

Control of Reactive Distillation Process using Intelligent Controllers

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ABSTRACT

The objective of the present work is precise control of distillate quality using the temperature profile of reactive distillation process. The temperature profile of the reactive process may be controlled using intelligent controller. The paper presents the methodology for the design of various intelligent controllers and its application on distillation process. Four intelligent controllers are designed based on fuzzy logic, adaptive linear network (Adaline) and hybrid of these two techniques i.e. Fuzzy-Neural Network and Fuzzy-Adaline Network. The Fuzzy Logic Controller (FLC) provides a better steady state response whereas the adaptive linear network controller (ADC) provides better transient response. The hybrid Fuzzy-Neural Network Controller (FNNC) and Fuzzy-Adaline Controller (HFADC) are proposed to combine the advantages of the two techniques. The results of the designed intelligent controllers are compared with the conventional PI controller. It is observed that the Hybrid Fuzzy-Adaline Controller (HFADC) outperforms all the controllers.

General Terms

Intelligent Controllers, Distillation Process, Reactive Process, Process control.

Keywords

Fuzzy Logic Controller, Adaline Controller, FNN Controller, Hybrid Fuzzy- Adaline Controller.

1. INTRODUCTION

Reactive distillation is a separation process that combines both chemical reaction and distillation in a single unit. The two feeds entering the column react to form the product components. These products must be removed from the column to increase the efficiency of the system. The removal is done with the help of distillation. The use of reactive distillation process has certain advantages such as utilization of heat of reaction, high gain, and compact nature etc. [1]. However the combination of reaction and distillation in a single unit increases the complexity that inhibits the design and tight control. Also reactive distillation is ideally suited for the systems where the reactant and product volatilities differ considerably.

Various intelligent control techniques are found in the literature for controlling the complex and nonlinear systems. S.R. Vijaya Raghavan et al. in 2011 [2] have presented the design and implementation of a recurrent neural network based inferential state estimation scheme for an ideal reactive distillation column. K. J. Jithin Prakash et al. in 2011[3] proposed an artificial neural network based nonlinear control algorithm for simulated batch reactive distillation column. The authors synthesized a neuro-

estimator based generic model controller (GMC) which consist of an ANN based state predictor and the GMC law. Fatima Barcelo-Rico et al. in 2011[4] applied the fuzzy control technique to control the continuous distillation tower. The designed fuzzy controller was able to keep the target output in the desired range for different input disturbances, changing smoothly from a predefined target output to another. Almila Bahar and Canan Ozgan in 2010 [5] used an Elman neural network to estimate and control the product composition values of the distillation column from temperature measurements inferentially. J. Fernandez de Canete et al. in 2010 [6] presented a robust stability analysis based on the harmonic balance and applied to a neural network controller in series with a dynamic multi variable nonlinear plant. Jeon lin and Ruey-Jing Lian in 2009 [7] developed a hybrid fuzzy logic and neural network controller for multi-input multi-output system. Swati Mohanty in 2009 [8] proposed a neural network based model which is used to design a model predictive controller for controlling the interface level in a flotation column. The controller was tested both for liquid–gas system as well as liquid–gas–solid system and was found to perform very satisfactorily. The performance of the controller was compared with that of a conventional PI controller for a two-phase system and was found to be better. Vijander Singh et al. in 2007 [9][10] developed a Neural Network estimator using Back Propagation and LM Technique for estimating the distillate composition from temperature profile of distillation column along with the pressure and heat input. Harun Taskin et al. in 2006 [11] proposed a fuzzy logic control of a fluid catalytic cracking unit to improve the dynamic performance. S. Gruner et al. in 2003 [12] proposed an observer based on asymptotically exact input/output linearization. The steady state observer offsets are compensated by an outer loop with simple PI controllers.

The present work proposes intelligent controllers based on fuzzy logic (FLC) and adaptive linear network (ADC). Further the two techniques are combined to obtain two hybrid controllers i.e. Fuzzy Neural Network Controller (FNNC) and Hybrid Fuzzy Adaptive linear network Controller (HFADC). FNNC is a combination of fuzzy logic and back propagation algorithm whereas HFADC is a switching controller which switches between the FLC and ADC.

1.1 Reactive Distillation Process

Reactive distillation shown in Fig.1 is a process of chemical reaction and separation of the products in the common chamber. It is a highly nonlinear and complex process. The chemical

industry has recognized the significance of reactive distillation due to its high gain and compact nature. Reactive Distillation Column (RDC) is an ideal two-reactant-two-product reactive distillation column proposed by Al-Arfaj and Luyben [13] and later developed into state space model. It consists of a reactive section in the middle and non-reactive rectifying and stripping sections at the top and bottom respectively.

The column consists of Reactive Trays (N_{rx}) in the middle, Rectifying Trays (N_r) in the top and Stripping Trays (N_s) in the bottom. The trays of the column are numbered from reboiler to condenser. The reaction takes place in the reactive zone is exothermic liquid-vapour in nature and is given by



During the distillation process, the reactant B which is one of the input feeds is recovered in the rectifying section from the output product C whereas the second feed i.e. reactant A, is recovered from output product D in the stripping section. The reactive section comprises the middle section of the reactive distillation column where the reactants A and B react to produce C and D. The reaction generates the heat which is then used for the distillation of the products. The products are separated to prevent any undesired reaction between reactants A and B and products C and D. The volatilities of the products and reactants are such that

$$\alpha_c > \alpha_a > \alpha_b > \alpha_d \quad (2)$$

where α_j is the volatility of the j^{th} component, $j = a, b, c, d$.

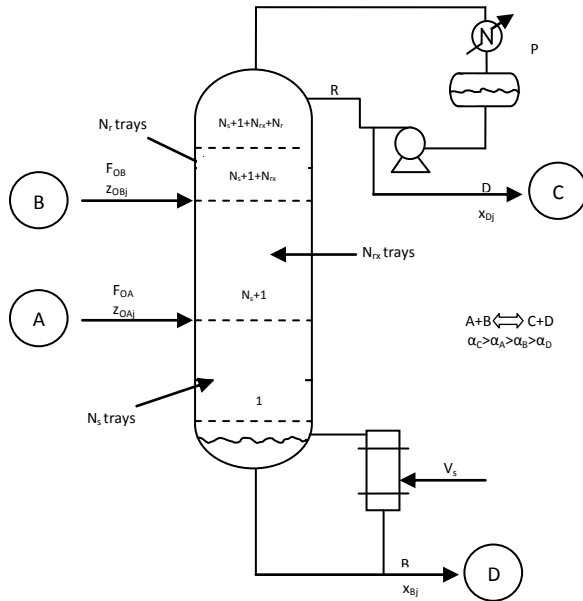


Fig 1: Basic structure of reactive distillation column

It is observed from the relation defined in eq. (2) that C is the lightest product with highest volatility, D is the heaviest product with lowest volatility and volatilities of A and B lie in between them. This relative volatility ensures that the products A and B have high concentration in the reactive section, which is typical example of an ideal reactive distillation column. The quality of products C and D is controlled by manipulating the feed flow rates. The controllers in the process are termed as dual end composition control structure. The purity of both products must be maintained at desired set point. The mathematical modeling of the reactive process is explained in the next section.

1.2 Mathematical Modeling

The net reaction rate for component j on tray- i in the reactive zone is given by

$$R_{i,j} = v_j M_i (k_{fi} x_{i,A} x_{i,B} - k_{bi} x_{i,C} x_{i,D}) \quad (3)$$

The steady-state vapour and liquid flow rates are constant through the stripping and rectifying sections because equimolar overflow is assumed. However, these rates change through the reactive zone because of the exothermic reaction. The heat of reaction vaporizes some liquid on each tray in that section; therefore, the vapour rate increases up through the reactive trays and the liquid rate decreases down through the reactive trays.

$$V_i = V_{i-1} - \frac{\lambda}{\Delta H_v} R_{i,c} \quad (4)$$

$$L_i = L_{i+1} + \frac{\lambda}{\Delta H_v} R_{i,c} \quad (5)$$

The dynamic component balance equations for the column are as follows:

Reflux drum:

$$\frac{d(x_{D,j} M_D)}{dt} = V_{NT} y_{NT,j} - D(1 + RR)x_{D,j} \quad (6)$$

Rectifying and stripping trays:

$$\frac{d(x_{i,j} M_i)}{dt} = L_{i+1} x_{i+1,j} + V_{i-1} y_{i-1,j} - L_i x_{i,j} - V_i y_{i,j} \quad (7)$$

Reactive trays:

$$\frac{d(x_{i,j} M_i)}{dt} = L_{i+1} x_{i+1,j} + V_{i-1} y_{i-1,j} - L_i x_{i,j} - V_i y_{i,j} + R_{i,j} \quad (8)$$

Feed trays:

$$\frac{d(x_{i,j} M_i)}{dt} = L_{i+1} x_{i+1,j} + V_{i-1} y_{i-1,j} - L_i x_{i,j} - V_i y_{i,j} + R_{i,j} + F_i z_{i,j} \quad (9)$$

Column base:

$$\frac{d(x_{B,j} M_B)}{dt} = L_1 x_{1,j} - B x_{B,j} - V_s y_{B,j} \quad (10)$$

The forward and backward specific reaction rates on i^{th} tray is given as follows:

$$k_{f,i} = a_f e^{-E_f/RT_i} \quad (11)$$

$$k_{b,i} = a_b e^{-E_b/RT_i} \quad (12)$$

Temperature on i^{th} tray is calculated by the following expression:

$$T_i = B_{vp} / [A_{vp} - \ln(\alpha_j P / \sum_{k=1}^{N_C} \alpha_k x_{i,k}) - B_{vp}] \quad (13)$$

The ideal vapour–liquid equilibrium is assumed and column pressure P is optimized for each tray. With pressure P and tray liquid composition $x_{i,j}$ known at each tray, the temperature T_i and the vapor composition $y_{i,j}$ is calculated. This bubble point calculation is made by Newton-Raphson iterative convergence method.

$$P = \sum_{j=1}^{N_C} x_{i,j} P_j^S \quad (14)$$

$$y_{i,j} = \frac{P_j^S}{P} x_{i,j} \quad (15)$$

The mathematical model of the reactive distillation column described in this section is simulated in MATLAB and then used for control and analysis purpose as shown in Fig. 2. A conventional controller is designed to control the temperature profile of the distillation process and hence the distillate quality. Various intelligent controllers are also designed based on fuzzy logic, neural network and hybrid of these two techniques. These control schemes are applied to control the temperature of the 14^{th} tray as explained in the next section.

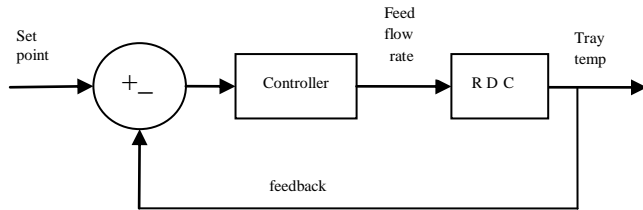


Fig 2: Basic block diagram of RDC control

2. CONTROL SCHEMES

A control system design problem is to obtain a nonlinear vector value function $h()$ given as [14],

$$\mathbf{u}(t) = \mathbf{h}[t, \mathbf{x}(t), \mathbf{r}(t)] \quad (16)$$

Where $\mathbf{u}(t)$ is the control input to the process, $\mathbf{x}(t)$ is the system state vector and $\mathbf{r}(t)$ is the reference input. The feedback control law \mathbf{h} is selected in such a way that the closed loop system is stable and meets the performance indices.

In case of single input single output system, the function \mathbf{h} takes the following form for a proportional plus derivative plus integral or PID controller.

$$e_a(t) = k_p * e(t) + k_i \int e(t)dt + k_d * \frac{de}{dt} \quad (17)$$

The possible combinations of the three controller terms can be used depending upon the nature of the system. Thus the control system design problem in case of PID controller is reduced to obtaining coefficients $k_p, k_i,$ and k_d . The product quality of reactive distillation process depends upon the temperature

profile of the column thus controlling the temperature will indirectly regulate the product quality. In the present control system problem the temperature of 14^{th} tray of the reactive distillation process is controlled by using the proportional plus integral (PI) controller. The PI controller designed is tuned by using Tyreus-Luyben method and the values of k_p and T_i obtained are 2.94 and 113.182 respectively.

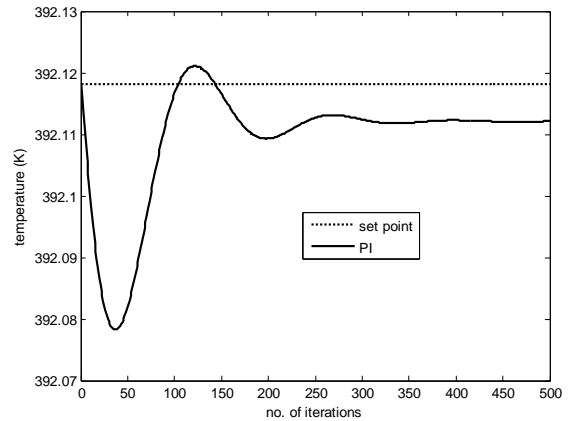


Fig 3: Tray temperature control with PI controller

The tuned PI controller is used to control the reactive process. It is observed from Fig. 3 that there is a steady state error and a large undershoot in the response of the system. Thus both the transient response and steady state response need to be improved. The overall response of the system may be improved with the help of intelligent controllers. Therefore it is desired to control the tray temperature in a more efficient manner and for that purpose advanced control techniques are proposed. The different control schemes used are as follows.

2.1 Fuzzy Logic Controller

The fuzzy logic controller is applied to control the tray temperature of the reactive distillation process. In this case the Fuzzy rule base system uses a set of fuzzy conditional statements which are derived from system's knowledge base to approximate the control input to the plant. The calculation of control input is based on interpolative and approximate reasoning. Simple fuzzy logic controllers for given system can be depicted in the form of a block diagram as shown in Fig. 4. The steps involved in designing a simple fuzzy control system are as follows:

1. The inputs, states and outputs of the plant are identified.
2. The universe of discourse of each variable is partitioned into a number of fuzzy subsets and each subset is assigned a linguistic label.
3. Membership function for each fuzzy subset is selected depending on the nature of the system.
4. The fuzzy relationships are defined between the inputs fuzzy subsets and the outputs fuzzy subsets in the form of IF-THEN rules and thus forming the rule base.

5. Appropriate scaling factor is chosen for input and output variables so that the variables are normalized to [0,1] or [-1,1] interval.
6. Inputs to the controller are fuzzified.
7. The fuzzy approximate reasoning is used to infer the output contributed from each rule.
8. Aggregation and defuzzification of the fuzzy output is done to obtain a crisp output.

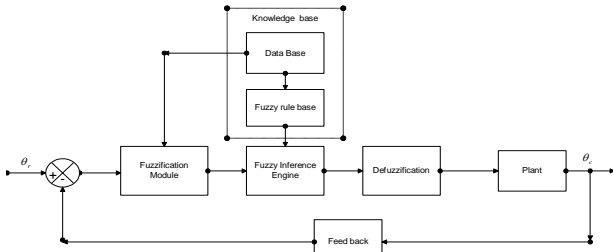


Fig 4: Block diagram of fuzzy logic control system

Based on the above procedure, a fuzzy controller is designed. The knowledge base required for the fuzzy controller is developed using the simulation results of the PI controlled reactive distillation process. Here, the error, change in error and output are fuzzified using triangular membership functions for the tray temperature control. The membership functions are as shown in Table 1, Table 2 and Table 3.

Table 1: Membership functions for error of 14th tray

Membership function	Lower limit	Middle limit	Higher limit
ESP	-0.0150	0	0.0150
VVSP	0	0.0150	0.03
VSP	0.0150	0.03	0.045
SP	0.03	0.045	0.06
NP	0.045	0.06	0.075
VNP	0.06	0.075	0.09
LP	0.075	0.09	0.105
VLP	0.09	0.105	0.12
VVLP	0.105	0.12	0.135
ELP	0.12	0.135	0.15

The rule base selected for the temperature control of the tray is shown in Table 4. Mamdani inference technique is selected for inferring the output results and centroid method is used for

defuzzification. The designed fuzzy controller is applied on reactive distillation process for testing purpose and results are obtained.

Table 2: Membership functions of rate of change of error of 14th tray

Membership function	Lower limit	Middle limit	Higher limit
ESD	-0.1	-0.05	0
VSD	-0.05	0	0.05
SD	0	0.05	0.1
ND	0.05	0.1	0.15
VND	0.1	0.15	0.2
LD	0.15	0.2	0.25
VLD	0.2	0.25	0.3

Table 3: Membership functions for output of controller

Membership function	Lower limit	Middle limit	Higher limit
ESC	-0.1	-0.05	0
VSC	-0.05	0	0.05
SC	0	0.05	0.1
NC	0.05	0.1	0.15
VNC	0.1	0.15	0.2
LC	0.15	0.2	0.25
VLC	0.2	0.25	0.3

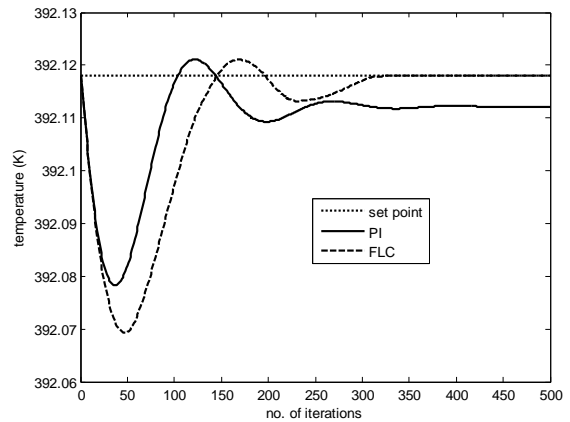


Fig 5: Tray temperature control with PI and FLC

Table 4: Rule Base

Membership Functions	ESP	VVSP	VSP	SP	NP	VNP	LP	VLP	VVLP	ELP
ESD	ESC	ESC	ESC	VSC	VSC	VSC	VSC	SC	SC	NC
VSD	VSC	NC	VSC	VSC	SC	SC	NC	NC	NC	VNC
SD	LC	LC	VLC	VLC	VLC	VLC	VLC	VLC	LC	LC
ND	NC	NC	LC	LC	VLC	VLC	LC	LC	LC	LC
VND	NC	NC	VNC	VNC	LC	VLC	VLC	VLC	LC	LC
LD	NC	NC	NC	VLC	VLC	VLC	VLC	VLC	VLC	LC
VLD	VLC	VLC	VLC	VLC	VLC	LC	LC	VNC	VNC	NC

From above results, it is observed that the fuzzy logic controller reduces the steady state error significantly but undershoot is larger than PI controller. On other hand the PI controller has poor steady state response but small undershoot as compared to the FLC. Thus to improve the transient response of the system a better controller needs to be designed. Therefore another intelligent technique i.e. adaptive linear network is used to design the controller which is discussed in the next section.

2.2 Adaptive Linear Network based Controller (ADC)

Adaptive Linear Network (Adaline) developed by Widrow and Hoff is found to use bipolar activation functions for both the input signals and target output (1960)[15]. The architecture of an Adaline is shown in Fig. 6. The Adaline has only one output unit which receives input from several units and also from bias whose action is always +1. The Adaline resembles a single layer network. In Fig. 6 an input layer with x_1, \dots, x_n and bias and an output layer with only one output neuron is present. The input and output neurons possess weighted interconnections. These weights are trained using suitable learning rules.

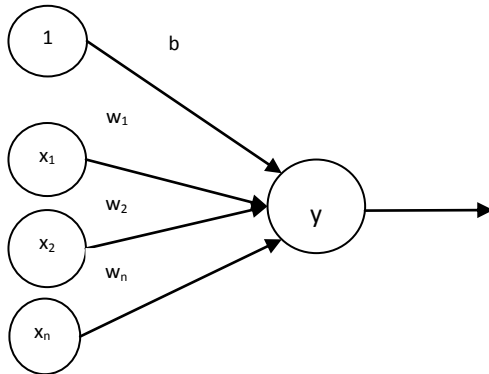


Fig 6: Architecture of an Adaline

The output y of the adaline is given as

$$y = \sum_{i=1}^n w_i x_i + b \quad (18)$$

The Adaline controller (ADC) is designed to control the temperature profile of reactive distillation process. The inputs to the controller are change in temperature (i.e. difference between set point temperature and measured tray temperature) and rate of change of temperature. The target input to the controller is the change in feed flow rate. These input and target patterns are generated by simulating the closed loop reactive distillation column with PI as the controller. The proposed controller is trained with the help of the generated input and target patterns. The designed Adaline controller is then tested by replacing the PI controller with the adaline controller. It is observed from the results of Fig. 7 that the transient response of the Adaline controller is better as compared to the PI controller and FLC but there is an offset error which is more as compared to FLC. Therefore from the above observations it can be concluded that fuzzy provides better steady state response whereas neural network controller i.e. Adaline controller provides better transient response. Therefore a hybrid controller is proposed

which uses both the fuzzy and neural network controller to get the overall improved performance of the system. In the present work two types of hybrid controller are proposed and are discussed in the next section.

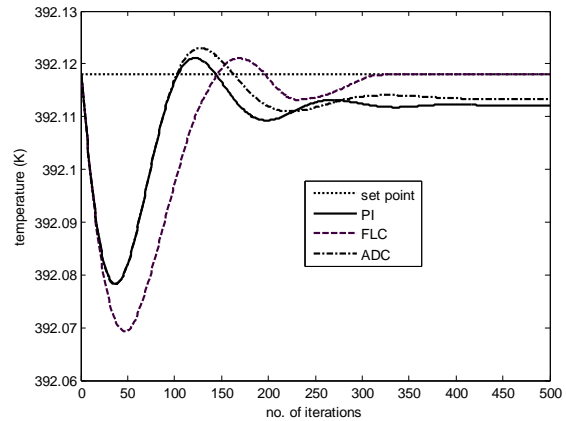


Fig 7: Tray temperature control with PI, FLC and ADC

2.3 Hybrid Controllers

2.3.1 Fuzzy-Neural Network Controller (FNNC)

A Neuro-fuzzy approach gets the benefits of neural networks as well as of the fuzzy logic systems and it also removes the individual disadvantages when combined on the common features. Neural network and fuzzy logic have certain common features for example model free estimation, handling uncertain and imprecise data, distributed representation of knowledge etc. Neural networks can handle noisy data while fuzzy logic has the ability to handle imprecise data. Fuzzy Neural Network (FNN) is an approach in which a fuzzy inference system is constructed using a given set of input and output. The membership functions and rules of these systems are adjusted using various computational algorithms to make them learn from the data they are modeled.

To present the FNN architecture, let us consider two-fuzzy rules based on a first-order Sugeno model.

Rule 1:

If x is A_1 and y is B_1 THEN $f_1 = p_1 x + q_1 y + r_1$

Rule 2:

If x is A_2 and y is B_2 THEN $f_2 = p_2 x + q_2 y + r_2$

A possible FNN architecture to implement the above two rules is shown in Fig. 8. In Fig. 8 a circle indicates a fixed node whereas a square indicates an adaptive node (the parameters are changed during training). Different layers of Fig. 8 are described as follows:

Layer 1: In this layer all the nodes are adaptive, i is the degree of the membership of the input to the fuzzy membership function (MF) represented by the node. The output of each node is given by

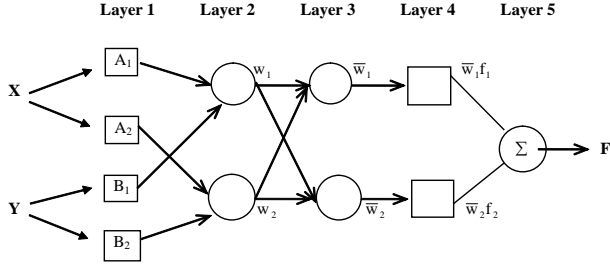


Fig 8: Layers of FNN

$$O_{1,i} = \mu_{A_i}(x) \quad \text{for } i = 1,2 \quad (19)$$

$$O_{1,i} = \mu_{B_{i-2}}(y) \quad \text{for } i = 3,4 \quad (20)$$

where, $O_{1,i}(x)$ is essentially the membership grade for x and y . A_i and B_i can be any appropriate fuzzy sets in parameter form. For example, if bell MF is used then

$$\mu_A(x) = \frac{1}{1 + \left| \frac{x-c_i}{a_i} \right|^{2b_i}} \quad (21)$$

where a_i , b_i and c_i are the parameters for the MF.

Layer 2: The nodes of this layer are fixed (not adaptive) and their work is to simply provide a gain. The outputs of these nodes are given by

$$O_{2,i} = w_i = \mu_{A_i}(x)\mu_{B_i}(y), \quad i = 1,2 \quad (22)$$

Layer 3: This layer also has fixed nodes. At this stage the nodes normalize the firing strength of previous layer. The output of a node in this layer is given by

$$O_{3,i} = \bar{w}_i = \frac{w_i}{w_1 + w_2} \quad (23)$$

Layer 4: All the nodes in this layer are adaptive nodes. The output of a node is the product of the normalized firing strength and a first-order polynomial

$$O_{4,i} = \bar{w}_i f_i = \bar{w}_i(p_i x + q_i y + r_i) \quad (24)$$

where p_i , q_i and r_i are design parameters.

Layer 5: This is a single node layer performing the function of a summer. The output of this node is given by

$$O_{5,i} = \sum_i \bar{w}_i f_i = \frac{\sum_i w_i f_i}{\sum_i w_i} \quad (25)$$

The FNN architecture is not unique. Some layers can be combined and still produce the same output. In this FNN architecture, there are two adaptive layers (1 and 4). Layer 1 has three modifiable parameters (a_i , b_i and c_i) pertaining to the input MFs. These parameters are called *premise* parameters. Layer 4 has also three modifiable parameters (p_i , q_i and r_i) pertaining to the first-order polynomial. These parameters are called *consequent* parameters.

A learning algorithm is used to update the parameters associated with the membership function. The updating of these parameters is facilitated by a gradient vector which provides a measure of how well the fuzzy inference system is modeling the input/output data for a given set of parameters. In this paper the hybrid algorithm is used for its non complexity and high

efficiency in training. The output error is used to adapt the premise parameters by means of a standard back propagation algorithm.

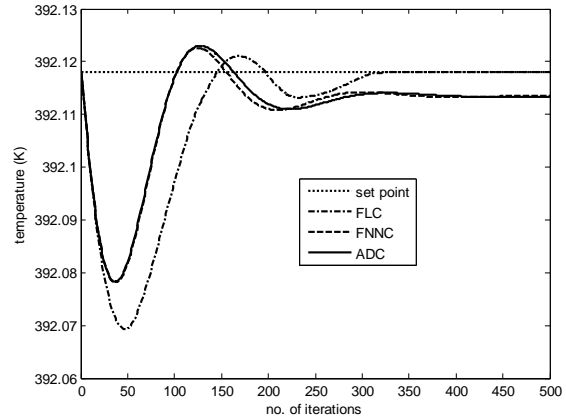


Fig 9: Tray temperature control with FLC, FNNC and ADC

A FNN controller is designed for reactive distillation process control. The data used for training the network is same as for ADC. The structure of the network has two membership functions for inputs and output. The designed controller is then tested to control the system and the results are obtained as shown in Fig. 9. It is seen from the above results that FNN controller is slightly better than the ADC. The FNN has better performance because it has the advantages of both the fuzzy as well as neural network. Still the performance is not up to the mark so a new hybrid is proposed which uses the switching option as discussed in the next section.

2.3.2 Hybrid Fuzzy-Adaline Controller (HFADC)

As discussed in the previous section neural network and fuzzy logic combination provides the advantages of both the techniques and the individual disadvantages are overcome. As observed from Fig. 9. FLC provides a response with large undershoot and oscillations, but the steady state error in the response is reduced to a very large extent. On the other hand if the behaviour of ADC is analyzed, it is found that it has lesser undershoot and less oscillations but a finite steady state error exists. The control strategy includes a FLC and a switching neural network as shown in the block diagram of Fig. 10. The design of the proposed hybrid fuzzy-adaline controller (HFADC) involved designing an adaline controller and a fuzzy logic controller. Already designed FLC and ADC are used for this purpose and a strategy is devised to switchover from FLC to ADC. This strategy is to find the switching time which is based upon the responses of the two controllers. The ADC controls the system response during transients i.e. the peak time and later on the control is switched over to the fuzzy controller (FLC) to control the steady state response of the system.

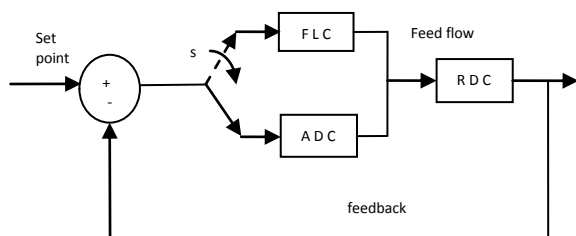


Fig 10: Block diagram of hybrid fuzzy-adaline control system

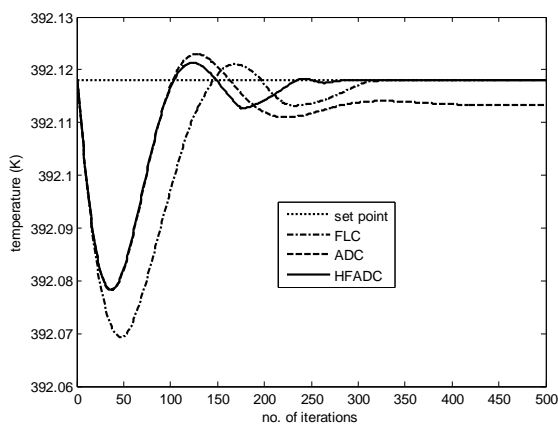


Fig 11: Tray temperature control with FLC, ADC and HFADC

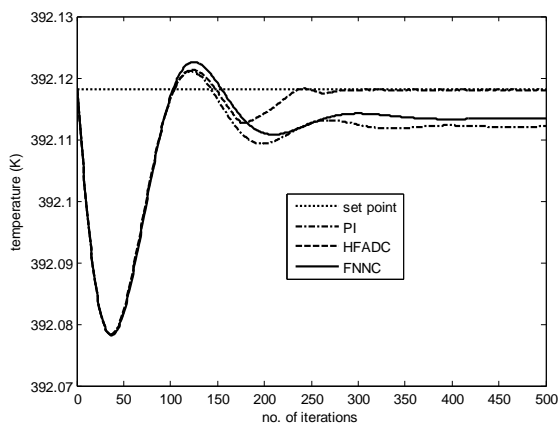


Fig 12: Tray temperature control with PI, HFADC and FNNC

The HFADC is designed and applied to control the temperature of reactive distillation process. It is observed from the Fig. 11 that the hybrid controller HFADC provides less overshoot and oscillations as compared to FLC. Also HFADC has very less steady state error as compared to ADC. Therefore the HFADC improves the transient as well as steady state response of the reactive distillation process. Finally the hybrid controller thus proposed reduces the settling time to a large extent. The response of the system using HFADC and FNNC are obtained and compared with the PI controller as shown in Fig. 12. It is observed from the results that the HFADC outperforms the PI and FNNC. The performance indices of all the designed

controllers are shown in Table 5. It is analyzed from the performance indices that the HFADC proves to be the best controller.

Table 5: Performance indices of controllers

Controller	Undershoot	Settling time (iterations)	Steady state error
PI	0.03983	310	0.0059
FLC	0.04876	310	0.000045
ADC	0.03989	275	0.0048
FNNC	0.03988	280	0.003465
HFADC	0.03979	230	0.00004

3. CONCLUSION

In this article the intelligent controllers are designed for reactive distillation column. The tray temperature used for distillate quality control is selected by conducting a sensitivity analysis. The necessary data for designing the controller is obtained using a dynamic reactive distillation model.

For a comparative study a PI controller is designed. The performance of PI controller is analyzed and it is found that the peak undershoot is large, response is oscillatory and there is an offset error. In an effort to improve the control performance, the intelligent controllers FLC and ADC are designed. The results showed that the transient performance of ADC is better whereas the steady state performance of FLC is better. Utilizing this information two hybrid controllers are proposed to combine the advantages of fuzzy logic and neural network. The first hybrid controller is a FNNC in which membership function parameters are updated using output error by means of a standard back propagation method. The second hybrid control scheme HFADC consists of a switching controller where ADC works during the transients whereas FLC takes over the control after the peak time. The comparison of control performance of all the controllers is shown in Table 5. It is concluded from the above observations that the combination of fuzzy logic and adaptive linear network (HFADC) provides a significant improvement in transient as well as steady state performance in comparison to the designed intelligent controllers.

Abbreviations:

- $y_{B,j}$ Vapour composition of reboiler of j^{th} component (mole fraction)
- L_1 Liquid flow rate leaving 1st tray (lb-mole/h)
- $x_{1,j}$ Liquid composition on 1st tray of j^{th} component (mole fraction)
- E_b Activation energy for backward reaction (Btu/mole)
- E_f Activation energy for forward reaction (Btu/mole)
- F_i Input feed flow rate (lb-mole/h)
- L_{NT} Liquid flow rate leaving NT^{th} tray (lb-mole/h)
- M_i Molar holdup on i^{th} tray (lb-mole)
- $R_{i,j}$ Rate of reaction on the i^{th} tray
- T_i Temperature on i^{th} tray (K)
- k_{bi} Backward specific reaction rate on i^{th} tray
- k_{fi} Forward specific reaction rate on i^{th} tray
- v_j Stoichiometric coefficient of component j
- $x_{D,j}$ Liquid composition in reflux drums of j^{th} component (mole fraction)

$x_{NT,j}$ Liquid composition on NT^{th} tray in j^{th} component (mole fraction)
 $x_{i,A}$ Mole fraction of component A on i^{th} tray (mole fraction)
 $x_{i,B}$ Mole fraction of component B on i^{th} tray (mole fraction)
 $x_{i,C}$ Mole fraction of component C on i^{th} tray (mole fraction)
 $x_{i,D}$ Mole fraction of component D on i^{th} tray (mole fraction)
 $y_{NT,j}$ Vapour composition on NT^{th} tray of j^{th} component (mole fraction)
 A_{vp} Antoine constant for component A
B Bottom flow rate (lb-mole/h)
 B_{vp} Antoine constant for component B
D Distillate flowrate (lb-mole/h)
L Liquid flow rate (lb-mole/h)
NC Number of component
NT Total number of trays
P Pressure in the column (psia)
 P_j^s Pure vapour pressure of components j (psia)
R Reflux flowrate (lb-mole/h)
V Vapour flow rate (lb-mole/h)
 α Relative volatility
 ΔH_v Heat of vaporization (Btu/lb_m)
 λ Heat of reaction (Btu/lb-mole)

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