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Application of Feed Forward and Recurrent Neural Network Topologies for the Modeling and Identification of Binary Distillation Column

Amit Kumar Singh, Barjeev Tyagi and Vishal Kumar

Department of Electrical Engineering, Indian Institute of Technology Roorkee, Roorkee, India

ABSTRACT

This paper presents identification of artificial neural network model of a Binary Distillation Column (BDC). In this paper, the two most common topologies of artificial neural networks in the area of control are introduced: Feed forward neural network and recurrent neural networks. The training of neural network has been performed by the data set acquired from real 9-tray continuous BDC setup available in laboratory. The network model is composed of two layers. A hyperbolic tangent sigmoid function and a pure linear function have been utilized as activation functions in the first and the second layers, respectively. The developed neural network model has been validated by an extensive data set of practical data received from real BDC setup.

Keywords:

Binary distillation column, Feed forward neural network, Identification, Modelling, Recurrent neural network.

1. INTRODUCTION

Distillation columns are widely used in chemical processes, such as crude oil refinery and hydrocarbon processing industries. The control of the overhead and bottom compositions in a binary distillation column (BDC) using reflux and steam flow rates has shown to be a particularly difficult problem because the product quality cannot be measured economically on line. This is because the instrumentation is either very expensive and/or measurement lags and sampling delays make impossible to design an effective control system. A solution to this problem is the use of secondary measurements which replaces a mathematical model of the process with the input/output relationship-based model to predict the product quality. Neural network can be used as a model identification technique to fulfill this purpose.

Artificial neural networks (ANNs) are very effective for modeling and control applications. The ANN-based approach has some significant advantages over conventional methods such as adaptive learning ability and nonlinear mapping ability, since it is more flexible and easy to be implemented in practice. A number of applications of NNs to process control problems have been reported. Piovoso *et al.* [1] have compared NN to other modeling approaches for Internal Model Control (IMC), global linearization, and generic model Control. Seaborg and co-workers have used radial basis function NN for nonlinear

control and they have applied their approaches to simulated systems [2,3].

Most of neural networks that have been applied to the identification of nonlinear dynamical systems are based on multilayer feed-forward neural networks with back-propagation learning algorithm. A novel multilayer discrete-time neural network is presented in [4] for identification of nonlinear dynamical systems. A new scheme [5] for online states and parameters estimation of a large class of nonlinear systems using RBF (Radial Basis Function) neural network has been designed. A new approach [6] has been presented to control nonlinear discrete dynamic systems, which relies on the identification of a discrete model of the system by a feed-forward neural network with one hidden layer. A study has been given [7] regarding nonlinear system identification via discrete-time recurrent single layer and multilayer neural networks.

An identification method [8] is introduced in the form of Fuzzy-Neural Networks for nonlinear models. The Fuzzy-Neural Networks combines fuzzy "if-then" rules with neural networks. The adaptive time delay neural network is used and four architectures are proposed for identifying different classes of nonlinear systems in [9]. The identification of nonlinear systems by feed-forward neural networks, radial basis function neural networks, Runge-Kutta neural networks, and adaptive neuro-fuzzy inference systems is investigated in [10]. The simulation result reported in this paper indicates that adaptive

neuro-fuzzy inference systems give the good results for identification purposes.

In the latest work, the Levenberg–Marquardt (LM) approach is proposed by [11] for predictive inferential control of distillation process. The developed estimator using LM approach predicts the composition of distillate using column pressure, reboiler duty, and reflux flow, along with the temperature profile of the distillation column as inputs.

This paper presents two neural network identification topologies, i.e., feed forward neural network (FFNN) and recurrent neural network (RNN) for the model identification of binary continuous 9-tray distillation column. The output results of developed models have been validated and compared with the experimentally acquired results by the operation of laboratory setup of BDC. A brief discussion is given on the laboratory setup of BDC in Section 2. Section 3 presents the neural network-based algorithm for the model identification. This section also gives the introduction to the considered neural network topologies and their application for the model identification of distillation column. In this section, training of neural network model of BDC is also discussed. Section 4 contains simulation and results. The work has been summarized and concluded in Section 5.

2. LABORATORY SETUP OF BINARY DISTILLATION COLUMN

In order to get the sufficient data for the validation of the developed model, it is necessary to run experiments on a distillation column large enough in diameter to have realistic hydraulics and thermal behavior, and with a number of trays sufficient to have acceptable values of the process characteristic times. The pilot plant used has a diameter of 0.15 m and nine bubble cap trays with tray spacing of 0.15 m (total height, 1.5 m). The reboiler is of the shell-and-tube natural circulation termo-syphon type with the 25-l capacity. The overhead vapor is totally condensed in a water-cooled condenser and the reflux drum is open to atmosphere. The feed is introduced on the fifth tray from bottom.

A schematic of column setup of 9-tray continuous BDC unit with the instrumentation can be seen in Figure 1. A 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 setup, bubble cap trays have been placed; however, flexibility has been provided to change them to sieve trays. A 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 4 kW, 2 kW, and 2 kW. One condenser is also 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. Total twelve resistance temperature detectors (RTD) are used, of which nine are fitted in the trays, one in reflux drum, one in condenser inlet, and one in condenser outlet. Every RTD is 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. The specifications of laboratory setup of BDC can be seen in the Appendix 1.

3. NEURAL NETWORK DEVELOPMENT

A neural network [12] is composed of simple elements (artificial neurons) operating in parallel. The network function is determined by the connections (weights) between the elements. The neural network can be trained to approximate a given function by adjusting the values of the connections between elements. Neurons are arranged in "layers." There are a variety of neural networks suitable for different purposes. Here, the two most commonly used network topologies are introduced: FFNN and RNN.

In FFNN, the data direction is from input to output units, i.e., strictly feed-forward.

The data processing can extend over multiple (layers of) units, but no feedback connections are present. The developed feed forward model can be seen in Figure 2.

RNN contain feedback connections. Contrary to feed-forward networks, the dynamical properties of the

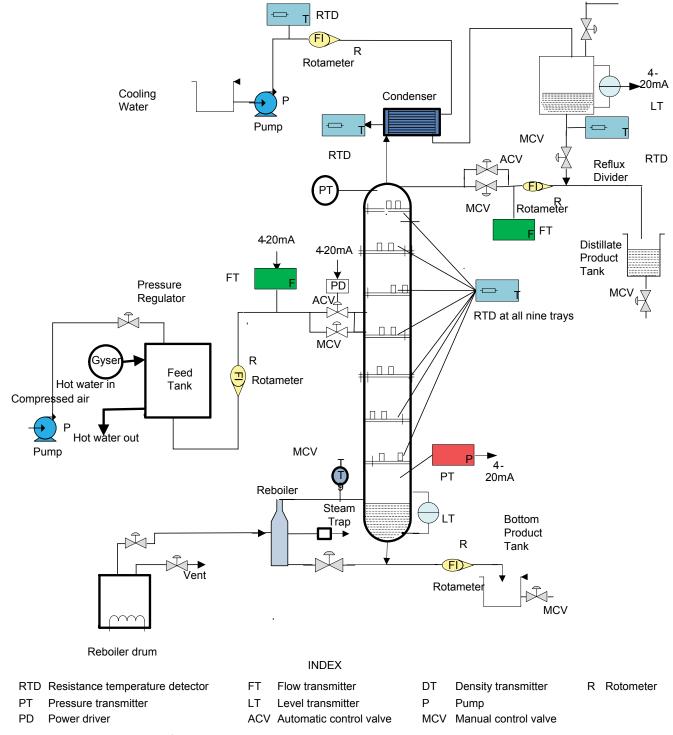


Figure 1: Schematic diagram of distillation column with instrumentation.

network are important in RNN network. Figure 3 shows the RNN model of distillation column. These are the steps of neural network model development. The flow diagram of neural network algorithm can be seen in Figure 4.

Step 1: Select proper neural network architecture like FFNN, RNN, etc

- Step 2: Vary the input variables (manipulated variables), collect the input and output data from process simulators which is normally available for any plant
- Step 3: Start training based on standard neural network training algorithm such as the LM optimization algorithm. The optimal number of hidden layers

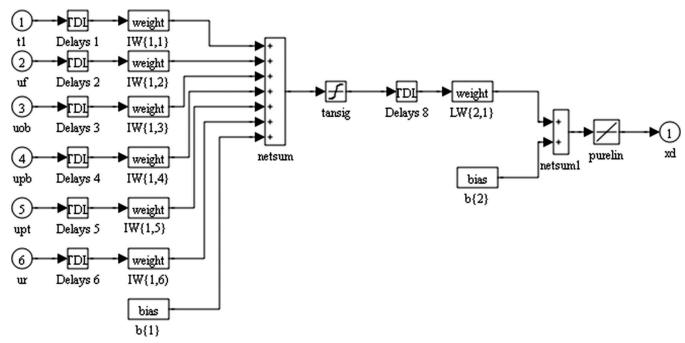


Figure 2: Feed forward neural network model of binary distillation column.

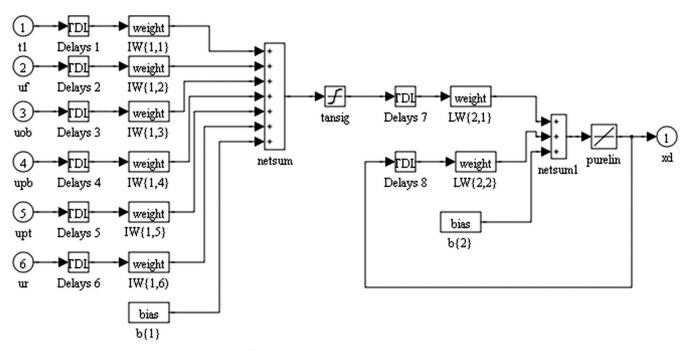


Figure 3: Recurrent neural network model of binary distillation column.

is selected based on the minimum mean square error (MSE) value

Step 4: Update weights between input-hidden as well as hidden output layers until stopping condition is reached.

The stopping condition may be number of epochs, minimum mean square error, etc.

The developed neural network has two layers, one is input or hidden layer and another is output layer.

Number of neurons in the hidden layer affects the performance of the training. There is not a definite method to select the number of neurons in hidden layer. Neurons in the input layer have been decided by trial and error method. Hidden neurons have been selected since on this value, the mean-squared error between the trained output and desired target output is minimum. In the two-layer network, a hyperbolic tangent sigmoid function has been chosen as activation function in the first layer, whereas a pure linear function has been taken in the second layer. Pure linear

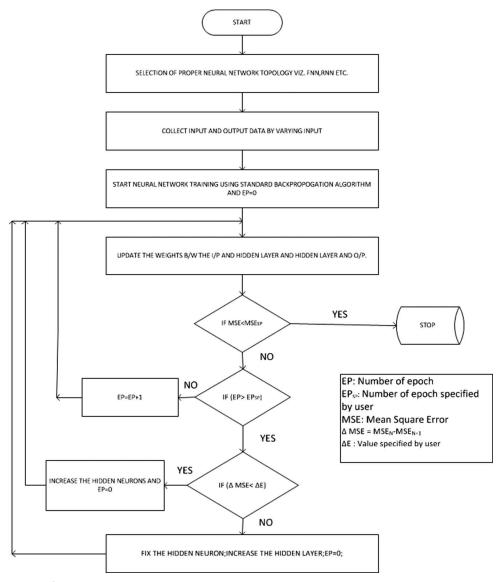


Figure 4: Flow diagram of neural network algorithm.

function in the output layer has been used to model most non-linearities.

The following are the input variables of neural network: u_p : Reflux flow rate,

u_E: Feed flow rate,

u₁₁: First tray temperature,

u_{OB}: Reboiler duty,

 $u_{PT}^{(2)}$: Reflux drum top pressure and,

u_{pp}: Reboiler bottom pressure

The output of the neural network model is x_D , the distillate output composition. The relationship between s_1 , the output of the first layer, and the input variables is given by (1)

$$\begin{split} s_1 &= IW\{1,1\}u_R + IW\{1,1\}u_F + IW\{1,1\}u_{T_1} \\ &+ IW\{1,1\}u_{Q_R} + IW\{1,1\}u_{P_T} + IW\{1,1\}u_{P_R} + b\{1\} \end{split} \tag{1}$$

Where, s_1 is the weighted sum of the input variables, which is fed to hyperbolic tangent sigmoid transfer function. The output of the hyperbolic tangent sigmoid function is x_1 which is given by (2)

$$x_1 = \tan sig(s_1) = \left[\frac{2}{1 + e^{-2s_1}} - 1\right]$$
 (2)

The difference between the structure of FFNN and RNN starts after (2). For FFNN model, x_1 multiplies with the weight and sum up with the bias. It gives s_2 as shown in (3).

$$s_{2(FNN)} = LW\{2,1\}x_1 + b\{2\} \tag{3}$$

Now, $s_{2(FFNN)}$ goes to the activation function of second layer A pure linear function is chosen to be the activation function of the second layer.

For FFNN model, the output of the activation function is the distillate composition x_D as shown in (4).

$$x_{D(FNN)} = \operatorname{purelin}(s_{2(FNN)}) \tag{4}$$

For RNN model, the output of the first layer x_1 is then fed to the second layer. $s_{2(RNN)}$ is the weighted sum fed to the linear function in the second layer of the network, as shown by (5)

$$s_{2(RNN)} = LW\{2,1\}x_1 + LW\{2,2\}x_{D(RNN)} + b\{2\}$$
 (5)

Where, $x_{D(RNN)} = purelin(s_{2(RNN)})$

The output $x_{D\ (RNN)}$ is fed back at the input of the second layer to create the recurrent network that helps in quicker convergence. The linear activation function is chosen in the output layer, as it can distribute the target values.

The data for training of the neural network model are real data acquired from the operation of BDC in laboratory. Input–output data sets with different values of $u_{R'}$, $u_{F'}$, $u_{TI'}$, $u_{QB'}$, $u_{PT'}$, and u_{PB} are used as the training data sets.

Each input vector consists of 579 data samples. Each input variable vary in a range as given below

 u_R : 0.82 to 1.41 kmole/h

 u_{E} : 2.5 to 3.5 kmole/h

 u_{T_1} : 80 to 99°C

 u_{OB} : 0.019 × 10⁶ (5.5 kW) to 0.0241 × 10⁶ kJ/h (7.0 kW)

 u_{PT} : 101.42 to 106 kPa u_{PR} : 115.21 to 120 kPa

For output data set, there is one output x_D , i.e., output distillate composition. x_D is varied from 0.84 to 0.92%. Overall, 3 447 data samples are used to train the neural network model for the BDC. The LM back propagation algorithm is used for training, which is performed using the neural network toolbox of MATLAB[13].

4. SIMULATION AND RESULTS

4.1 Training Performance

Table 1 shows the gradient value and the MSE of FFNN and RNN architectures of neural network with the different number of hidden neurons. These two characteristics represent the performance of the model and are used for validation and testing of the developed neural network model. The numbers of hidden neurons considered are six to twenty two because the neural network did not converge when the numbers of neurons were taken less than six. Training the network with more than twenty-two neurons produces the non-convergence.

Table 1 shows that the optimal number of hidden neurons for FFNN model are 14 because gradient and MSE both are minimum for these number of hidden neurons. For RNN model, the optimal number of hidden neurons is 18. It can be understand by analyzing Table 1 that further increment or decrement in the number of neurons will not help in the optimization.

4.2 Comparison with Experimental Data

The data for training, testing, and validation of FFNN and RNN have been experimentally acquired from the BDC in laboratory. For modeling of the neural network, NEURAL NETWORK TOOLBOX [13] of MATLAB has been used. Here, 60% data have been taken for training, 20% data for testing, and 20% data for validation. The validation of FFNN with the experimental results can be seen in Figure 5. By analyzing the results, one can conclude that the results are satisfactory.

Now for RNN, the comparison with experimental results is given in Figure 6. Here, the results are seen well than the results by FFNN. Figure 7 analyzes the performance of FNN and RNN model with the experimentally acquired results in a better way.

Table 1: Gradient and MSE of the FFNN and RNN model with different number of neuron

Architecture	Gradient		MSE for recurrent network			MSE for feed forward network		
	Recurrent network	Feed forward network	Training	Testing	Validation	Training	Testing	Validation
6-6-1	8.09274e-008	7.08754e-007	4.62041e-007	6.18119e-006	5.76232e-007	5.38178e-007	8.0423e-007	1.2104e-007
6-8-1	2.51694e-008	4.40621e-006	2.51693e-008	1.81347e-007	1.31297e-007	1.12582e-007	4.4063e-006	4.0231e-006
6-10-1	7.65893e-008	6.63989e-007	8.37572e-008	2.30491e-007	5.72831e-008	6.50383e-007	9.5467e-007	5.2435e-007
6-12-1	4.60608e-008	7.74967e-007	4.60607e-008	4.04947e-008	3.89503e-008	2.7823e-007	5.55703e-007	4.3213e-007
6-14-1	4.27704e-008	1.13615e-007	4.27703e-008	1.27959 e-007	3.49057e-008	4.19688e-007	1.13728e-007	1.1256e-007
6-16-1	4.5796e-008	3.13599e-006	4.5796e-008	1.34004 e-007	4.42589e-008	3.86997e-006	4.3219e-006	2.3251e-006
6-17-1	3.58982e-008	4.64871e-007	3.58982e-008	9.37122e-008	5.95519e-008	3.00008e-006	4.6488e-007	3.0412e-007
6-18-1	2.36800e-008	1.08061e-005	2.36800e-008	6.12864e-008	8.94861e-008	2.10534e-007	2.13081e-005	1.9229e-005
6-20-1	2.42435e-007	5.53205e-007	7.60179e-007	1.17440e-006	6.94123e-007	1.52098e-007	3.64351e-007	2.6511e-007
6-22-1	5.80767e-008	5.63932e-006	5.80766e-008	1.49045e-007	3.92859e-008	6.98418e-006	5.63980e-006	4.8965e-006

MSE - Mean square error; FFNN - Feed forward neural network; RNN - Recurrent neural network

It is observed from the Figures 5-7 that the RNN model closely follows the real data than the FFNN model.

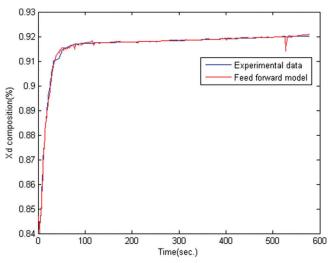


Figure 5: Comparison of FFNN with experimental results.

The MSE is 2.36800e-008 for RNN and 4.19688e-007 for FFNN for the estimation of distillate product composition. The results show that the developed neural network was in good agreement with the experimental results, but the error between the FFNN model and experimental results is greater than the error between RNN model output and experimental results.

The comparison of errors can be seen in Figure 8. Error converges fast to zero in the case of RNN. In FFNN model case, it shows that model takes more time to minimize the error between the neural outputs and targets but is still unable to converge the error to zero.

5. CONCLUSION

In this paper, two neural network topologies, FFNN and RNN, are applied for the identification of model of a continuous BDC. The presented two-layer FFNN and RNN model incorporates the non-linear behavior

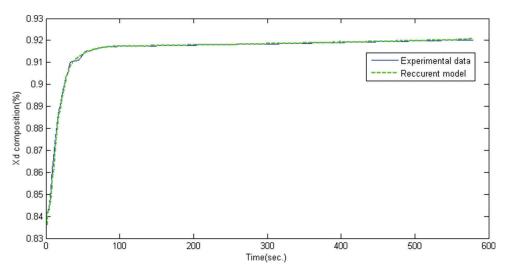


Figure 6: Comparison of RNN with experimental results.

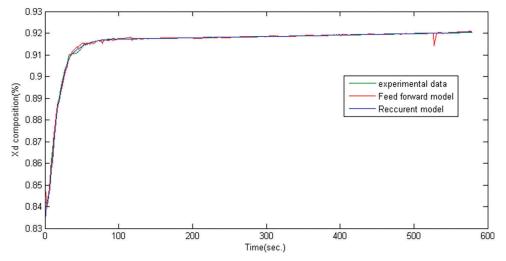


Figure 7: Comparison of FNN and RNN with experimental results.

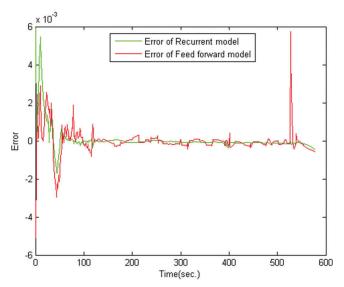


Figure 8: Error of FNN and RNN model with experimental results.

of BDC. The training of the neural network has been done by the experimentally acquired real data from the laboratory setup of continuous BDC. The trained NN outputs distillate composition. The comparison between FFNN and RNN model outputs confirmed that RNN model precisely identify the parameters of BDC with a faster convergence rate than FFNN. The model has been validated with the experimentally acquired results. It is found that the RNN topology is more suitable than FFNN topology for the identification of model of BDC.

6. ACKNOWLEDGMENT

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Appendix

Number of trays	9
Weir height in stripping section	0.47 inch
Weir length in stripping section	0.47 inch
Column diameter in stripping section	4.80 inch
Weir height in rectifying section	5.91 inch
Weir length in rectifying section	5.91 inch
Column diameter in rectifying section	4.80 inch
Volumetric hold up in column base	0.5414 ft ³
Volumetric hold up in reflux drum	0.0001 ft ³
Liquid feed rate	2.5 kg-moles/hr
Liquid feed temperature	34.5°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 moles/hr
Vapor distillate product flow rate	0.0 kg-moles/hr
Murphree vapor efficiency	0.60

AUTHORS



Amit Kumar Singh is currently working toward his Ph.D. degree in Department of Electrical Engineering at Indian Institute of Technology, Roorkee (India). His research interests include control system, process control and application of evolutionary techniques to chemical processes.

E-mail: akschauhan.amit@gmail.com



Barjeev Tyagi received B. Tech. degree in Electrical Engineering from University of Roorkee (India) in 1987 and Ph. D. degree from IIT Kanpur in 2006. Presently, he is an Associate professor faculty member in Electrical Engineering Department at Indian Institute of Technology, Roorkee (India). His research interests include control system, power system deregulation,

power system optimization and control.

E-mail: btyagfee@iitr.ernet.in



Vishal Kumar received the Ph.D. degree in power system engineering from the Indian Institute of Technology, Roorkee, India, in 2007. Currently, he is an Assistant professor in the Department of Electrical Engineering, Indian Institute of Technology, Roorkee, India. His research interests include power distribution system operation and protection, and digital design and verification.

E-mail: vksaxfee@iitr.ernet.in

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