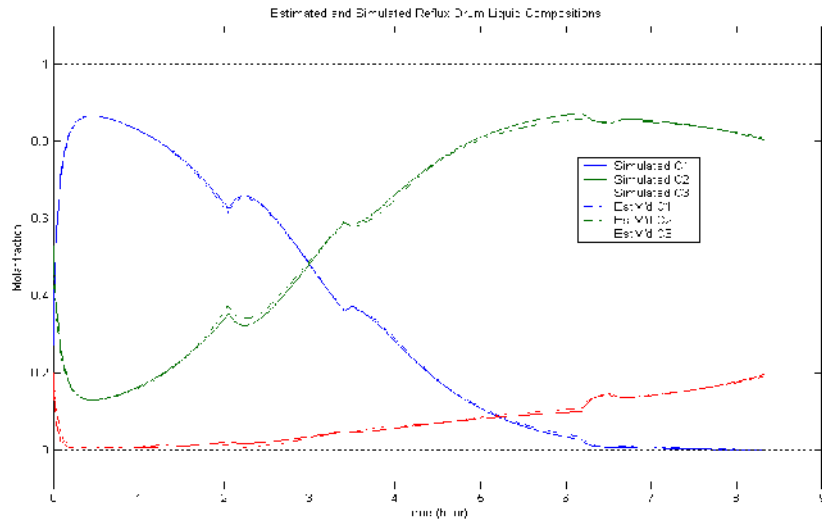


Fig 5.24 Generalization of Tri3con structure; C_{init} [0.27; 0.53; 0.20] with the IAE scores 0.0292, 0.0583 and 0.0349, respectively

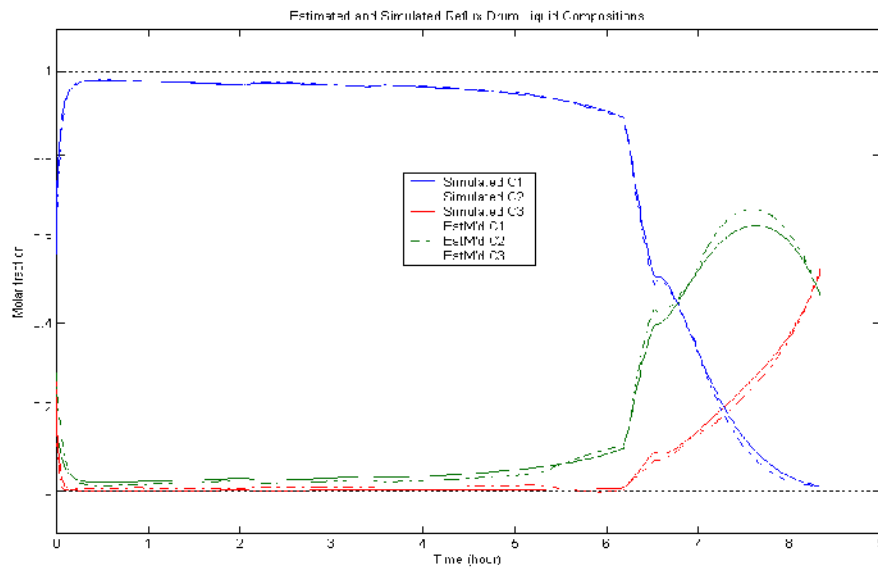


Fig 5.25 Generalization of Tri3con structure; C_{init} [0.58; 0.16; 0.26] with the IAE scores 0.0389, 0.1073 and 0.0741, respectively

Yidiz (2003) designed an Extended Kalman Filter (EKF) to estimate the compositions in the reflux drum for the batch distillation column under study. Figure 5.26 illustrates the performance of the EKF estimator for the reflux drum compositions with the initial fractions of feed C_{init}

[0.407; 0.394; 0.199]. For the same initial fractions, Tri3con ANFIS estimator performance was already given in Figure 5.19. Estimators's performances are shown in Figure 5.27.

EKF is the optimal state estimator while ANFIS can be used in estimation studies of distillation columns. If the sensors provide perfect and complete data about a system without any measurement corruption by noise and without device inaccuracies, trained ANFIS structures can be implemented to the system for online estimation of the state variables. Also, there is no need for a simplified mathematical model of the system; that is needed for the EKF design.

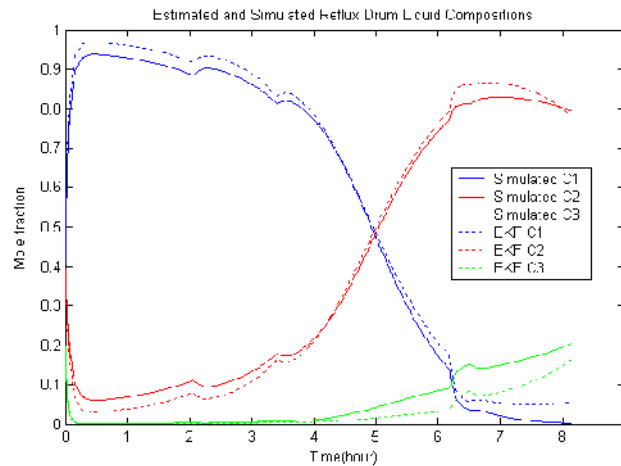


Fig 5.26 EKF estimator performance; C_{init} [0.407; 0.394; 0.199] with the IAE scores 0.2211, 0.1933 and 0.1966, respectively

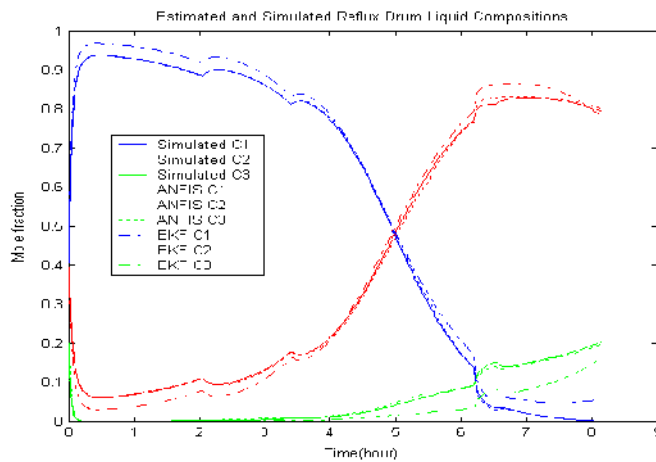


Fig 5.27 Comparison of ANFIS and EKF estimators

In this study, design parameters of the system are selected as the ANFIS structure parameters. Temperature sensors locations were not investigated in detail. Actually, number of tray temperature is sufficient to use as the estimator inputs. Therefore, in the system under study, only two tray temperatures can be used. However, as stated previously in the batch distillation column study, three temperature locations were selected as 2nd, 5th and 9th trays (one from bottom, one from middle and one from top of the column) to represent the column dynamic well. The designed ANFIS estimator performances with two tray temperatures are shown in Figure 5.28 and 5.29. Figure 5.28 illustrates the performance of the estimator with the initial feed fractions of 0.58, 0.16 and 0.26. The estimator performance with three inputs for the same initial feed fractions was shown in Figure 5.25. When these two Figures 5.25 and 5.28 and IAE scores are compared, it is observed that two input estimator performance is as good as than three input estimator. However, initial fraction estimation of C₂ and C₃ is not very close (0.1677/0.64, 0.2822/-0.101). Figure 5.29 also illustrates the performance of the estimator with the initial fractions of 0.407, 0.399, and 0.199. The estimator performance with three inputs for the same initial fractions was shown in Figure 5.17. It can be seen from the Figure 5.17 and 5.29 that the estimator performance with two inputs is as good as three input estimator with the IAE comparison but initial fraction estimation of C₃ (0.20/-0.10) is not achieved. When the total IAE scores are compared in these two runs tested with different initial feed composition, it can be concluded that the estimation can be done using only two tray temperatures but initial composition fractions cannot be estimate accurately.

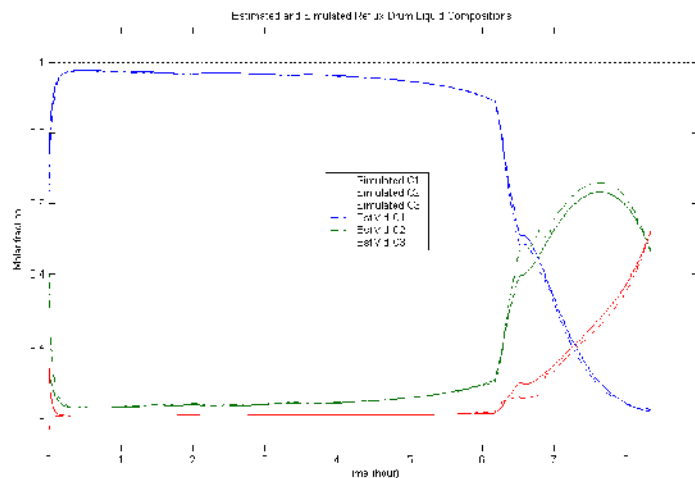


Fig 5.28 ANFIS estimator performance with two estimator inputs with the initial fractions; C_{init} [0.58; 0.16; 0.26] and with the IAE scores 0.0441, 0.0938 and 0.0569, respectively

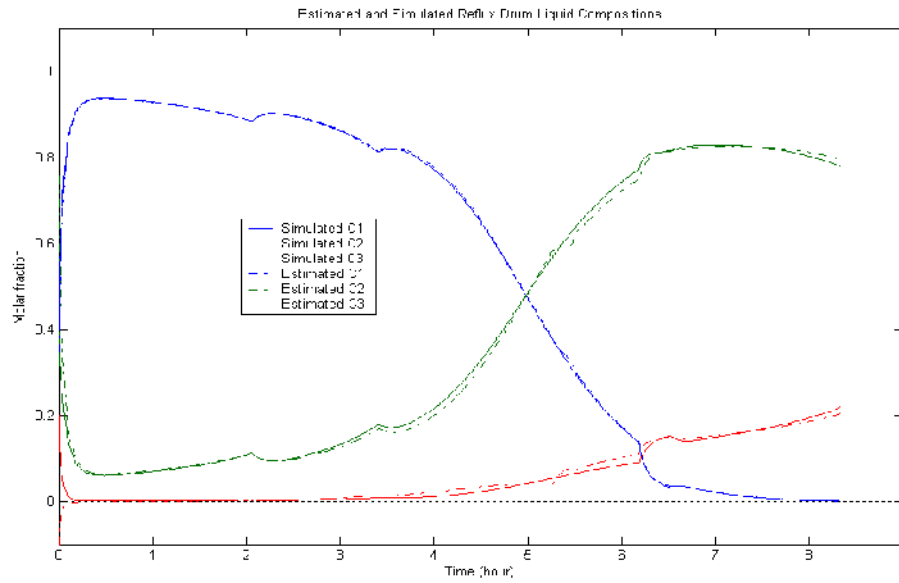


Fig 5.29 ANFIS estimator performance with two estimator inputs with the initial fractions; C_{init} [0.407; 0.394; 0.199] and with the IAE scores 0.029, 0.076 and 0.045, respectively

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

In this study, estimation of the compositions from the trays temperature measurements in continuous and batch distillation columns, are achieved by using the ANFIS architecture.

1. In continuous distillation column, ANFIS structures are trained and tested to infer one of the components of the top and bottom product compositions. It is concluded that all estimators' structures verification and generalization capabilities are very good especially in feed flow rate changes. Triangular structures are better than Gaussian structures that are used in membership functions (MF).

2. Best performance is obtained by Tri3lin (three triangular MFs for each input and linear output MF) ANFIS structure for both top and bottom product estimation. Tri3lin ANFIS estimator performance is compared with NN estimator and it is seen that performance of the ANFIS is better than that of NN.

3. In batch distillation column, three parallel Triangular ANFIS structures are trained and tested for the three components in reflux drum. It is seen that, structures that have constant output MF performances are better. The best performance is obtained by Tri3con ANFIS structure for all compositions in reflux drum. Tri3con ANFIS estimator is compared with EKF estimator and it is seen that ANFIS is better than EKF.

4. In batch distillation column, designed estimator using two tray temperatures is also evaluated. It is seen that, the estimator performance with two tray temperatures is as good three tray temperatures. However, initial composition values are not estimated accurately.

5. ANFIS controller performance is compared with NN controller. It is concluded that convergence of ANFIS with backpropagation algorithm is slower than that of NN.

6. As a recommendation for further studies, using hybrid-learning algorithm that combines the backpropagation learning algorithm and least squares estimates can increase the performance of the ANFIS especially in controller applications.

7. If sufficient process input-output data is collected from the system, ANFIS methodology can be used for estimation and modeling purposes in chemical processes.

8. ANFIS can be also used for control purposes in chemical processes especially in Neuro-Fuzzy control structures.

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