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Neural Network Technique in the Study of Selected Chemical Engineering Unit Operations Data using MATLAB

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Abstract:- The concept of Artificial Neural networks was of McClloch and Pitts in 1943 and since then it has been studied in details by scientists and engineers alike. This is a study of the use of artificial neural network in analysis of selected chemical engineering unit operations. In this paper several networks were developed and trained for three different unit operations. This paper deals with the training of neural networks to perform predictions of several chemical unit operations.

The feedforward neural network was trained to model the bubble point temperature and pressure of the water ethanol-water vapor-liquid equilibrium system. It was found that the neural network predicted values with high accuracy. Focused time-delay neural network was used to model and predict the change in concentration of the batch saponification reaction of ethyl acetate. The response of the network in one step in time ahead predictions was quite accurate. The dynamics of a CSTR with a cooling jacket was also modeled with the NARX neural network. The NARX model developed gave multi step on time predictions with enormous aplomb.

Keywords:- *artificial neural network; feedforward; supervised learning; cstr; batch reactor; VLE; dynamic network.*

I. INTRODUCTION

The concept of Artificial Neural Network is largely motivated by the recognition that the human brain computes in an entirely different way from the conventional digital computer [1]. It is applied in a wide variety of chemical engineering problems including fault detection of CSTR [2], the real time optimization of the distillation column [3], Monitorization and Control of Multivariable Systems with Application to Distillation Columns[4], Predicting Oil Content in Wax[5]; Predictive control of Chemical reactor[6]; modeling and simulation of reactive packed columns[7]; data rectification in dynamic process[8].

The solution to chemical engineering problems almost always involves complex and nonlinear systems. This makes it quite difficult for them to be solved accurately and quickly by the conventionally used methods of modeling. Recent results show that neural network technique seems to be very effective to model a broad category of complex nonlinear systems when we do not have complete model information [9]. The use of Artificial Neural Network has been a growing field and can solve these problems with a certain level of ease. Neural networks have been applied very successfully in the identification and control of dynamic systems. The universal approximation capabilities of the multilayer perceptron make it a popular choice for modeling of nonlinear systems and for implementing of nonlinear controllers [6].

This paper is aimed at present simple forms of ANN and their applications in certain chemical engineering unit operations. In this work the following ANNs will be briefly discussed: (1) Feedforward Neural Network, (2) Focused Time-delay Neural Network, (3) NARX Neural Network. Also the applications of these types of ANN are discussed for simple predictions (VLE bubble point prediction) to multi-step ahead prediction for batch saponification reaction and jacketed CSTR.

II. ARTIFICIAL NEURAL NETWORK

A brief description of ANNs will be given here. As the term artificial neural networks implies, early work in the field of neural networks centered on modeling the behavior of neurons found in the human brain. Engineering systems are considerably less complex than the brain; hence from an engineering viewpoint ANN can be viewed as nonlinear empirical models that are especially useful in representing input-output data, making predictions in time, classifying data, and recognizing patterns [8].

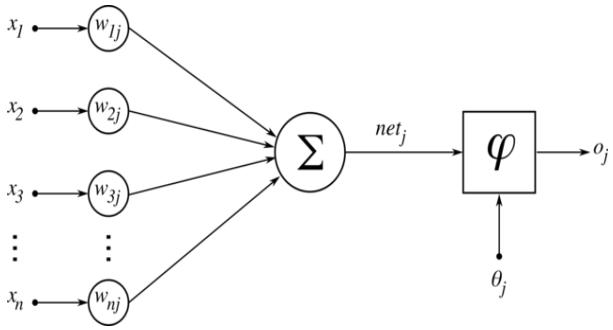

Fig. 1: Structure of a neuron

Fig 1. Shows a single neuron which is the fundamental unit of every artificial neural network and as the name implies, is also analogous to the neuron of the human brain. Here, the neuron has inputs x_1, x_2, x_3 …, x_n which may be direct input signals or input from another neuron. Each input to the neuron is weighted by its corresponding weight i.e. w_{1j}, w_{2j}, w_{3j} …, w_{nj}. The weights of the artificial neuron have a similar function to the synapse that connects two neurons in the brain. Weighted inputs are summed and sent to the transfer function ($_\varphi$). The transfer function may need an extra

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bias, Θ_j if the value of net_j is not strong enough. The transfer function may be any mathematical function. The output from one neuron may be the input to another or may be the final output of the ANN.

A single neuron however, cannot work independently just as is the case of the human brain: neurons work together to achieve a common goal. When neurons combine in this way, they form an artificial neural network.

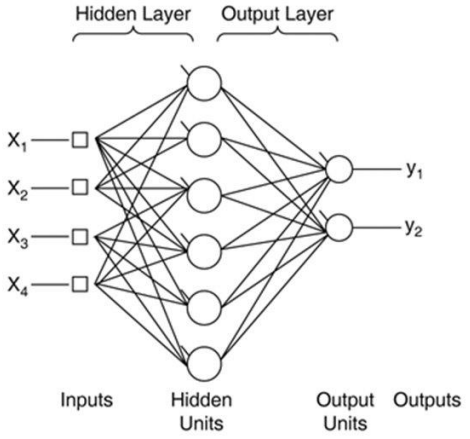

Fig. 2: A Simple artificial Neural Network

Fig. 2 shows a simple artificial neural network having four input signals and two ouput signals. The network has two layers of neurons (in some literature, the input signals are regarded as a layer of neuron). The output layer is fixed by the number of output signals the network is to give while the number of hidden layers takes a rather tedious process to determine. For a detailed description of the determination of the number of neurons in the hidden layer, see [10].

A. Types of Artificial Neural Network

There are quite a number of artificial neural networks identified as in [schakolf, haykin]. But the ones applied in this paper are briefly explained.

- Feedforward artificial neural network, as the name implies is connection of several neurons with the output of each neuron directed to the input of the next neuron or set as the output of the network. In essence a feedforward artificial neural network has its neurons all pointing in one direction.
- Dynamic network contains delays and the output is determined not only by the current input to the system, but also on the current or previous inputs, outputs, or states of the network. Dynamic networks can be categorized as forward-dynamic (where there is no feedback) and recurrent-dynamic (where there is feedback). They are more difficult to train than static networks like the feedforward networks discussed; however, they are generally more powerful than static networks. They include: (1) Focused Time-Delay Neural Network – in this case, the network dynamics occur only at the input layer. (2) Distributed Time-Delay Neural Network – here, delays are distributed throughout the network. (3) NARX Network – this is a recurrent dynamic network, with feedback connections enclosing several layers of the network.

B. Training of Artificial Neural network

The networks explained above are trained by a supervised learning: where inputs and outputs are presented to the network during training so that the network can map out the relationship between them. There are networks that are trained by unsupervised learning but these are not considered here see[11, 12].

Supervised learning steps are summarized by [13, 8], they are:

- for a given ANN architecture, the values of the weights in the network are initialized as small random numbers;
- the inputs of the training set are sent to the network and the resulting outputs are calculated;
- some measure (an objective function) of the error between the outputs of the network and the known correct (target) values is calculated;
- the gradients of the objective function with respect to each of the individual weights are calculated;
- the weights are changed according to the optimization search direction and step length determined by the optimization code;
- the procedure returns to step 2;
- the iteration terminates when the value of the objective function calculated using the data in the test set starts to increase.

C. Design of Artificial Neural network

In design of any ANN, data preprocessing, data division and data post processing are key factors that would affect the performance of the network created.

Data Preprocessing: ANN training requires the use of data which are often gotten from differnet sources and may have some discrepancies in them. Prepocessing requires that the data used for ANN training are properly organized before they are used so that the designed network can learn the actual relationship between the inputs and the outputs. In order to achieve this, the following steps should be taken:

- Data Cleaning: this is often – but not always – required due to flaws often associated with experimental data. These flaws could be missing values in the data set due to unavailable data during data entry/collection. Another often encountered flaw during data collection is noisy data.
- Data Integration: combining data from different sources is often a difficult task, as most times different ways can be used to represent the same data type; care is taken to check all the sources and ensure that the units of each data used are all converted to a single form that will be used throughout the training.
- Data Transformation: often it is desirous that data used for network training be tailored so that the inputs can better match the outputs. This also puts the data into a certain distribution range that can be easily processed by the network.
- Data division: the ratio of the data and the way in which this data is shared is into training, validation and testing data sets. For a comprehensive treatment of data division, see [11].
- Data post-processing: this must be done whenever data pre-processing is done. This is usually done after the network

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has been trained and it is most typically carried out on the initially transformed output data.

III. APPLICATIONS OF ARTIFICIAL NUERAL NETWORK

A. Ethanol-water vle predictions

Chemical Processes such as distillation, absorption, and extraction bring phases of different compositions in contact, and when the phases are not in equilibrium, mass transfer between them alters their compositions. Both the extent of change and the rate of transfer depend on the departure of the system from equilibrium. Thus, for qualitative treatment of mass transfer the equilibrium T, P, and compositions must be known. The most commonly encountered coexisting phases in industrial practice are vapour and liquid[14, 15].

When thermodynamics is applied to VLE, the goal is to find by calculation the temperatures, pressures, and compositions of phases in equilibrium. Indeed, thermodynamics provides the mathematical framework for the systematic correlation, extension, generalization, evaluation and interpretation of VLE data. The the simplest and most widely model for the behavior of systems in VLE is Raoult's law[15].Raoult's law is expressed mathematically as (1).

$$y_i P = x_i P_i^{sat} \quad (1)$$

$$\ln P_i^{sat} = A_i - \frac{B_i}{T + C_i} \quad (2)$$

$$P_i \emptyset_i = P_i^{sat} \gamma_i x_i \quad (3)$$

In order to apply (1), two assumptions are made:

- The vapour phase is an ideal gas: this means that Raoult's law is only applicable for low and moderate pressures;
- The liquid phase is an ideal solution: i.e. it can have approximate validity only when the species that comprise the system are chemically similar.

In order to calculate P_i^{sat}, the Antoine's equation (2) is applied. The form of (1) may mislead one to think that the VLE calculations would be easy; however this is not the case. Imagine simple dew temperature calculations with (1). Here the vapour-phase mole fraction, x_i and the total pressure, P are given and the liquid-phase mole fraction, y_i and temperature, T are required. This would require the following iterations:

- guess T;
- calculate P_i^{sat} using the Antoine equation;
- P_i^{sat} is used to calculate the total pressure;
- this value is then checked with the given pressure;
- the initial guess of T is adjusted and iteration processed is repeated until the total pressure calculated matches the given pressure.

This is algorithm is rather time consuming and eventually fails when there exist intermolecular interaction of the molecules of the mixtures. In this case, the modified/extended Raoult's law (3) is used. This would lead to more iterations due the need for correlations like the Wilson's equation[14].

The use of ANN would greatly reduce computation time and the errors that are inevitable with the thermodynamic equations [14]. In principle ANN would involve less model mismatch for a real process and would reduce the computation time to predict outputs from inputs [8].

Thus Artificial Neural Network is applied to the ethanol-water vapor-liquid equilibrium system for the determination of bubble point temperatures (Given x_i and P, calculate y_i and T) and bubble point pressures (Given x_i and T, calculate y_i and P). Data was obtained from [16]. The total number of data points is 241 and the pressure range for the data set is 4.4130kPa to 101.3247kPa and that for temperature is 303.1500K to 373.1500K. For these prediction calculations, a static feedforward neural network with two layers was developed. According to Cybenko, a single hidden layer is sufficient to represent any function and a single hidden layer is enough to represent any continuous function [10, 8]. The data division was in the ratio of 1:1:2 for test, validation and train. The Levenberg-Marquardt Training algorithm was used to train the network with mean-square error performance function. The output layer has a linear transfer function and it has two neurons – as fixed by the number of outputs. The other training parameters were determined after trying several combination and the number of neurons in the hidden layer was also determined by a hill climbing method [10, 12] of continuously adding one neuron after each training run. The feedforward networks were built in MATLAB by employing the use of the neural network toolbox.

For the bubble point temperature predictions (BUBL T), the optimum network topology for the created feedforward network was 2-5-2. When this network was trained, the following plots were obtained:

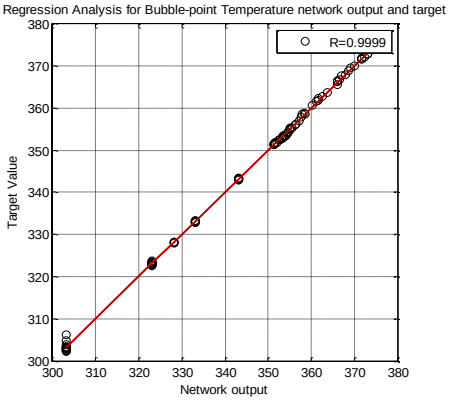

Fig. 3: BUBL-T Temperature Regression Plot for 5 Hidden Layer Neurons

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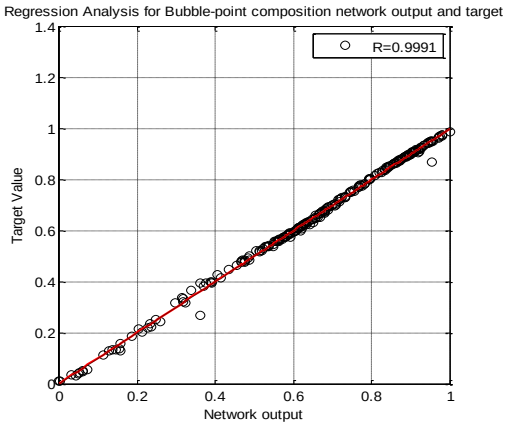

Fig. 4: BUBL-T Composition Regression Plot for 5 Hidden Layer Neurons

Fig. 3 shows that the network output value matched the desired target very closely. It gave a regression value of 0.9999. Fig. 4 represents the regression plot for the BUBL-T composition prediction; the network gave a regression value of 0.9991. From the foregoing, it can be concluded that the proposed network can be used to predict BUBL-T values for the ethanol-water VLE system for values with the pressure range of 4.4130kPa to 101.3247kPa and temperature range of 303.1500K to 373.1500K.

For the bubble point pressure predictions (BUBL P), the optimum network topology for the created feedforward network was 2-4-2. When this network was trained, the following plots were obtained:

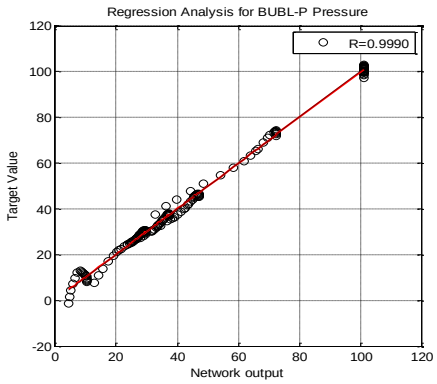

Fig. 5: Figure 4-11: BUBL-P Pressure Regression Plot for 4 Hidden Layer Neurons

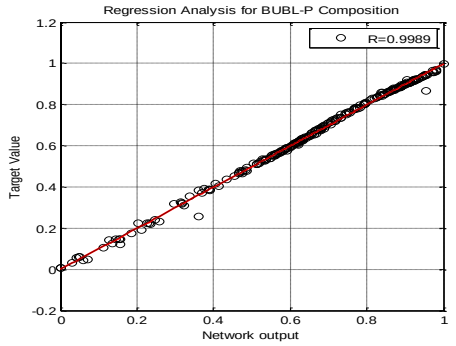

Fig. 6: Figure 5: Figure 4-11: BUBL-P Composition Regression Plot for 4 Hidden Layer Neurons

For the BUBL-P pressure, Fig. 5 showed that the regression coefficient obtained was 0.9990. This further justifies the network structure of 2-4-2 for the prediction of the BUBL-P pressure based on the levenberg-marquardt training algorithm and the other parameters selected for the ethanol-water vapor-liquid equilibrium system. Fig. 6 also gave a high regression coefficient of 0.9989 when the network targets were plotted against the network outputs for the BUBL-P composition prediction. It is therefore concluded that a 2-4-2 feedforward network structure with the parameters fixed according to BUBL-P can be used for the BULB-P prediction of ethanol-water vapor-liquid equilibrium given that it falls within pressure range of 4.4130kPa to 101.3247kPa and temperature range of 303.1500K to 373.1500K.

B. batch saponification concentration prediction

Here, the use Focus Time-Delay Neural Network will be used for one-step ahead prediction of a batch reactor. The reactor modeled is the SOLTEQ Batch reactor (Model: BP 109) which is designed as an isothermal and adiabatic reactor[17]. Here, the reaction considered is the saponification reaction between ethyl acetate and sodium hydroxide.

The data used for this study was gotten from UCSI University, it is an unpublished data. For further details contact UCSI University or [17].

The network built to model the concentration change uses the default values for the FTDNN as found in MATLAB. The training algorithm used is the levenberg-marquardt. The following plot is the actual change in concentration with time for the saponification reaction at 40^{o}C:

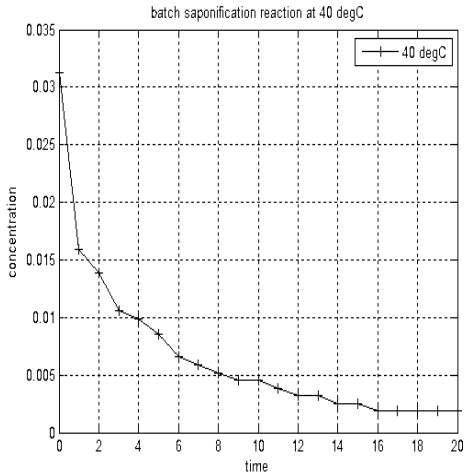

Fig. 7: Actual Concentration-time Profile for Batch Saponification Reaction

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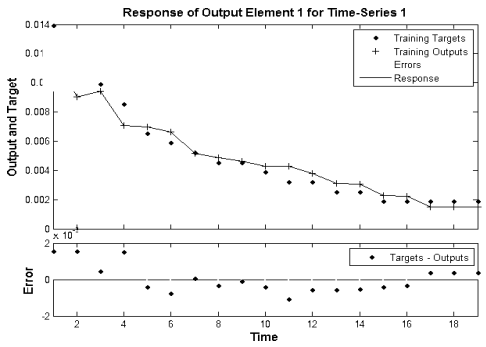

Fig. 8: FTDNN Time Series Response for 40^0C

Fig. 8 is clearly seen to follow the same path as Fig. 7. The errors in predictions are indicated in Fig. 8 and it can be seen that they are of the order of 10^{-13} which shows that the FTDNN can predict one step ahead in time of the batch saponification reaction of ethyl acetate. For a further check on the FTDNN's performance, the following regression plot was made:

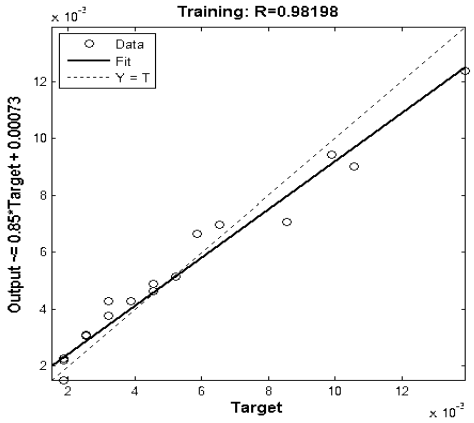

Fig. 9: Regression plot for the propose FTDNN for the batch saponification

The output obtained by using the FTDNN closely matched the network target yielding a regression value of 0.98198 and a root mean square error of 0.0011.

Reaction Temp. (^{o}C)	Hidden Neuron	Regression Coefficient	Root mean square error
40	7	0.98198	0.0011
50	8	0.3163	0.0057
60	8	0.97451	0.0045
70	6	0.9672	0.0067

Table 1: Summary Of Regression And Rmse Values Obtained

C. CSTR MODELING WITH NARX NEURAL NETWORK

In an ideal Continuously Stirred Tank Reactor (CSTR), the conditions are uniform throughout and the condition of the effluent is the same as the condition in the tank[15]. Flow reactors are used for greater production rates when the reaction time is considerably short and when uniform temperature is desired[14].

Chemical reactors often have heat effects, so it is important to be able to add or remove heat from them[18]. In a jacketed CSTR, the heat is added or removed by virtue of the temperature difference between a jacket fluid and the reactor fluid. In order to model the jacketed CSTR, the following assumptions are made: (1) Perfect mixing in reactor and jacket (2) Constant volume reactor and jacket and (3) Constant parameter values. The reaction is first order in propylene oxide concentration – since water is supplied in excess. The equations give a detailed model of the CSTR with the cooling jacket dynamics are given by (4), (5) and (6).

$$\frac{dC_A}{dt} = 0 = \frac{F}{V}\left(C_{Af} - C_A\right) \quad (4)$$

$$\frac{dT}{dt} = 0 = \frac{F}{V}\left(T_f - T\right) + \left(\frac{-\Delta H}{\rho C_p}\right) k_0 exp\left(\frac{-E}{RT}\right) C_A - \frac{UA}{V\rho C_p}(T \quad (5)$$

$$\frac{dT_J}{dt} = \quad (6)$$

The parameters are given in Table II below:

Parameter	Description	Value
k_0	frequency factor	16.96×10^{12} hr^{-1}
-ΔH	heat of reaction	39000Btu/lbmol
E	Activation energy	32400Btu/lbmol
U		75Btu/(hr.ft^2 ^{0}F)
ρC*P	ρ: Reactant Density C_P: Reactant heat capacity	53.25Btu/$(ft)^3$ ^{0}F
R	Molar gas constant	Btu/(lbmol)^{0}F
V/F	Residence Time	0.25hrs
C_{Af}	Reactor feed concentration	0.132lbmol/$(ft)^3$
T_f	Reactor feed temperature	60^0F
V	Reactor operating volume	500ft^3
A	Heat transfer area	309ft^2
V_j/V	jacket to reactor volume ratio	0.25
T_{jf}	Jacket coolant feed temperature	0^0F
ρ_j *C_{pj}	ρ_j: Coolant density C_{pj}: Coolant heat Capacity	55.6Btu/$(ft)^3$ ^{0}F

Table 2: Reaction Parameters For Jacketed Cstr

The jacketed CSTR shown below (Fig. 10) would be used to model the hydrolysis of propylene oxide with sulfuric acid as catalyst as found in [18].

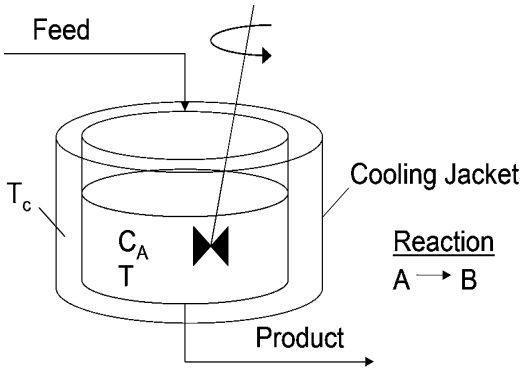

Fig. 10: CSTR with Jacket

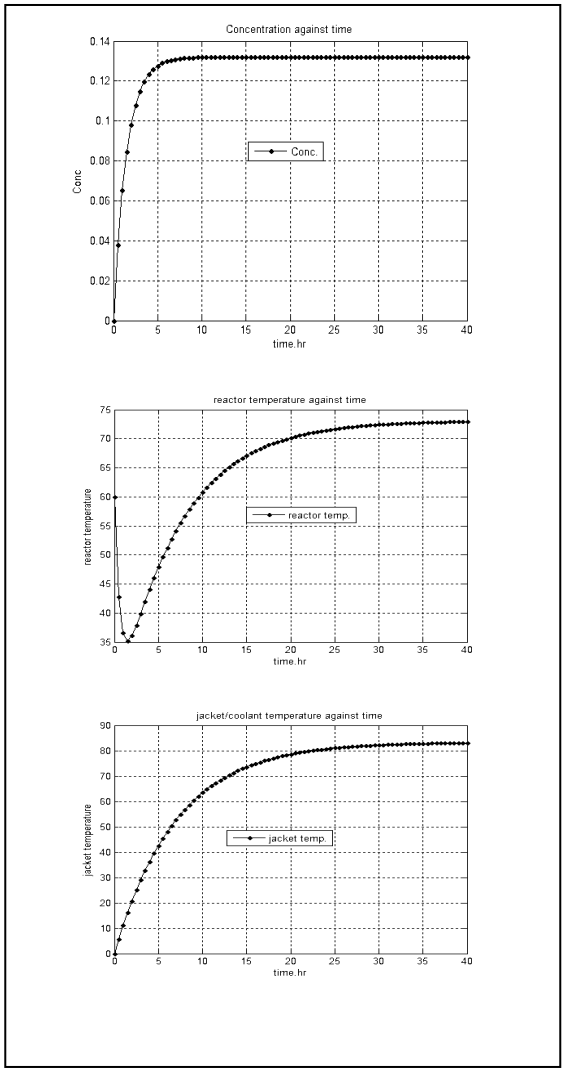

Fig. 11: Actual Dynamics of CSTR

The actual dynamics of the CSTR after modeling with MATLAB is shown in Fig. 11. When the NARX neural network was used to predict the concentration of the product form, it was found that the outputs of the network closely matched the actual targets (Fig. 12).

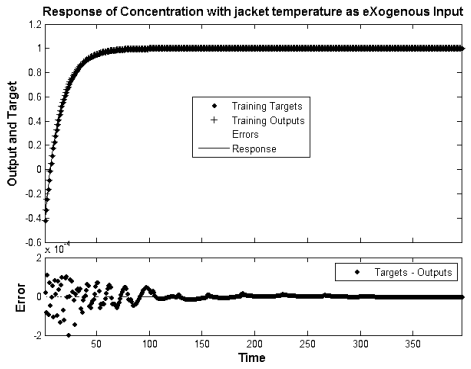

Fig. 12: Time-series response of NARX for concentration

This response led to the use of the developed NARX network to predict multi-step in time and the Fig. 13 was obtained.

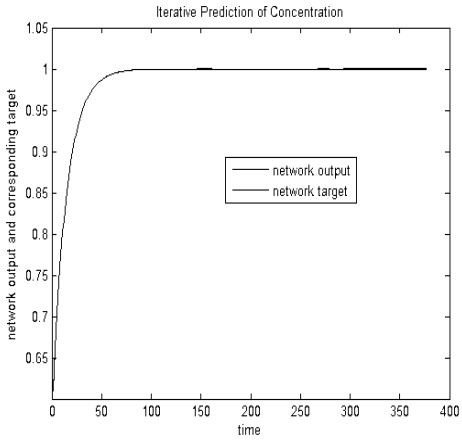

Fig. 13: Iterated Prediction of the Concentration

From Fig. 13, it can be seen that the network output closely matched the target values for the concentration even though it was used to predict 30 steps ahead.

When the NARX neural network was used to predict the reactor temperature, it was found that the outputs of the network closely matched the actual targets (Fig. 14).

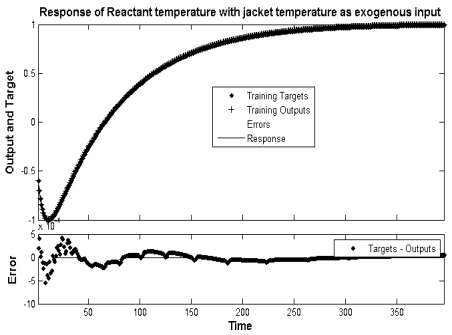

Fig. 14: Time-series response of NARX for Reactor Temperature

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With such high response, the trained NARX network was used to predict the temperature of the reactor with a time delay of 35. This yielded Fig 15.

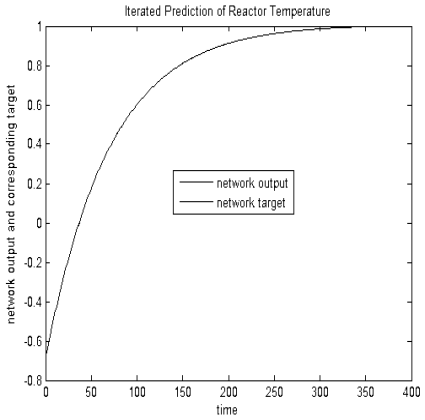

Fig. 15: Iterated Prediction of the Temperature of reactor

From Fig. 15, it can be seen that the network output closely matched the target values for the temperature of the reactor even though it was used to predict 35 steps ahead.

The jacket coolant dynamics were also closely matched when the NARX network was applied to the values obtained by MATLAB simulation of the CSTR Dynamics.

IV. CONCLUSION

Artificial Neural Networks have been shown here to model chemical engineering processes with some high level of accuracy as opposed to the conventional methods and it also takes very little time to make these accurate predictions.

For the VLE system of ethanol and water, the feedforward neural network gave very high correlations when applied to predict the BUBL-T and BUBL-P values.

Dynamic neural networks applied to a jacketed CSTR also proved to be very good in terms of predicting future values in the dynamics of the CSTR. The NARX neural network was used in this case.

In conclusion, there are countless applications to which artificial neural network can be used and with the highly non-linear systems found in chemical engineering unit operations, the use of ANN is justified.

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