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Application of Neural Network based Control Strategies to Binary Distillation Column

Amit Kumar Singh *, Barjeev Tyagi,
Vishal Kumar

Electrical Engineering Department,
Indian Institute of Technology, Roorkee, India.
**Corresponding Author email: akschauhan.amit@gmail.com*

Abstract: This paper presents three different neural network based control schemes to the control of the Distillate composition of binary distillation column. The main goal is to control a single output variable, the Distillate composition, by changing two manipulated input variables, reflux flow rate and steam flow rate. A first-principle equation based model of binary distillation column is developed in SIMULINK® and validated by the experimental results. This model is used here as a reference model on which the developed neural control schemes have been applied. Three approaches Neural Network based Direct Inverse control (NN-DIC), Neural network based model reference adaptive control (NN-MRAC) and Neural network based internal model control (NN-IMC), are simulated and their performances are assessed. Comparison was also made with conventional PID cascade control. The results demonstrate that NN-IMC strategy provides a better performance than PID, NN-DIC and NN-MRAC for the cases analyzed.

Keywords: Direct inverse control (DIC), feed forward networks (FFN), internal model control (IMC), model reference Adaptive control (MRAC), distillation column

1. INTRODUCTION

Artificial neural networks (ANNs) have shown an excellent ability to model any nonlinear function to a desired degree of accuracy (Hornik et al., 1989). This property makes ANN suitable for the identification and control of nonlinear plants (Hunt et al., 1992). Systems based on ANNs are able to model highly nonlinear processes, to detect changes in process conditions (monitoring) and to stabilize closed-loop systems (Haber et al., 2002). Different classifications are found in the literature for neuro controllers (Hagan et *al.*, 2002; Chowdhury et al., 2001; Willis et al., 1992). In the late 1980s, artificial neural networks were employed to map the measured output to the control command. In this article, it is assumed that, in neuro control systems, neural networks are directly involved in generating the control command. Thus, control Systems with ANN observers without neuro controllers (Hornik et al., 1989; Scardovi et al., 2007) are not addressed. ANNs, trained using such data, could produce a control command which would lead to a desired output. This approach is called inverse dynamics or the inverse modeling method and used to be the dominant approach in the era of the pioneers of neuro control (Miller et al., 1989; Andersen et al., 1990) without directly mentioning the word "inverse" as the name of the method. The term "inverse" gradually appeared to introduce this approach in the early 1990s (Hunt et al., 1991; Lee et al., 1992).

In general the inversion of nonlinear models is not an easy task and analytical solutions may not exist, so solutions have to be found numerically. There are several strategies for obtaining the inverse model so that the nonlinear performance can be fully exploited in order to cope with a complex plant (Carotenuto et al., 2001). Narendra and Parthasarathy used two ANNs for modeling and control at the same time and devised model reference neuro control (Narendra et al., 1990). Few researchers were employed ANNs to generalize well known nonlinear control methods (Kuttisupakorn et al., 2001). From the early 2000s, in some research works, after ANN compensation, the resultant dynamics was still nonlinear and was controlled using well-known nonlinear control methods (Gong et al., 2001). Neural network based estimator is developed for the estimation of methanol composition on the application of distillation column in the recent research works (Singh et al., 2007; Singh et al., 2013).

The internal model control (IMC) strategy is considered in this paper, due to its excellent robustness and stability (Morari et al., 1989). The IMC-based ANN (IMC-NN) strategy consists in training a network to learn the process dynamics. Another ANN is trained to learn the inverse dynamics so that it can be used as a nonlinear controller. Lightby and Irwin (Lightbody et al., 1997) have shown how Multi Layer Perceptron (MLPs) is used for providing controllers on the basis of the IMC principle. An internal model is linearised and an inverse controller is obtained via Kalman's method. Recently, Kambhampati et al. (Kambhampati et al., 2000) have suggested the utilization of recurrent neural networks (i.e., Hopfield neural networks) in the IMC strategy. Some interesting work has been done in the field of neural control schemes recently (Mohammadzaheri et al., 2011; Yu et al., 2011). In this paper, following three neuro control methods are briefly introduced in chronological order, so as to cover both well-established and emergent methods.

1. ANN Direct inverse control systems (NN-DIC)

2. ANN model reference control systems (NN-MRAC)

3. ANN Internal model control systems (NN-IMC)

A conventional cascaded PID controller was also compared with these schemes in order to provide some further insight into the performance of the neural-network control. These control schemes are used to produce an efficient control to get the desired distillate composition. The main goal is to control a single output variable, distillate composition, by changing two manipulated variables, the reflux flow rate and steam flow rate. This paper is organized as follows. Sect. 2 gives a brief introduction to the lab setup of binary distillation column on which the experimental work has been done. A brief introduction along with design and implementation of direct inverse control, internal model control and model reference adaptive control strategy is given in Sect. 3. In Sect.4 some simulation results and the comparison of NN-DIC, NN-IMC and NN-MRAC strategies are given. Finally, the authors' conclusions are presented.

2. PILOT PLANT OF BINARY DISTILLATION COLUMN

The lab set up of nine-tray continuous binary distillation column unit with a single feed and two product streams can be seen in fig. 1. Mixture of methanol and water is taken as feed to the column. The BDC contains a vertical column that has nine equally spaced trays mounted inside of it. Every tray has one conduit on alternate side, called down comer. Liquid flows through these down comers by gravity from each tray to the one below. Every tray has a weir, which is present on one side of the tray to maintain the liquid level at a suitable height. In the present laboratory set-up, bubble cap trays have been placed, however flexibility has been provided to change them to sieve trays. One reboiler is connected to the vertical shell suitable piping. It provides necessary heat for vaporization for distillation column operation. It has three electric heaters of 4kW, 2kW and 2kW.One condenser that is connected to the column through another piping so as to condense the overhead vapors. Water is used as coolant in condenser. There are two feed tanks for storing and supplying the feed to the distillation column whenever required. Three rotameters are provided for measuring the liquid flow rate as well as for controlling the liquid flow of feed, the bottom product and the cooling water. a pressure regulator is provided to set the pressure in the column. An Automatic Control Valve is provided to fix and control liquid flow of feed. A Compressor is provided to develop necessary pressure for circulating the feed.

Transducers are interfaced in the BDC to facilitate monitoring and control of various parameters of the column under consideration. There are total twelve Resistance Temperature Detectors (RTD) are used, out of which nine are fitted in the trays, one in reflux drum, one in condenser inlet and one in condenser outlet. Every RTD has attached with an isolator to convert the output of the RTD into current outputs for the corresponding Resistance Temperature. A level transmitter is attached with the column to sense the level of the reflux drum. There are two pressure transmitters available to sense the vapor pressure at the bottom and at the top of the distillation column. A flow transmitter is attached for sensing the feed flow.

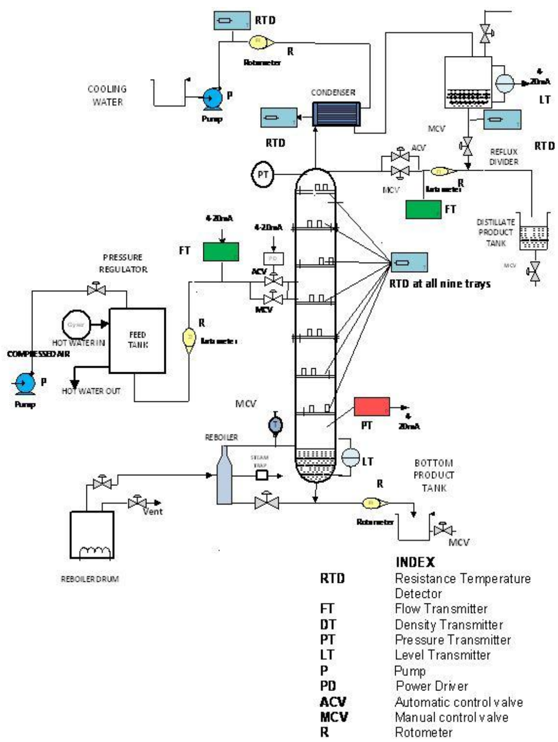

Fig. 1. Schematic Diagram of Distillation Column with Instrumentation.

A First principle equation based model of binary distillation column has been developed in the environment of SIMULINK® .The detail regarding the model is given in Appendix A. The specifications of experimental setup of binary distillation column are annexed in Appendix B.

3. INTRODUCTION TO DEVELOPED CONTROL APPROACHES

There are several schemes that have been proposed for the neural control of nonlinear systems (Scardovi et al., 2007).Three schemes took into consideration here, NN-DIC scheme, NN-IMC scheme and NN-MRAC scheme. In this section the brief introduction to each scheme is given.

3.1 NN-DIC Scheme

Inverse models provide the neural net structure which represents the inverse of the system dynamics in the region of the training/identification. Here identification process has been carried out by the generalized inverse learning technique (Hagan et al., 2002b).

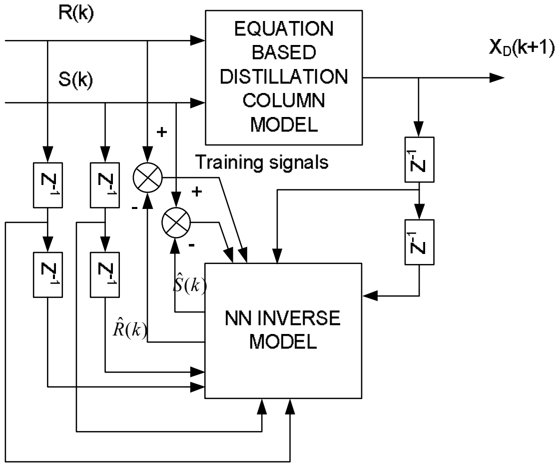

Fig. 2. Schematic of NN-DIC strategy.

Here, the required future or reference output together with the past inputs and the past outputs are fed to the network to predict the current input or control action, $u(k)$ i.e. R(k) and S(k). The trained network represents the inverse model of the system. The desired value of the output, $X_D(k + 1)$ corresponds to the required set point or reference signal. Although various prediction horizons can be used for both the forward and inverse models, this study concentrates on a simple one-step ahead horizon which assumes that there are no additional time delays between the control action and the output. fig. 2. illustrates the NN-DIC Strategy. The inverse model can be expressed mathematically in functions of inputs as Shown below in (1): -

$$\hat{u}(k)=f(R(k-1),R(k-2),S(k-1),S(k-2),X_D(k-1),e_R(k),e_S(k)) \tag{1}$$

where $u(k)=\hat{R}(k)$ and $\hat{S}(k)$

$e_R(k)=R(k)-\hat{R}(k)$ and ,

$e_S(k)=S(k)-\hat{S}(k)$

3.2 NN-IMC Scheme

Internal model control (IMC) (Hagan et al., 2002a) incorporates approximations of both the system model and its inverse in the control algorithm. Here, the inverse model which generates the required input(s) which would take the current system to the desired output(s) is used as the controller for the process. Nonlinear Internal Model Control (NIMC), shown in fig. 3, consists of a neural network controller, a neural network plant model, and a robustness filter with a single tuning parameter.

In this scheme, both the forward neural network model (that is, one which predicts future outputs given previous inputs and outputs) and the inverse model (that is, one which predicts the required inputs given previous inputs and outputs and a desired future output) are used in the feedback loop.

The relationship between the forward and inverse neural network models is illustrated in Fig. 3. When the network inverse model acting as a controller it gives the appropriate control action, *R(k)* and *S(k)* , to drive the system towards its desired set point, X_{DSP}. The desired set point is fed to the network together with the past plant inputs and outputs to predict the required current plant inputs. The plant and the forward neural network model are placed in parallel to cater for plant/model mismatch and this error is subtracted from the set point before being fed back into the inverse model. The forward model is fed with the proposed input to the plant (that is, the output of inverse model) as well as with the past inputs and past outputs of the plant. In cases of noisy plant output data, the forward model can also be fed with its own past outputs instead of the plant outputs. A filter, F can be introduced prior to the controller in this approach in order to incorporate a degree of robustness in the feedback system this can be especially important where it is difficult to get exact inverse models. This NN-IMC strategy is normally formulated in input-output form for ease of implementation. Here, the inputs to the network are past and current states. In this way, one can obtain a state space representation of the closed loop inverse neural network-based IMC control configuration. The result assumes that the forward model is an exact representation of the system model.

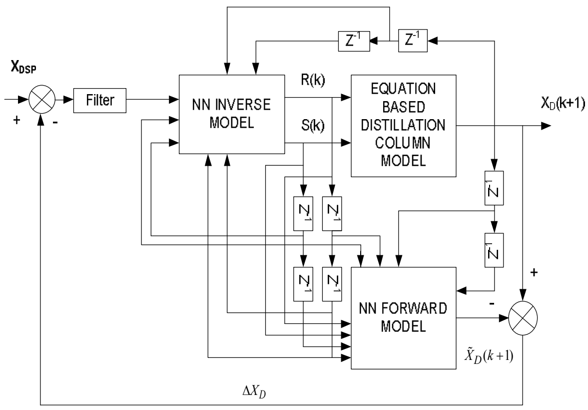

Fig. 3. Schematic of NN-IMC strategy.

The most popular and straightforward approach for the identification of forward model is to augment the network inputs with corresponding discrete past inputs and past output data signals from the model or system being identified as seen in fig. 4.

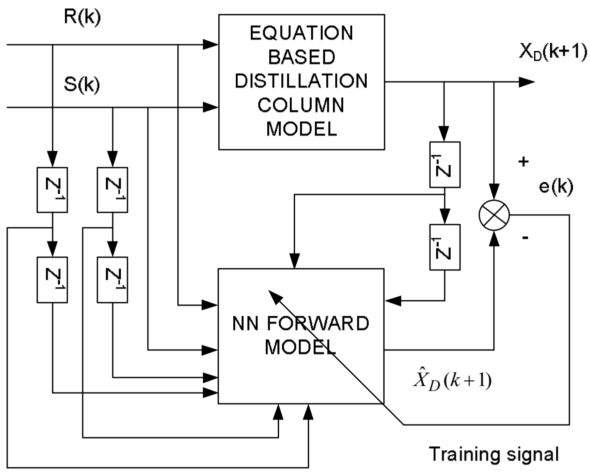

Fig. 4. Structure for the training of forward neural network model.

Other available state variables, considered as part of the inputs, can also be fed into the network as was done in this study. The neural network is placed in parallel with the model or system and the error between the system output and network output (i.e. prediction error) is used as the training signal for the inverse neural network. The forward model can be expressed mathematically in functions of inputs as Shown below in (2): -

$$\hat{x}_D(k+1) = f(R(k),R(k-1),R(k-2),S(k),S(k-1),S(k-2),X_D(k),X_D(k-1))$$

Where $\hat{x}_D(k+1)$ = Plant output, (2)

This identification includes various important steps to be followed: selection of model structure and size, data set, input excitation signal, weight initialization, training method and model validation. One point which deserves special attention is the appropriate number of past inputs and outputs which are provided to the network for the purposes of identification. Here two past values and two future values have been taken into consideration. Identification of inverse model is same as given in section 3.1.

3.3 NN-MRAC Scheme

As with other techniques, the Neural Network Model Reference Adaptive Control (NN-MRAC) (Scardovi et al., 2007) configuration consists of a neural network controller, a neural network plant model and a reference model as shown in fig. 5.

The difference between NN-IMC and NN-MRAC configuration is that there is no robustness filter in NN-MRAC scheme but instead of that there is a reference model which output is compared with the neural network controlled plant. The differences between these two models give control error. Here NN forward model is attached in the same manner as in the NN-IMC configuration. The model network can be trained off-line using historical plant measurements.

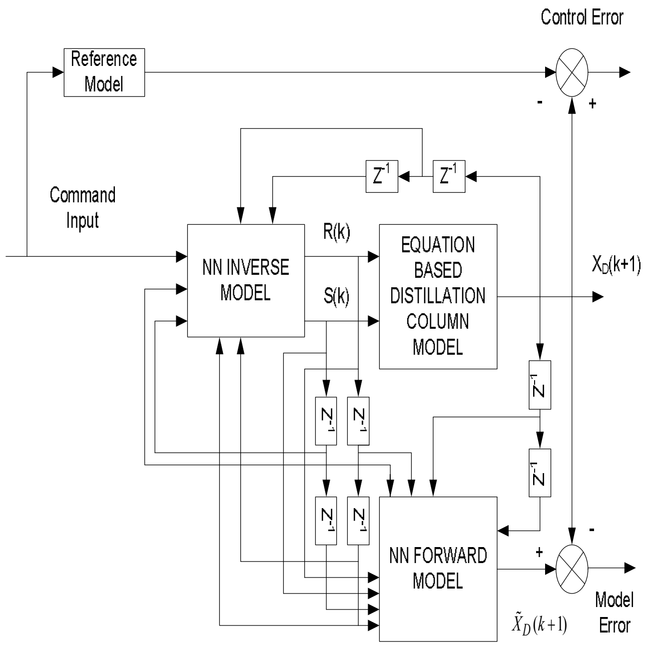

Fig. 5. Structure of the NN-MRAC strategy.

3.4 Classical PID Controller

The PID controller (Aström et al., 1995) is consists of proportional, integrative and derivative elements. It is widely used in feedback control of industrial processes. Here the PID controller is designed to control the purity of methanol composition of distillation column. To design the PID controller the environment of Matlab®/ Simulink® is used. Two PID controllers are designed because there are two manipulated variables reflux flow rate and reboiler heat duty to control the controlled variable (methanol composition) in distillation column. Designed PID controllers are applied to the equation based distillation column model as discussed in appendix A.

The PID scheme and terminology as follows:

$$u(k+n) = K_P\left[e(k+n) + \frac{\Delta k}{\tau_i}.\sum_{i=0}^{n} e(k+n) + \frac{\tau_d}{\Delta k}(e(k+n) - e(k+n-1))\right] \quad (3)$$

Where K_P, τ_i and τ_d are the tuning parameters of PID controller. u(k+n) is the output of the PID controller. e(k+n) is the difference between the desired methanol composition and measured methanol composition at n^{th} time interval. Here the inputs are same for both of the PID controllers i.e. e(k+n) but the outputs are different. Outputs of the PID controllers are reflux flow rate and reboiler heat duty respectively. The tuning parameters of PID controllers are acquired by the Ziegler-Nichols method (Ziegler et al., 1942). To apply the Ziegler-Nichols method step responses of distillation column are used. A unit step input is applied to both of the inputs of distillation column and checked the step responses one by one. The final tuning parameters of each controller computed by Ziegler-Nichols method are summarized in Table 1.

Table 1. PID controller tuning parameters.

Tuning parameters	PID controller 1 (Reflux flow rate loop)	PID controller 2 (Reboiler heat duty loop)
K_P	2	5
τ_i	10	15
τ_d	0.01	0.02

4. SIMULATION AND EXPERIMENTAL STUDIES

4.1 Validation of Equation based model with the experimental setup

First of all the developed model has been validated with the real experimental results so that the developed control strategies can be applied on that model. The model has been developed in the environment of SIMULINK® .The model details has been illustrated in appendix A. For the simulation of a distillation column the quantities such as feed composition, flow rate, temperature and pressure, column pressure, stage efficiencies are assumed to be specified and for this purpose the formulation of dynamic equations for the composition response with L and V as independent variables is required. The nonlinear model contains two manipulated inputs (R, V_B), a disturbance (F) and 18 states (state1: liquid composition in reboiler x_1=X_B, then follow the stage compositions x_i up the column, state 9: composition stage 9 (condenser) x_9= Y_D, state 10: holdup reboiler M_B, then follow the stage holdups up the column M_i, state 18: condenser holdup M_D).

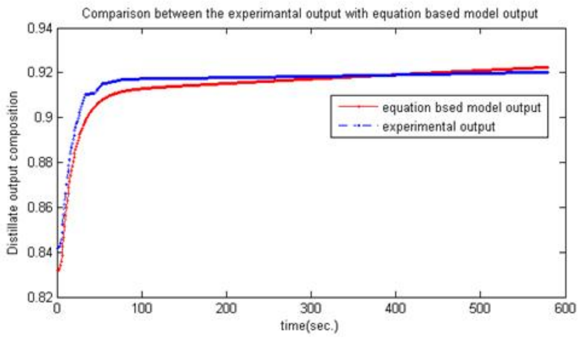

Fig. 6. Comparison between real data and equation model output.

The output of the model is distillate output. The comparison of distillate output composition of equation based model and the lab setup of binary distillation column can be seen in fig. 6. The error between the models output is shown in fig. 7.

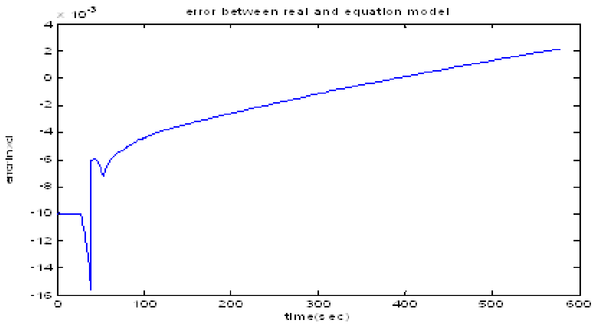

Fig. 7. Error between real data and equation model output.

The result shows that the developed model is closely working as the experimental setup. These results have been acquired from the experimental operation of binary distillation column in the open loop manner it means that there was no controlling action.

4.2 Application of NN-DIC, NN-IMC and NN-MRAC Strategies to Binary Distillation Column Model

4.2.1 Neural Network Training

In order to implement the neural-net inverse control methods on-line, the plant was first operated open-loop in order to generate the relevant data for training the neural-net forward and inverse models of the system. The open loop data were generated by varying the control input signal to excite the system adequately and extract its dynamic behaviour. In the experimental system, these could not be chosen randomly as in simulation studies but had to be compatible with the operating conditions, operating constraints and response time of the system. Because of these limitations, more structured signals were used for training. The data for training the network were sampled at 5 second intervals with 2700 data sets collected. This frequency was fast enough to capture the system dynamics for training the forward and inverse models. Similarly, several test data sets were generated for further training of the models and `validation' sets for observing the performance of the models when faced with unknown situations or dynamic changes of different amplitudes.

The same data sets were used for training both the forward and inverse models; it is only the input/output patterns of these models that are different. The data collected included the present and past values of the control inputs (Reflux flow rate and steam flow rate), Output distillate composition as required for the forward and inverse models. Note that although in a real plant accurate composition measurements would not generally be available on-line, some estimate of Composition (via an estimator, Kalman filter or other `soft sensor') periodically updated by sample measurements, might will be implemented as part of an advanced control algorithm. Training was performed for both the forward and inverse models using the fast back-propagation method. An adaptive learning rate (as found in the Neural Network Matlab toolbox) was used in the initial stages of learning to speed up the convergence rate due to the large amount of data being processed. When the convergence was close to an acceptable value, the learning rate was kept constant and applied until the end of training. The final neural network forward model chosen has 8 input nodes, 20 hidden nodes and 1 output node with sigmoid activation functions. An identical topology was used for the inverse model.

4.2.2 Simulation Studies

The forward and inverse models will be incorporated in the IMC strategy in on-line experiments only after they were tested first in simulation using a developed model of the Distillation column illustrated in appendix A. The simulation study has been done to examine the accuracy of the forward and inverse models in closed-loop situations and to observe the performance and stability of the developed controllers in the case of plant/model mismatch. Mismatches were introduced in this simulation due to inherent differences between the simulated plant and the neural network forward and inverse models (which were identified from real experimental data).

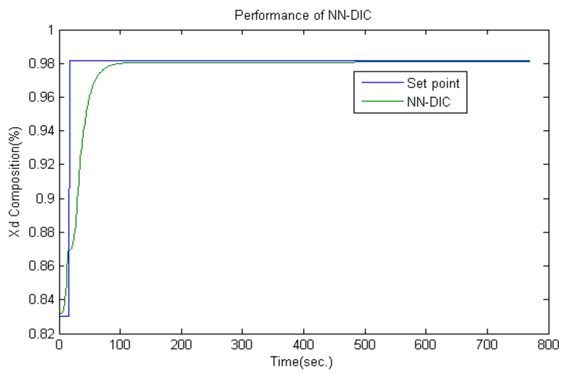

Fig. 8. Performance of NN-DIC scheme.

Two typical simulation results were discussed here one for set-point tracking and another for disturbance rejection. The set point is desired distillate composition which is varied from the nominal steady state value 83% to 98 % distillate composition. For set point tracking the performance of NN-DIC scheme is shown in fig. 8.

NN-IMC and NN-MRAC have introduced some good results as can be seen in the fig. 9 and 10.

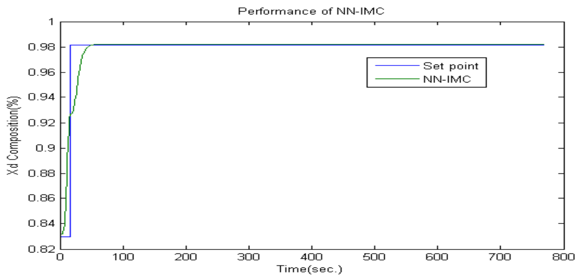

Fig. 9. Performance of NN-IMC scheme.

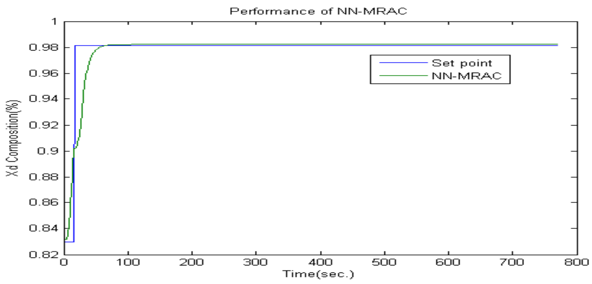

Fig. 10. Performance of NN-MRAC scheme.

In NN-MRAC scheme control error and model error also came into picture as shown in fig. 11.

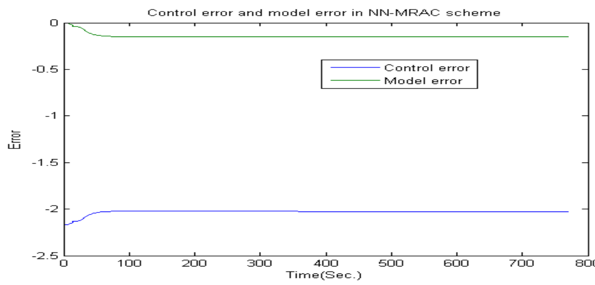

Fig. 11. Control error and model error in NN-MRAC scheme.

Control error defines the controller performance and model error shows the mismatch between the plant model and developed neural network forward model. Here both control and model errors are in the desired limits.

A conventional cascaded PID controller was also tested in the same circumstances in order to provide some further insight into the performance of the neural-network controller. Here, the error between the desired distillate composition and acquired distillate composition is fed to PID and reflux flow rate and steam flow rate are the outputs. Figure 12 illustrates the performance of PID controller. It shows that PID gives more undershoot and larger settling time than the neural based schemes. The comparison of performances of neural schemes to get the better understanding illustrated in fig. 13.

It can be seen here that NN-IMC performs better than the other schemes to track the set-point.

Fig. 14 shows the graph of errors produced by different neural schemes. NN-IMC produced the least error and PID produced largest error.

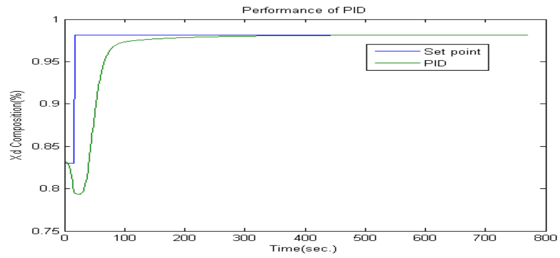

Fig. 12. Performance of conventional PID controller.

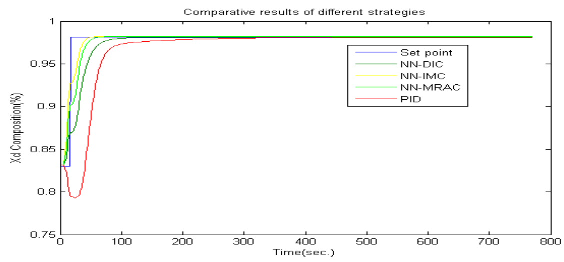

Fig. 13. Comparison of performance of different control schemes.

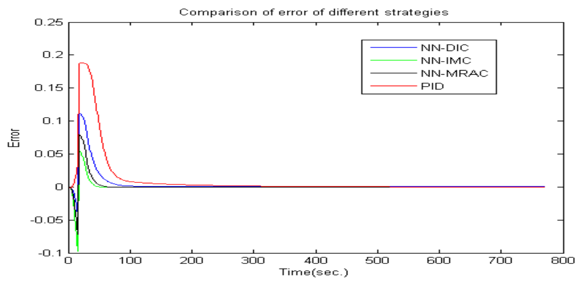

Fig. 14. Errors of different control schemes.

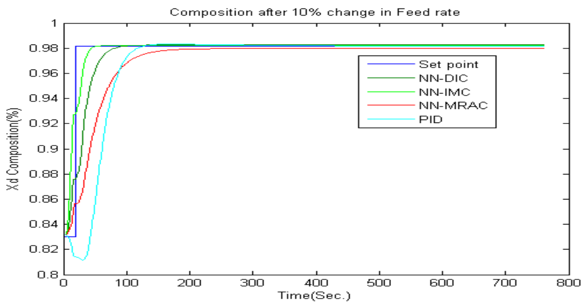

Fig. 15. Comparison of performance of different control schemes after 10% change in feed flow.

The developed neural schemes were also tested for the disturbance rejection. To test this 10% change has been incorporated in the feed flow. Change in feed flow worked as a disturbance for the distillation process and it upset the thermal equilibrium of the distillation column.

Fig. 15 shows the comparative performance of neural schemes when 10% change has been incorporated in feed flow. Error was also graphed in figure 16 to trace the changes in performance of neural schemes.

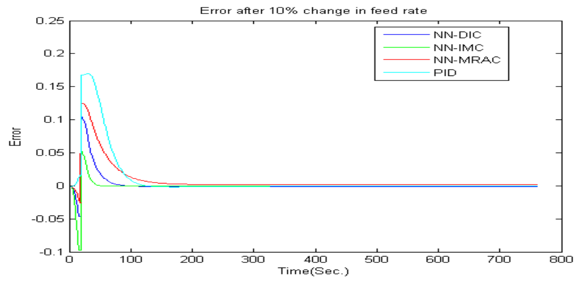

Fig. 16. Error of different control schemes after 10%b change in feed flow.

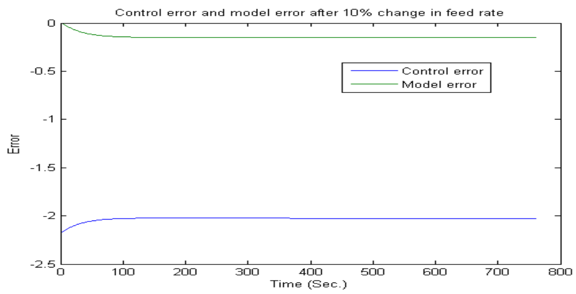

Fig. 17. Control error and model error in NN-MRAC scheme after 10% change in feed rate.

By The fig. 15 and 16 it concludes that NN-IMC scheme rejects the disturbance in better manner than the other schemes. Model error and control error are shown in fig. 17 in the case of NN-MRAC scheme.

5. CONCLUSION

The main purpose of performing this experimental investigation was to develop and test the different neural network control strategies under real plant conditions. The developed schemes have been applied on the developed equation based model. The validation of this developed model has been done by the experimentally acquired data of the existing model of binary distillation column. NN-DIC, NN-IMC and NN-MRAC strategies have been developed and investigated here. Earlier theoretical work indicated that NN-IMC configuration had some positive advantages when compared with other forms of neural network based control schemes. Here two cases have been investigated for all the developed neural schemes, one is set-point tracking and another is disturbance rejection. Result shows that NN-IMC scheme performed better for both the cases. Comparisons were also made with PID/cascade control, an existing classical control strategy normally implemented in the process industries. So, finally this paper concludes that NN-IMC scheme maintain its performance objective (to control the distillate composition at the desired set point) in a better way than the conventional PID controller, NN-DIC and NN-MRAC schemes.

NOMENCLATURE

A_{net}	Net area of the tray, m^2	M_B, M_D, M_i	Liquid molar hold up reboiler , reflux drum and on i^{th} tray respectively
B	Bottom product rate, kmols/h	NC	No. of components
D	Distillate product rate kmols/h	NT	Total no. of trays in distillation column
F_i	Total feed flow rate into i^{th} tray kmols/h	Q_B,Q_C	Heat duty of reboiler and condenser respectively, kj/hr
h_B	Total molar enthalpy of bottom kj/kmol	R	Reflux flow rate , kmol/hr
h_f	Total molar enthalpy of feed kj/kmol	S	Steam flow rate, kmol/hr
h_i	Total molar enthalpy of liquid mixture kj/kmol	V_i	Total vapour flow rate from the tray kmol/hr
h_w	Height of the weir, m	x	Liquid composition of more volatile component, mole fraction
H_i	Total molar enthalpy of vapour, kj/kmol	y	Vapour composition of more volatile component, mole fraction
L_i	Total liquid flow rate leaving the tray, kmols/h	y_{ij}*	Equilibrium vapour composition of j^{th} component on i^{th} tray, mole fraction
l_w	Length of the weir, m	η_{ij}	Murphree stage efficiency on tray I of component j

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APPENDIX A

Equation Based Modeling

Dynamic simulation of distillation is characterized by stiff set of differential algebraic equations of material and efficiency equilibrium relationships. The dynamic model to be developed in this work is expected to meet the following objective: The model should be easy to use for the design of distillation column control schemes, online identification and optimization purposes.

To develop the equation based model, the following information has been taken directly from the existing experimental setup of binary distillation column:

(1) Liquid composition on each tray
(2) Liquid flow rates from each tray
(3) Temperature of each tray
(4) Condenser and reboiler duties

To simplify the model, the following assumptions have been considered (Luyben, 1990):

1) The relative volatility **α** is constant throughout the column.
2) The vapor - liquid equilibrium relationship can be expressed by

$$y = \frac{\alpha x}{1 + (\alpha - 1)x}$$

Where
α = Relative volatility
x= Composition of more volatile component in liquid, mole fraction,
y= Composition of more volatile component in vapor, mole fraction

3) The overhead vapor is totally condensed in the condenser.
4) The holdup of vapor is negligible throughout the system(i.e., the same immediate vapor response, $dV_1 = dV_2 = \ldots = dV_{N+1} = dV$) , where N= total number of trays
5) The molar flow rates of the vapor and liquid through the stripping and rectifying sections are constant: $V_1 = V_2 = \ldots = V_{N+1}$; $L_2 = L_3 = \ldots = L_{N+2}$
6) Reboiler and condenser are also considered as a tray. Numbering of trays is done from the bottom i. e. boiler is considered as a first tray and condenser is considered as a last tray. This means that if there is N number of trays then boiler is first tray and condenser is (N+1)th tray.

Distillation column is divided into three different sections for the modeling point of view as shown in fig. A.1. I[st] section is reboiler section, II[nd] section is Tray section, and III[rd] section is condenser section. The material and enthalpy balance equations are obtained by applying conservation laws to these sections.

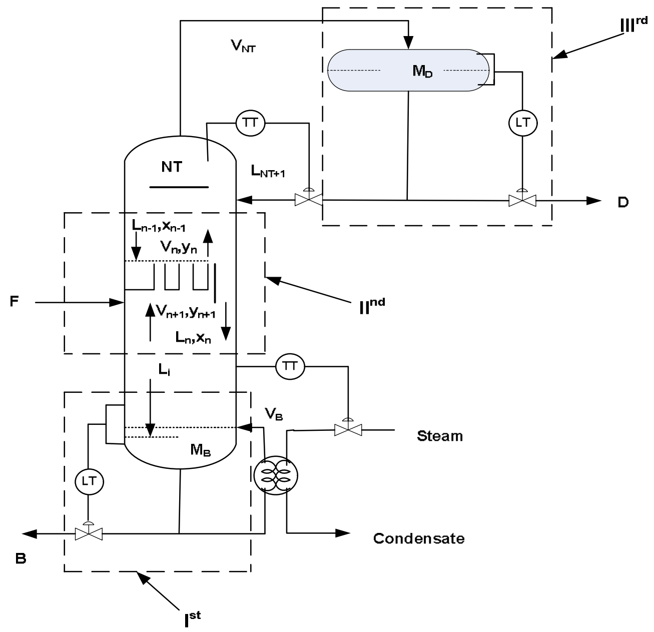

Fig. A.1. Distillation column used in modelling.

<u>*Ist Section*</u>

Component material balance Equations

The constant molar holdup in reboiler has been considered i.e. $dM_B/dt=0$, so by this
$B = L_l - V_B$
Component material balance around reboiler is given by

$$M_B \frac{dx_{B,j}}{dt} = L_1 x_{1,j} - V_B y_{B,j} - (L_1 - V_B) x_{B,j} \quad \text{(A.1)}$$

Where M_B= Liquid molar hold up in reboiler, kmoles ,
L_l= Total liquid flow rate from tray-1 entering to reboiler, kmole/hr,
$x_{B,j}$ = Liquid fraction of component j in bottom product ,% mole fractions,
V_B = Total vapor flow rate leaving reboiler, kmole/hr,
$y_{B,j}$ = Vapor fraction of component j in bottom product ,% mole fractions,
B = Total bottom product rate, kmole/hr,

The vapor fraction of component j from reboiler is given by

$$y_{B,j} = \eta_{1,j}^{v} . k_{1,j} x_{B,j} \quad \text{(A.2)}$$

where
$\eta_{1,j}^{v}$ = vaporization efficiency of component j in reboiler,
$k_{1,j}$ = Equilibrium constant of component j in reboiler

Total enthalpy balance equations

Total enthalpy balance equation for reboiler is given by

$$M_{B.} \frac{dh_B}{dt} = L_1 h_1 - V_B H_B - (L_1 - V_B) h_B + Q_B \quad \text{(A.3)}$$

Where
h_1 = Total molar enthalpy of liquid entering from tray-1 to reboiler, kJ/kmole,
h_B = Total molar enthalpy of liquid leaving reboiler, kJ/kmole,
H_B = Total molar enthalpy of vapor leaving reboiler, kJ/kmole,
Q_B = Reboiler heat duty, kW

II[nd] Section

In the second section modeling for general i-th tray is considered. Material balance and energy balance equations is obtained for this section.

Component material balance Equations

Component material balance Equation for i^{th} tray is given by

$$\frac{d(M_i x_{ij})}{dt} = L_{i+1}x_{i+1,j} - L_i x_{ij} - V_i y_{ij} + V_{i-1}y_{i-1,j} + F_i x_{Fij} \quad (A.4)$$

y_{ij} is calculated as

$$y_{ij} = \eta_{ij}(y_{ij}^* - y_{i-1,j}) + y_{i-1,j} \quad (A.5)$$

Where M_i= Molar liquid hold up on tray I, kmole
x_{ij} = Liquid fraction of component j, leaving the tray i , % mole fraction
L_i = Total liquid flow rate leaving tray-i, kmole/hr
V_i = Total vapor flow rate leaving tray-i, kmole/hr
F_i = Total feed flow rate injected to tray-i, kmole/hr
x_{Fij} = Liquid fraction of component j in feed on tray i ,% mole fractions,
y_{ij} = vapor fraction of component j leaving the tray i ,% mole fractions,
η_{ij} = Murphree stage efficiency based on vapor phase of component j on tray i
y_{ij}^* = Equilibrium vapor fraction of component j on tray i
L_i is an additional variable and it is related to M_i through

$$L_i = 3.33 l_w \left[M_i / (A_{net} . M_{Di}) - h_w \right] \frac{3600}{2.204} M_{Di} \quad (A.6)$$

Where l_w = Length of the weir, ft
A_{net} = Net area of the tray, ft^2
h_w = Height of the weir, ft
M_{Di} = Average molar density of liquid on tray I, kmole/ft^3
Total Material Balance Equation for i^{th} general tray is calculated as

$$\frac{dM_i}{dt} = L_{i+1} - L_i - V_i + V_{i-1} + F_i \quad (A.7)$$

Where
L_{i+1} = Total liquid flow rate entering to tray i, kmole/hr,
V_{i-1} = Total vapor flow rate entering to tray i, kmole/hr,
F_i = Total feed flow rate injected on tray i, kmole/hr

Enthalpy balance equation for general tray i

Enthalpy balance equation for general tray-i is given as

$$\frac{d(M_i h_i)}{dt} = L_{i+1}h_{i+1} - L_i h_i - V_i H_i + V_{i-1}H_{i-1} + F_i h_{Fi} \quad (A.8)$$

Where
h_i = Total molar enthalpy of liquid leaving tray I, kJ/kmole,
H_i = Total molar enthalpy of vapor leaving tray I, kJ/kmole

Enthalpy on any tray are calculated by mixing rule as given by

$$h_i = \sum_{j=1}^{NC} hl_{ij} x_{ij} \quad (A.9)$$

$$H_i = \sum_{j=1}^{NC} Hv_{ij} y_{ij} \quad (A.10)$$

Where
hl_{ij} = Pure component enthalpy of component j in liquid, kJ/kmole,
Hv_{ij} = Pure component enthalpy of component j in liquid, kJ/kmole
Next section i. e III[rd] section produces the modeling of condenser.

III[rd] Section

Component material balance Equations

Reflux drum level is considered constant. This means at any time $D=V_{NT}-R$
Component material balance around condenser is given by

$$M_D \frac{dx_{D,j}}{dt} = V_{NT} y_{NT,j} - V_{NT} x_{D,j} \quad (A.11)$$

Where
M_D= Liquid molar hold up in the reflux drum, kmole,
D = Distillate flow rate, kmole/hr,
$x_{D,j}$ = Liquid fraction of component j in reflux drum, % mole fractions
$y_{NT,j}$ = Vapor fraction of component j leaving tray NT ,% mole fractions,
R = Total liquid flow rate entering to the tray NT from reflux drum, kmole/hr,
V_{NT} = Total vapor flow rate leaving the tray NT, kmole/hr,

Enthalpy balance equation

The enthalpy balance equation for liquid and vapor for condenser is

$$M_D \frac{dh_D}{dt} = V_{NT} H_{NT} - V_{NT} h_D - Q_c \quad (A.12)$$

Where
h_D = Total molar enthalpy of liquid leaving the reflux drum, kJ/kmole ,
H_{NT} = Total molar enthalpy of vapor leaving the last tray NT, kJ/kmole,
Q_C = Condenser duty, kW

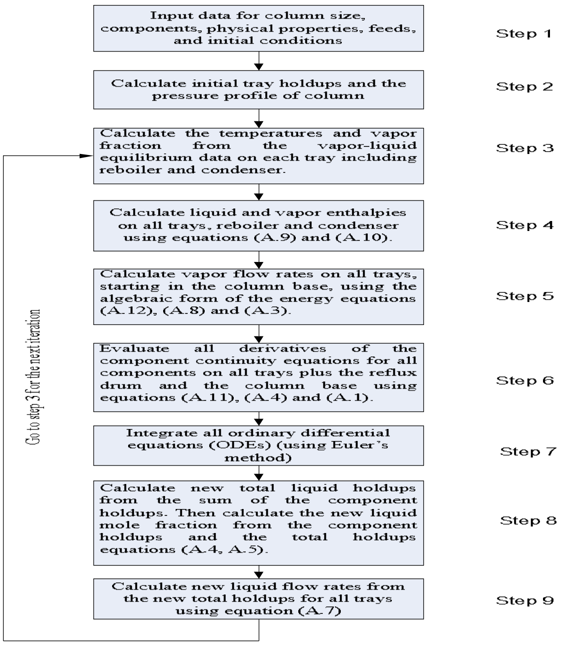

Fig. A.2. Simulation Algorithm.

All the above equations have been used to develop the model. The flow diagram of the simulation algorithm to develop the equation based model of binary distillation column is given in fig. A.2. To simulate open loop binary distillation column the environment of MATLAB®/SIMULINK® has been used.

APPENDIX B

Number of trays	9
Weir height in stripping section	0.47 inch
Weir length in stripping section	0.47 inch
Column diameter in stripping	4.80 inch
Weir height in rectifying section	5.91 inch
Weir length in rectifying section	5.91 inch
Column diameter in rectifying	4.80 inch
Volumetric hold up in column	0.5414 ft3
Volumetric hold up in reflux	0.0001 ft3
Liquid feed rate	2.5 kg-moles/hr
Liquid feed temperature	34.5 deg-C
Pressure in the bottom	115.21 kPa
Pressure in the reflux drum	101.42 kPa
Reboiler heat input	6.0 kW
Reflux flow rate	3.0 kg-moles/hr
Vapor distillate product flow	0.0 kg-moles/hr
Murphree vapor efficiency	0.60