Figure (7) shows neural network predictions together with real outputs. It is seen that neural network has been trained as well.
The error between neural network predictions and real outputs is presented in figure (8).

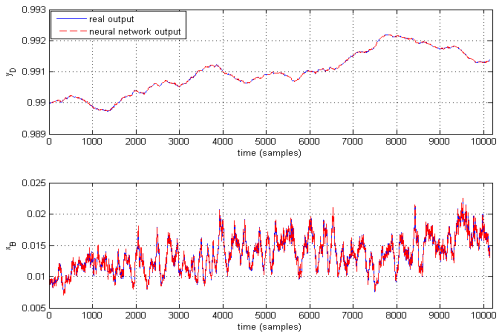

Fig. (7): Neural network predictions together with real outputs.

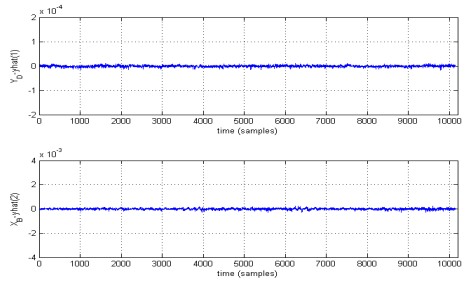

Fig. (8): Error between neural network predictions and real outputs.

3.4 Model validation

When a network has been trained, the next step is to evaluate it. To do this we should force another input to the model and check the predictions of neural network. To validate the model, we used the remaining 10150 samples of inputs and outputs that we did not use for training. Figure (9) shows the predictions of neural network together with real outputs. As it is seen the predictions of network follows the real outputs as well.
The error between neural network predictions and real outputs in validation phase is presented in figure (10).

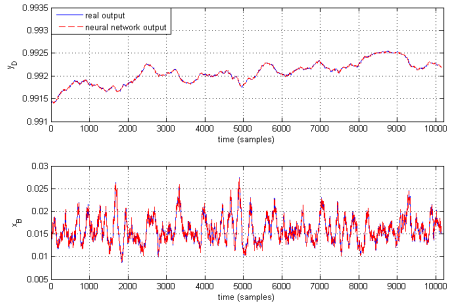

Fig. (9): Neural network predictions together with real outputs in validation phase.

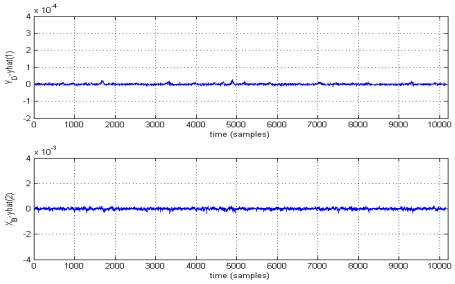

Fig. (10): Error between neural network predictions and real outputs in validation phase.

4. Conclusions

The purpose of this paper was to obtain a simple and reliable model for distillation column. We used black-box identification to determine the model. ARX model structure together with artificial feed forward neural networks was used to estimate the dynamics of system. Regarding the use of two layer feed forward neural networks we can declare that the obtained model is simple. The results in training phase and validation phase shows that predictions of neural network is very close to real outputs and the error is negligible. It ensures us that the obtained model is reliable.
As a future line of work we can study the possibility of combining empirical model that we obtained with dynamic model of distillation column.

Appendix

1- Auto Regressive with exogenous input
2- Neural network based system identification

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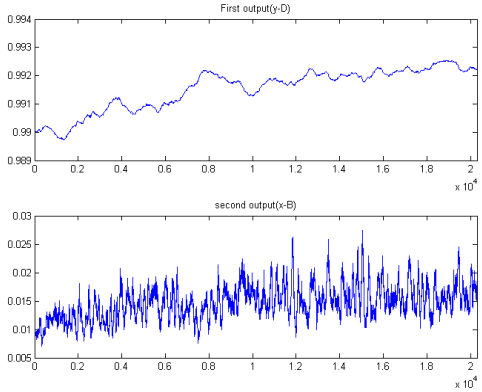

Fig. (3): Outputs of dynamic system.

3.2 Selecting model structure

After the data set has been acquired, the next step is to select a model structure. Unfortunately, this issue is much more difficult in the nonlinear case than in the linear case. Not only is it necessary to choose a set of regressors but also a network architecture is required. The approach used here is described in [7]. The idea is to select the regressors based on inspiration from linear system identification and then determine the best possible network architecture with the given regressors as inputs. The ARX model structure is selected because this model structure does not use predictions of model as its regressors. It means that our neural network is feed forward and we will not have the problems of high complexity and high computational costs of recursive networks.

The regressor vector is:

$$\varphi(t) = [y_1(t-1), y_1(t-2), u_1(t-1), y_2(t-1), y_2(t-2), u_2(t-1)]^T \quad (14)$$

Figure (4) shows the architecture of this model. As it is seen the neural network is used as the estimator.

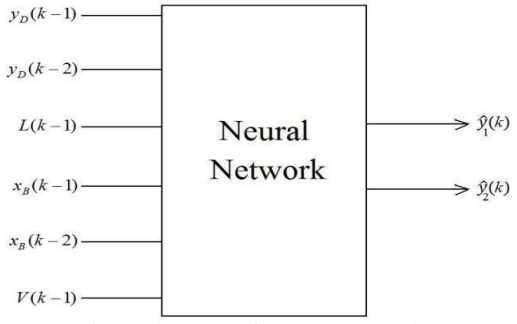

Fig. (4): Structure of neural ARX model.

3.3 Estimating model parameters by neural networks

A feed forward neural network with two layers is used to estimate model parameters. The number of neurons in each layer and the activation function of each neuron should be determined. The output layer has two neurons with linear transfer function. The number of neurons in the hidden layer is determined based on the trials .The variation of error with number of hidden neurons is shown in Figure (5).

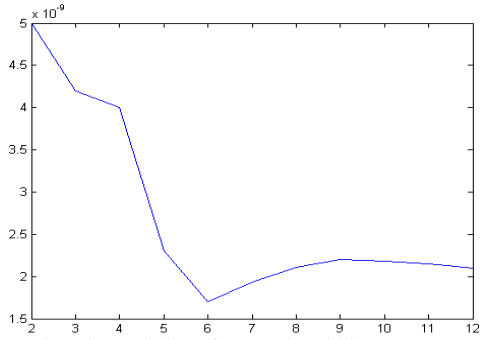

Fig. (5): Variation of error with hidden neurons.

The lowest error corresponds to 6 neurons in the hidden layer. Hence a two layer network with 6 neurons in the hidden layer and 2 neurons in the output layer is selected. Hyperbolic tangent activation function is used in hidden layer. The ANN architecture used is shown in Figure (6).

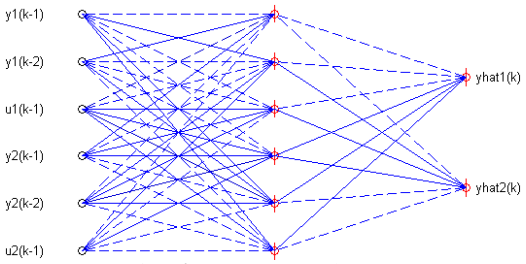

Fig. (6): Neural networks structure.

In order to determine neural network parameters and training the network we have used NNSYSID[2] [8] toolbox with MATLAB. 10150 samples of inputs and outputs are used to train the network and the remaining samples are kept to validate the model. The Levenburg-Marquardt algorithm was used to train the network. The parameters of training algorithm are presented in table 2.

Table (2): Parameters of training method

Step size	1×10^{-4}
Momentum	1
Maximum iterations	500
Stop if criterion is below this value.	0
Stop if change in criterion is below this value.	1×10^{-7}
Stop if largest element in gradient is below this value.	1×10^{-4}
Stop if largest parameter change is below this value.	1×10^{-3}
Weight decay	1×10^{-6}
Forgetting factor	9.95×10^{-1}
Min. eigenvalue of P matrix	10
Max. eigenvalue of P matrix	1×10^{-3}
Initial Levenberg-Marquardt parameter.	1

α is relative volatility between light and heavy component.

From the assumption of constant molar flows and no vapour dynamics, one obtains the following expression for the vapour flows

$$V_i = V_{i-1} \quad (5)$$

The liquid flows depend on the liquid holdup on the stage above and the vapour flow as follows

$$L_i = L0_i + \frac{M_i - M0_i}{\tau_L} + \lambda(V_{i-1} - V0_{i-1}) \quad (6)$$

Where $L0_i[kmol/\min]$ and $M0_i[\text{kmol}/\min]$ are the nominal values for the liquid flow and holdup on stage i and $V0_i$ is the nominal boil up flow. τ_L is time constant for liquid flow dynamics on each stage [min]. If the vapour flow into the stage effects the holdup then the parameter λ is different from zero. For the column under investigation $\lambda = 0$. The above equations apply at all stages except in the top (condenser), feed stage and bottom (reboiler).

1. For the feed stage, $i = N_F$ (it is assumed that the feed is mixed directly into the liquid at this stage)

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

$$\frac{d(M_i x_i)}{dt} = L_{i+1}x_{i+1} + V_{i-1}y_{i-1} - L_i x_i - V_i y_i + Fz_F \quad (8)$$

2. For the total condenser,

$$i = N_{tot}(M_{N_{tot}} = M_D, L_{N_{tot}} = L_T) \quad (9)$$

$$\frac{dM_i}{dt} = V_{i-1} - L_i - D \quad (10)$$

$$\frac{d(M_i x_i)}{dt} = V_{i-1} - L_i x_i - Dx_i \quad (11)$$

3. for the reboiler,

$$i = 1(M_i = M_B, V_i = V_B = V) \quad (12)$$

$$\frac{d(M_i x_i)}{dt} = L_{i+1}x_{i+1} - V_i y_i - B_i x_i \quad (13)$$

As a result, we obtain a nonlinear model of the distillation column of 82nd order. There are two states per tray, one representing the liquid composition and the other representing the liquid holdup. We need an overall model that describes the effect of the inputs (flows) on the outputs (product compositions). We make use of the so called LV-configuration of the distillation column in which L and V are inputs and Y-D and X-B are outputs. In order to find a linear model of the distillation column it is necessary to have a steady-state operating point around which the column dynamics is to be linearized.

The nonlinear model is linearized at the operating point given in Table 1 (the values of F, L, V,D,B, y_D, x_B and z_F). These steady-state values correspond to an initial state where all liquid compositions are equal to 0.5 and the tray holdups are also equal to 0.5 [kmol].

Table (1): Column data

N	40	B	0.5
N_{tot}	41	L	2.706
N_F	21	V	3.206
F	1	y_D	0.99
z_F	0.5	x_B	0.01
q_F	1	M_i	0.5
D	0.5	τ_L	0.063

The steady-state vector is obtained for t = 5000 min by numerical integration of the nonlinear model equations of the LV-configuration.

3. Modeling by neural networks

Modeling distillation columns by means of neural networks is reported in literature [6]. The network that they used was recursive. The recursive networks are proper for modeling purpose, but such models have the problems of high complexity and high computational cost. Our attempt is to find a model by using feed forward neural networks which will result in a simple model with less parameters and faster training time. Modeling of distillation column is done in four steps as follows.

3.1 Generation of input-output data

Having a proper data set is essential in each empirical modeling problem. In this work we generated such data set by forcing an input to dynamic model of distillation column and then obtaining the response of model to it. The type of input that we use is important because it should be an input that can excite all process dynamics. To achieve this goal a random signal was used as input of the system. Figure (2) shows the two inputs that we applied to dynamic model. Then the response of dynamic model to the inputs was obtained. Figure (3) shows two outputs of the system. Finally a data set of inputs and outputs with 20300 samples was obtained.

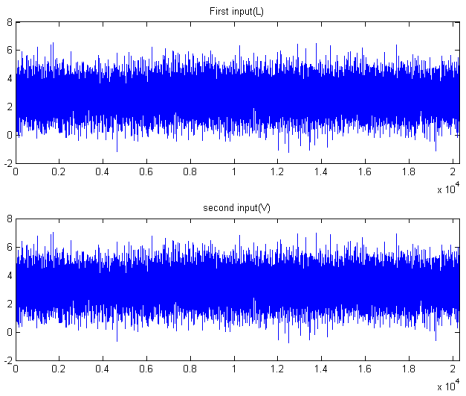

Fig. (2): Input sequences

This is because of two reasons: firstly, it has been shown that these networks are universal non-linear function approximators [3, 4], and secondly, their application does not require any knowledge about the structure of the system to be modeled. Moreover, the NNs can learn online, based on local information, can treat easily multi input multi output (MIMO) systems and their performance degrades gracefully due to the parallel, distributed processing structure and high degree of connectivity among the units. All these remarkable biologically inspired properties made the NNs successful alternative for dynamic modeling and estimation.

The purpose of this study is to obtain a powerful model of reference allowing to reproduce the dynamics of a complex process as a distillation column. This reliable model enables to reproduce the process dynamics under different operating conditions. The present study focuses on the development, and implementation of an ARX[1] neural model for the forecasting of the distillation column dynamics. A random input was forced to dynamic model and the response of model to the input was obtained in order to generate the data set that was needed for identification. Such data were used both to define and to validate the model. The performance of this neural model was then evaluated using the performance criteria. Results show that the ARX neural model is representative for the dynamic behavior of this nonlinear process.

This paper is organized as follows. Section 2 describes the distillation column and its dynamic model. Section 3 shows modeling of distillation column by means of neural networks. The validation of the model is also evaluated in section 3. Section 4 summarizes the conclusions and future lines of work.

2. Dynamic model of the distillation column

Distillation is an important process in the separation and purification of chemicals. The process exploits the difference at boiling points of multicomponent liquids. The distillation process is highly nonlinear and the corresponding linearized models are often ill-conditioned around the operating point. The dynamic model of distillation column is reported in different works in literature. One of the most important works has done by Sigurd Skogestad and Manfred Morari [5]. The dynamic model that we have used directly comes from that work.

A typical two-product distillation column is shown in Figure (1). The objective of the distillation column is to split the feed *F*, which is a mixture of a light and a heavy component with composition z_F, into a distillate product D with composition y_D, which contains most of the light component, and a bottom product B with composition z_B, which contains most of the heavy component. For this aim, the column contains a series of trays that are located along its height. The liquid in the columns flows through the trays from top to bottom, while the vapour in the column rises from bottom to top. The constant contact between the vapour and liquid leads to increasing concentration of the more-volatile component in the vapour, while simultaneously increasing concentration of the less volatile component in the liquid. The operation of the column requires that some of the bottom product is reboiled at a rate V to ensure the continuity of the vapour flow and some of the distillate is refluxed to the top tray at a rate L to ensure the continuity of the liquid flow. The notations used in the derivation of the column model are summarized in Table 11.1 and the column data are given in Table 11.2. The index *i* denotes the stages numbered from the bottom (i = 1) to the top ($i = N_{tot}$) of the column. Index B denotes the bottom product and D the distillate product. A particular high-purity distillation column with 40 stages (39 trays and a reboiler) plus a total condenser is considered.

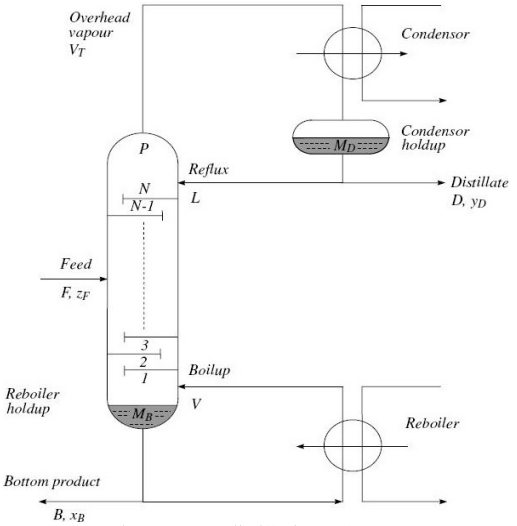

Fig. (1): The distillation column system

The nonlinear model equations are:

1. Total material balance on stage i

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

Where M_i is liquid holdup on stage *i* [kmol], L_i is liquid flow from stage *i* [kmol/min] and V_i is vapour flow from stage *i* [kmol/min].

2. Material balance for the light component on each stage i

$$\frac{d(M_i x_i)}{dt} = L_{i+1}x_{i+1} + V_{i-1}y_{i-1} - L_i x_i - V_i y_i \quad (2)$$

x_i and y_i are liquid and vapour composition of light component on stage i.

This equation leads to the following expression for the derivative of the liquid mole fraction

$$\frac{dx_i}{dt} = \frac{\frac{d(M_i x_i)}{dt} - x_i \frac{dM_i}{dt}}{M_i} \quad (3)$$

3. Algebraic equations

The vapour composition y_i is related to the liquid composition x_i on the same stage through the algebraic vapour-liquid equilibrium

$$y_i = \frac{\alpha x_i}{1+(\alpha-1)x_i} \quad (4)$$

Modeling Distillation Column Using ARX Model Structure and Artificial Neural Networks

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Abstract: Distillation is a complex and highly nonlinear industrial process. In general it is not always possible to obtain accurate first principles models for high-purity distillation columns. On the other hand the development of first principles models is usually time consuming and expensive. To overcome these problems, empirical models such as neural networks can be used. One major drawback of empirical models is that the prediction is valid only inside the data domain that is sufficiently covered by measurement data. Modeling distillation columns by means of neural networks is reported in literature by using recursive networks. The recursive networks are proper for modeling purpose, but such models have the problems of high complexity and high computational cost. The objective of this paper is to propose a simple and reliable model for distillation column. The proposed model uses feed forward neural networks which results in a simple model with less parameters and faster training time. Simulation results demonstrate that predictions of the proposed model in all regions are close to outputs of the dynamic model and the error in negligible. This implies that the model is reliable in all regions.

Index Terms: ARX model structure, Distillation column, Modeling, Neural networks.

1. Introduction

Advanced process control and supervision require accurate process models. Process models can be broadly divided into two categories: first principles models and empirical models. First principles models are developed based upon process knowledge and, hence, they are reliable. Whenever feasible, first principles models should be developed and utilized. The development of first principles models is usually time consuming and effort demanding, especially for complex processes. For some poorly understood processes, it is even impossible to build first principles models. However, in many nonlinear systems it is extremely difficult and expensive to obtain an accurate model of the process from first principles. This difficulty has limited the usage of nonlinear models to regions and systems where the model obtained is reliable. To overcome this difficulty, empirical models based upon process input output data can be developed.

Distillation is an important process in the separation and purification of chemicals. The distillation process is highly nonlinear and In industrial practice, it is not always possible in general to obtain accurate first principles models for high-purity distillation columns. Most industrial columns are used to separate multi-component mixtures whose constituent elements are often not known completely. the fundamental thermodynamics of multi-component vapour-liquid equilibrium, the physical property data, and other essential constitutive relations required for the successful development of a first principles model are not always available. And even when such knowledge is available, the resulting models usually occur in the form of a very large system of coupled nonlinear ordinary differential equations, and may therefore not always be the most convenient for controller or fault detection design.

Over the last 20 years, the NNs became a well-established methodology as exemplified by their applications to identification and control of nonlinear systems [1, 2].