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Research Article

Modeling Of Industrial Catalytic Naphtha Reforming Plant by Using Artificial Neural Network (ANN)

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Abstract: The prediction model of naphtha catalytic reforming plant using Artificial Neural Network (ANN) is developed. Industrial data from reforming plant in Al-Basrah refinery are collected for the simulation of prediction model. The total number of test cases (504) is used to train and test ANN model based on the various networks and architectures. The input parameters of the model consist of inlet reactors temperature, operating pressure, weight hour space velocity, and hydrogen to hydrocarbon molar ratio. The outputs of the network model include property parameters namely; yield and research octane number (RON) of the gasoline. Multilayered feed forward back propagation neural networks are used for this research. The performances of the **six** training algorithms are compared to select the most suitable training algorithm for naphtha reforming model. The results show that the optimum topology for reforming model is Levenberg-Marquardt Algorithm. The effects of the number of hidden layer (s), number of nodes in the hidden layer(s), the type and arrangement of transfer functions on the behavior of the neural network is investigated. The optimization carried out of ANN model by change architecture to become four input neuron, seven in first hidden, seven in second hidden layer and two neurons in output of network. As well as, the best arrangement of transfer function is (tansig, tansig, purelin). The optimized ANN model reduced prediction error for test sets to be 0.000413 while the regression is 0.99935; the results show that the developed model is capable of predicting the yield and RON of the gasoline for the unseen in training sets.

Keyword: Catalytic reforming; naphtha; artificial neural network; Modeling and simulation

INTRODUCTION

Naphtha catalytic reforming (NCR) is one of the main processes in oil refinery. Low octane hydrocarbons such as paraffin and naphthenes are converted to high octane aromatics through this process. Hydrogen and other light gases such as propane and butane are also produced^{1, 2}.

Over the last few decades the use of ANN has increased to cover a broad range of areas including engineering, economic and medical sectors³. The ANN is reduction techniques to improve the computational efficiency especially when large and complex structures are required to approximate and capture highly nonlinear models⁴. ANN has been applied for modeling of various oil refineries processes such as hydrodesulphurization, hydrocracking, catalyst regeneration, and thermal cracking of naphtha⁵⁻⁷.

In the catalytic reforming of naphtha, Silva⁸, used a mapping technique which consists of fitting a neural network model to the industrial data of reforming process. The model was able to evaluate operational conditions, feed and product streams quality, catalyst performance, and product yield. The model was then used to generate new values of the process with adequate resolution and uniformly distributed along the range of the variables⁸. Manamalli *et al.*⁹ developed a simple kinetic model of catalytic reformer to extract kinetic parameters from the reforming reactions. Also, optimal control of catalytic reformer has been carried out using ANN to maximize the aromatics yield.

Two neural networks, one in the forward path and the other in the feedback path, were trained to give optimal temperature set points. Zahedi *et al.*¹⁰ presented two ANN models for simulating the industrial NCRP and plant forming unit. The proposed model had predicted the volume flow rates of hydrogen, gasoline, and liquefied petroleum gas, outlet temperature, gasoline specific gravity, and RON of gasoline. In this study, 90 data sets were collected from Tabriz Refinery unit. The results showed that the predicted error of the networks was 1.07%.

Alves *et al.*¹¹ selected a mapping technique consists of fitting an ANN to the industrial data, and using this model to generate new values of the process variables with adequate resolution. The simulation results based on the proposed model agree very well with actual operating data of the industrial unit in a petroleum refinery. Hamed *et al.*¹² studied Adaptive Neuro-Fuzzy Inference Systems (ANFIS) for the system of naphtha reforming. In this research, 31 industrial data sets were used (21 data for training and the rest of the data used for generalization). The results showed that, hybrid method training algorithm in ANFIS has good agreements between industrial data and simulated results.

Sepehr and Mohaddecy¹³ used a ninety-seven data points were gathered from the industrial catalytic reforming plant during the complete life cycle of the catalytic bed. Ultimately, 80% of them were selected as past horizontal data sets, and the others were selected as future horizontal ones. The developed network was applied to predict the volume flow rate and research octane number of the future data versus days on stream.

Catalytic Reforming Unit of Basrah Refinery: Basrah reforming plant is considered as one of the most important industrial plants in Iraq. The productivity of the plant is **(8000 barrels /day)**. It is designed to produce reformate with high octane number through the process which contains three catalytic packed bed reactors and operates under adiabatic conditions with a central furnace. Each one of three reactors has been provided with **(Pt-Re/ Al₂O₃)** catalyst. The volume ratio of catalyst in reactors is **1:2:4**, this arrangement is important because the dehydrogenation reactions of naphthenes to aromatics which are nearly taking place in the 1st reactor. The 2nd and 3rd reactors contain more catalyst than the 1st reactor to

compensate for the loss in catalyst activities and allow more time in favor of higher yield of aromatics and branches^{14,15}.

However, the unit of the catalytic reforming process operates with a flow rate of **(38838 kg/hr)** of feedstock with low octane number (**about 65**). However, feedstock is fed to the 1st section of the furnace and then passed through to the first packed bed catalytic reactor. The endothermic reaction is carried out for converting naphthene to aromatic. So, the temperature of product stream will reduce to about **(40-50 °C)**. The product stream from the 1st reactor is then reheated to value of about **(505-530 °C)** inside the 2nd section of the furnace. The pre-heated mixture is then fed to the 2nd catalytic reactor. The reforming reactions still continue through the steps where the stream from the 2nd reactor will re-heated through the 3rd section of the furnace. The product stream from the last reactor contains reformat with high octane number¹⁶.

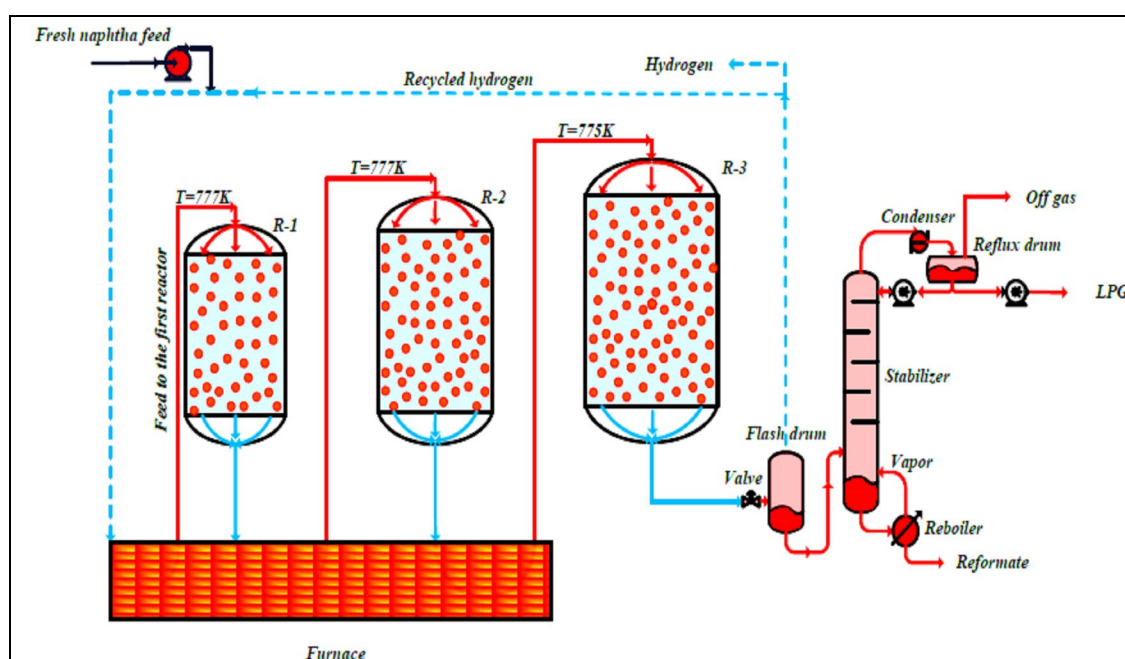


Figure 1: Process flow diagram of the catalytic naphtha reforming unit in Basrah refinery.

Artificial Neural Networks (ANN): The Artificial neural network (ANN) is an artificial intelligence technique that mimics the human brain's biological neural network in the problem solving processes. Neural Network consists of a number of interconnected processing elements, commonly referred to as neurons or nodes^{17, 18}.

Three layers including in ANN; there are input layer, hidden layer, and output layer as shown in **Figure 2**. The Input Layer is a layer of neurons that receives information from external sources, and passes this information to the network for processing. The hidden Layer is a layer of neurons that receives information from the input layer and processes them in a hidden way. The output Layer is a layer of neurons that receives processed information and sends output signals out of the system¹⁹.

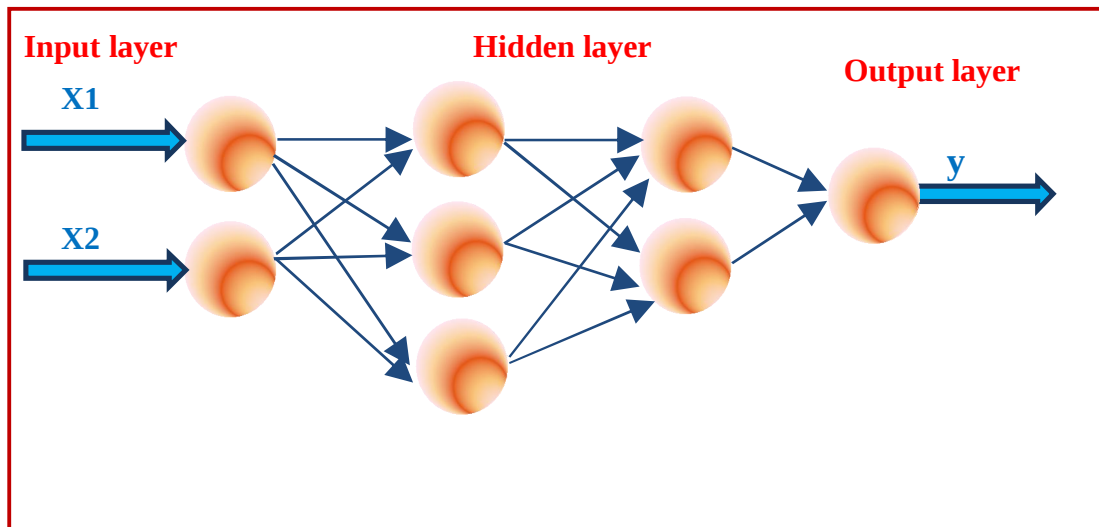


Figure 2: Basic structure of a multilayer feed forward neural network.

The number of input neurons corresponds to the number of input variables into the neural network, and the number of output neurons is the same as the number of desired output variables. The number of neurons in the hidden layer depends on the application of the network²⁰.

An artificial neuron is the basic element of a neural network. It consists of four basic components that include inputs and outputs, weighting factors, bias, and activation function. These elements are explained in the following **Figure 3**.

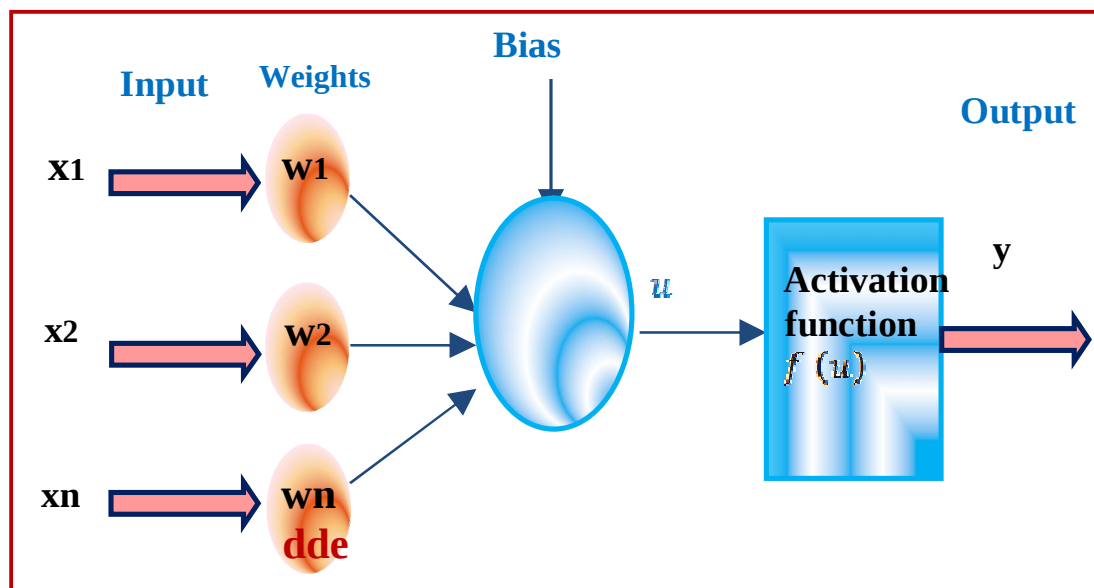


Figure 3: Basic elements of a neural network

It is a procedure for modifying the weights and biases of network to force a network to yield a particular response to a specific input, also referred to as training algorithm. Learning is certainly more complex than the simplifications represented by the learning rules used. We have two different types of learning rules, there are learning with supervision and learning without supervision²¹.

Artificial Neural Network Modelling: The experimental data used to train the neural network as training sets are those measured in catalytic reforming unit of Basrah refinery. The total number of (504) test cases are utilized. The loading case is represented by any six readings which have been selected from whole data. The industrial data of Basrah are divided into two sets: training set and testing set. The training set is used for computing the gradient and updating the network weights and biases to diminish the training error, and find the relationship between the input and output parameters. The testing set is used to evaluate the generalization ability of the learning process. The training set and test set consists of two-third and one-third of the total industrial data respectively. In this study, the parameters which may be introduced as the components of the input and the target vector as shown in **Table 1**.

Table-1: input and output parameters of the Proposed ANN

Item	Parameter	Symbol	Value
Input Parameters	Inlet Reactor temperature (C)	T	505-530
	Reactor Pressure (bar)	P	32-35 bar
	Hydrogen to hydrocarbon ratio	H ₂ /HC	5.5-8.7
	Weight hour space velocity (hr ⁻¹)	WHSV	1.4-2.1
Output Parameters	Gasoline yield (mol %)	Yield	78-91
	gasoline octane number	RON	67-86

Since there are a large number of training algorithms for feed forward neural network, it cannot be easily decide to estimate the best algorithm for a specific application. Thus the neural network model is trained by using six different training algorithms which are:

Gradient descent (traingd), Gradient descent with momentum (traingdm), Levenberg-Marquardt Algorithm (trainlm), Resilient (trainrp), Gradient descent with adaptive learning rule (traingda), and Gradient descent with momentum and adaptive learning rule (traingdx).

The computer program that is coded in **MATLAB.7** languages realizes the training and testing processes of the neural network with different training algorithm. The Structure of the program can be explained as a flow chart shown in **Figure 4**.

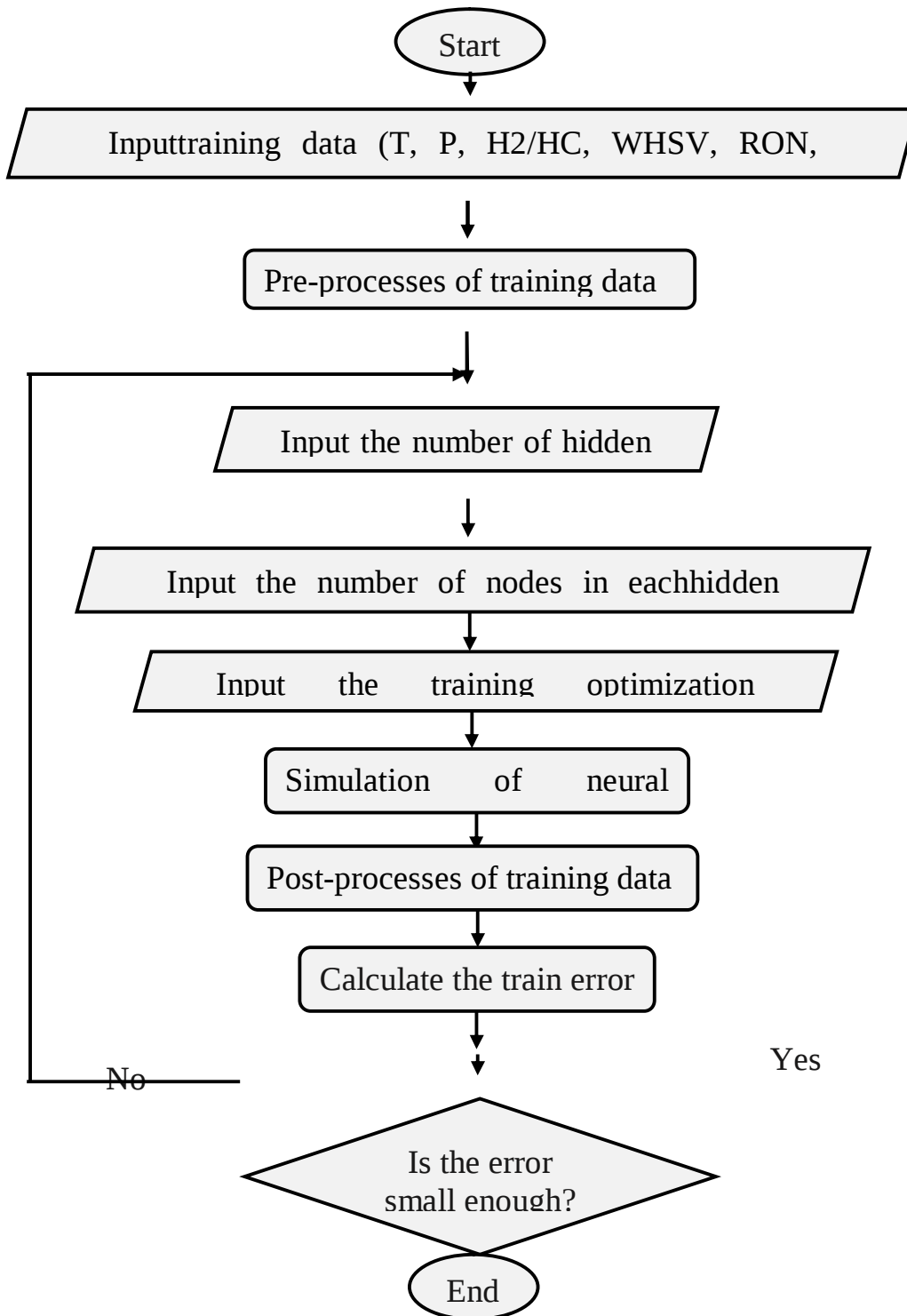


Figure 4: Flow chart of neural network program.

RESULTS AND DISCUSSION

In this study, various optimization algorithms of neural network are tested with one and two hidden layer configurations where the number of nodes in each hidden layer (s) is increased with a certain step. The results are divided into two parts; the first part related to use one hidden layer and the second part represents the use of two hidden layers in ANN modeling.

Using one hidden layer network: In this study, six training algorithms have been analyzed and tested there are (traingd, traingdm, traingdx, trainrp, traingda and trainlm). Also, the number of nodes in the hidden layer at each algorithm is discussed. However, different numbers of nodes for different algorithms are investigated to predict the best algorithm and best structure. All these algorithms are tested with activation function as hyperbolic tangent (*tansig*) function for hidden and linear (*purelin*) function for output layers.

Figure 5 gives comparisons between the different algorithms used in this study. This figure shows that, at the same number of iteration (Epochs), Levenberg-Marquardt Algorithm (trainlm) gives the lower value of mean square error and maximum value of regression at the same time. The number of nodes in a hidden layer drastically affects the outcome of the network training. Therefore, the various topologies of neural network are tested with an increasing number of nodes in hidden layer from (1 to 21) as shown in Figure 6. The figure shows that Levenberg-Marquardt algorithm with (19) nodes in the hidden layer gives best performance for testing than other networks which including different numbers of nodes in their hidden layers.

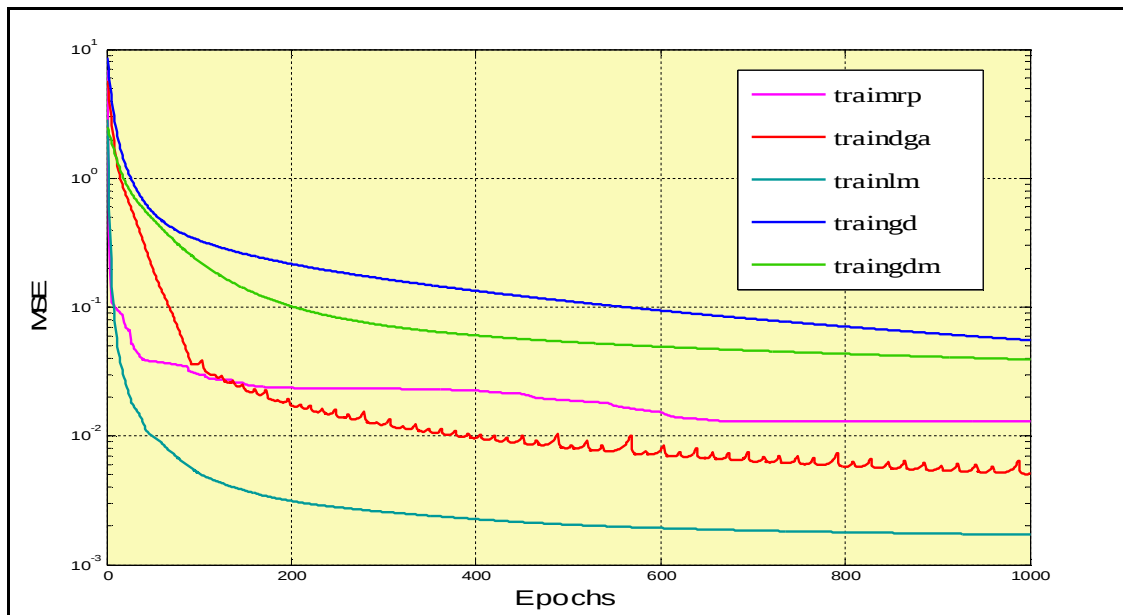


Figure 5: Compare various types of ANN algorithms with respect to Epoch.

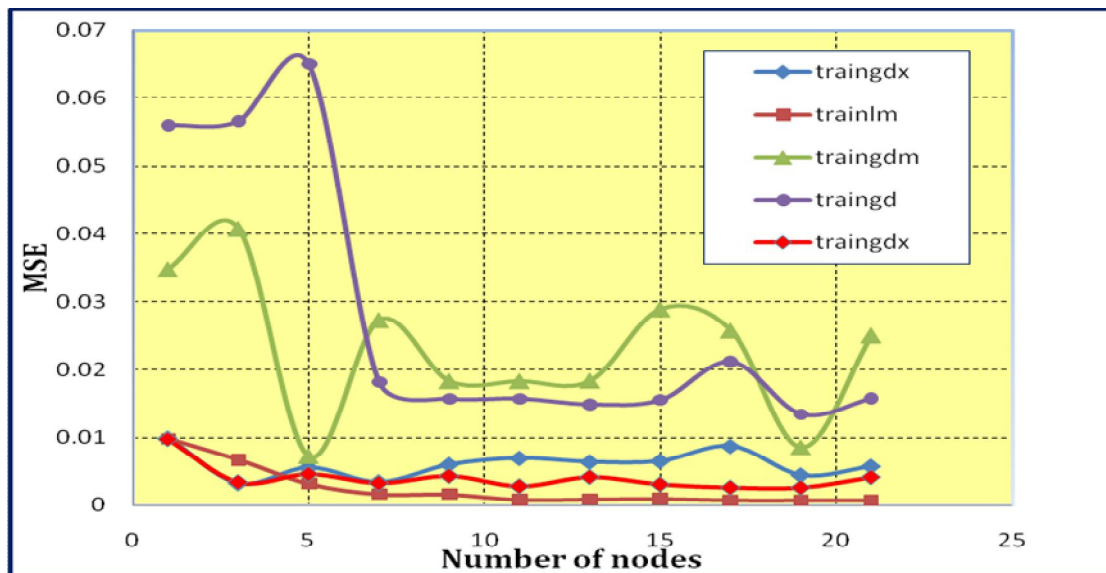


Figure 6: Comparison between Various types of ANN algorithms with respect to number of nodes

Additionally, the type and arrangement of activation functions have affected on the result. Therefore, different arrangements of activation function are analyzed where their results are shown in **Table 2** these arrangements including (*tansig, tansig*) and (*tansig, purelin*) type of activation functions arrangement. From the same table, it can be noticed from the shaded cell that the most networks with (*tansig, tansig*) arrangement have given the best performance and regression.

For this one hidden layer network, **Figure 7** shows the training session as the training error decrease versus number of iterations (*Epochs*) until goal error meeting. The performance parameter (*MSE*) at the final of iteration is 0.00067 that is a good value for total neural network error. Also, **Figure 8** show the regression analysis of the output of the proposed one hidden layer network and the corresponding target. It can be concluded from this result that an acceptable. Known that, the same result can be predicted from Table2, where the value of (*R*) approached to 0.99871.

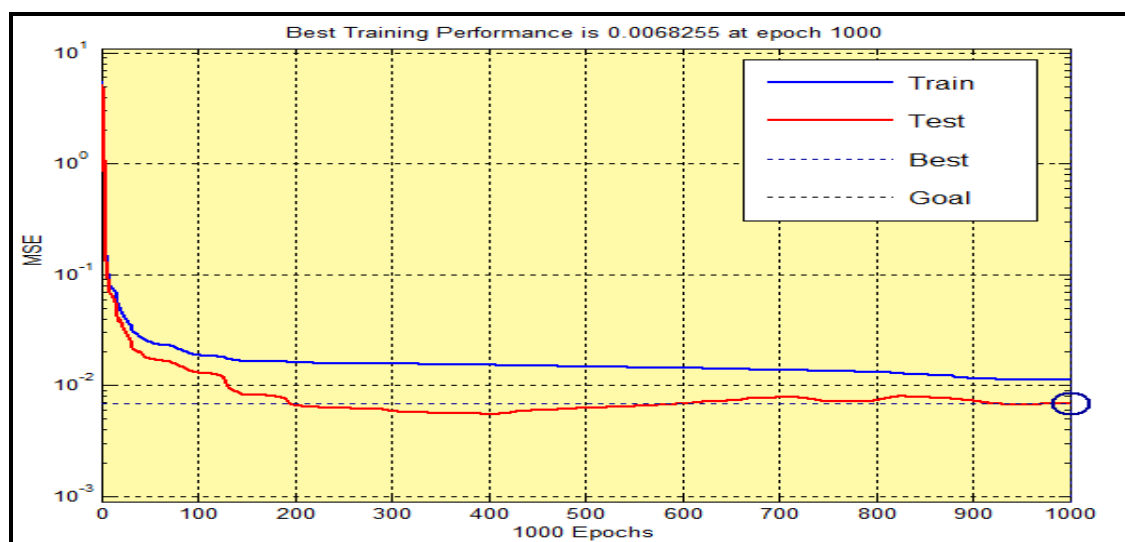


Figure 7: MSE for both training and testing data for one hidden layer

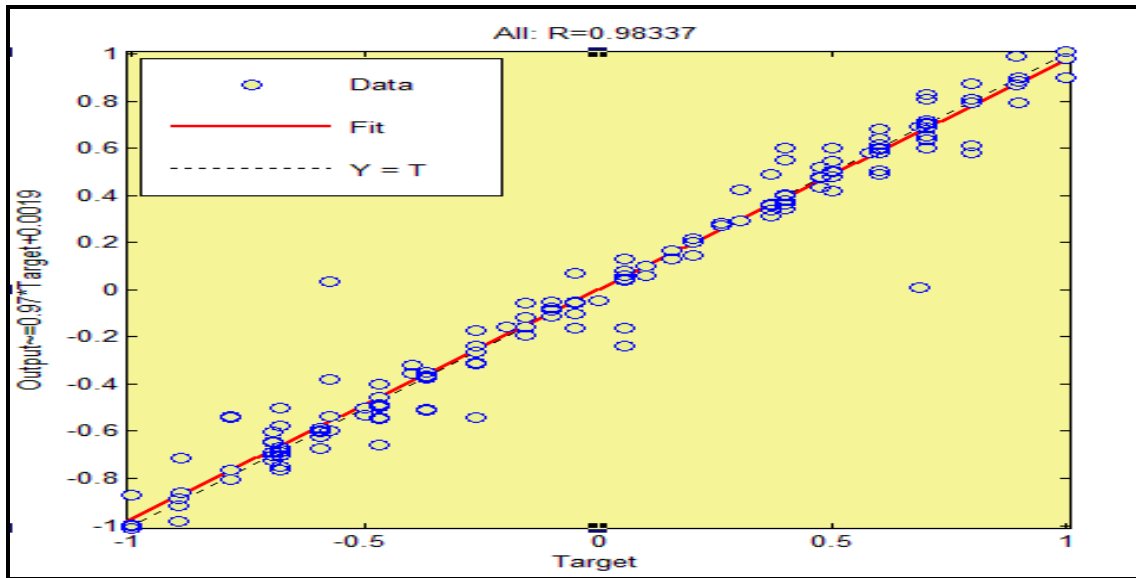


Figure 8: Regression for one hidden layer

Table 2: MSE and R for the one hidden layer Levenberg-Marquardt Algorithm.

No.of nodes	R and MSE	(tansig, tansig)	(tansig, purelin)
17	R	0.99804	0.94812
	MSE	0.00076	0.02123
18	R	0.99872	0.99875
	MSE	0.00051	0.00657
19	R	0.99871	0.95079
	MSE	0.00067	0.00135
20	R	0.99802	0.99878
	MSE	0.0007	0.00127
21	R	0.99809	0.93757
	MSE	0.00049	0.00158

From the previous analysis, the network configuration consisting 19 nodes for hidden layer with arrangement of (*tansig, tansig*) as activation function of hidden and output layers is chosen as a better network. However, this network can be compared with the best network of two hidden layer after investigation between the different types of two hidden layer network to estimate the proposed network.

Using one hidden layer network: After estimating the best algorithm of ANN for naphtha catalytic reforming model, then, neural network of two hidden layers is used with different activation functions for first hidden layer, second hidden layer and output layer. Also, various numbers of nodes in each hidden layer are used. The next important step had discussed the number of nodes at each layer of the two hidden layers with respect to their effect on the training performance and regression. Also, the effect of the number of nodes in the two hidden layers on the response of network as well as the optimum arrangements of activation functions is optimized in order to obtain the proposed network. Therefore, for

Levenberg-Marquardt Algorithm (trainlm), different arrangements of activation functions have been considered for the two hidden layers and the output layer.

Generally, use a two hidden layers configuration has improved the efficiency of the neural networks. Also, use various numbers of nodes in the both first and second hidden layers will be very useful to estimate the optimum number of these nodes to minimize the network error.

Therefore, the numerical values in **Table 3** explain that the network with structure 7-7 (7 nodes in the first hidden layer and 7 nodes in the second hidden layer) has given the best performance and regression for both training and testing mode.

Table 3: MSE and R for the two hidden layer networks with different arrangements of activation functions for Levenberg-Marquardt (trainlm) algorithm

No.of nodes	R and MSE	(tansig, urelin, purelin)	(tansig, ansig, purelin)	(tansig,tansig, tansig)	(purelin, tansig, tansig)	(tansig,purelin, tansig)
3-3	R	0.99353	0.99465	0.99183	0.99252	0.99436
	MSE	0.00298	0.00249	0.00404	0.00383	0.00259
3-5	R	0.99437	0.99624	0.99673	0.99544	0.99248
	MSE	0.00259	0.00177	0.00121	0.00205	0.00364
5-3	R	0.99458	0.99636	0.99474	0.48799	0.99555
	MSE	0.00266	0.00169	0.00127	0.00497	0.00220
5-5	R	0.99487	0.99774	0.99722	0.99522	0.44415
	MSE	0.00264	0.00081	0.00120	0.00230	0.00285
5-7	R	0.99539	0.99838	0.99808	0.99697	0.99561
	MSE	0.00201	0.00728	0.00088	0.00109	0.00199
7-3	R	0.99589	0.98597	0.99833	0.99433	0.99658
	MSE	0.00201	0.00655	0.00007	0.00259	0.00151
7-5	R	0.99666	0.98311	0.99826	0.99564	0.99689
	MSE	0.00146	0.00593	0.00075	0.00183	0.00133
7-7	R	0.99712	0.99932	0.99861	0.99661	0.98887
	MSE	0.00124	0.00043	0.00523	0.00141	0.00457
7-9	R	0.99671	0.99877	0.99874	0.99714	0.99607
	MSE	0.00133	0.00053	0.00055	0.00117	0.00194

However, the comparisons between the performances of one and two hidden layers network are very important to estimate the best network configuration. Therefore, **Figure 9** gives a comparison between the performances of one and two hidden layer (s) network based on (trainlm) algorithm. It can be noticed that from the plot, the efficiency of two hidden layer network is better than the other for the modeling of naphtha catalytic reforming. In the other hand, from the comparisons between the shaded cells in **Tables 2 and 3**, it is easy to conclude that, two hidden layers network consist of 7 nodes in the first layer and 7 nodes in the second hidden layer is better than that of 19 nodes with one hidden layer.

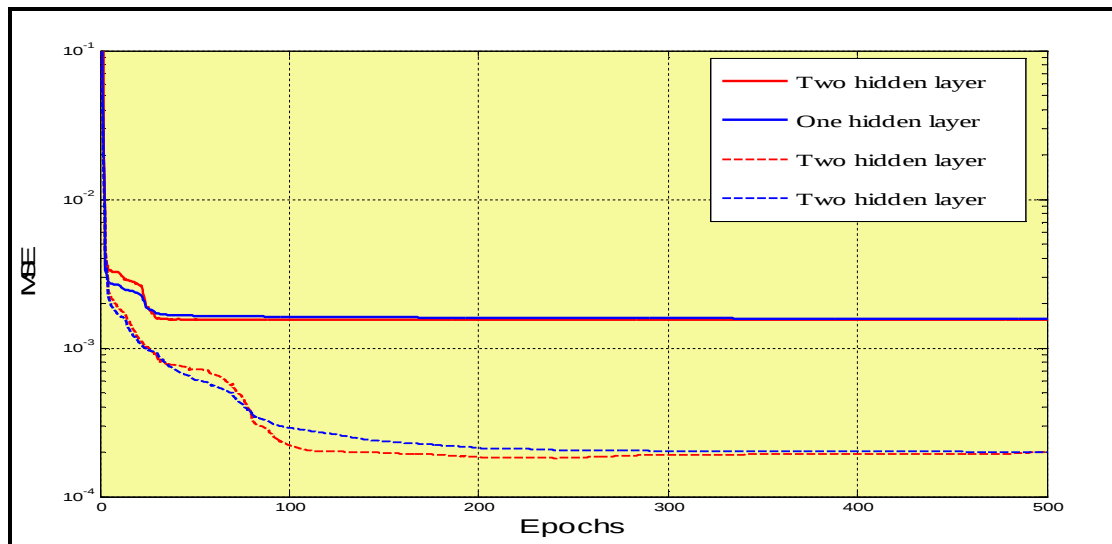


Figure 9: Comparison between one and two hidden layers of ANN Performance.

Consequently, at using one hidden layer in ANN, the shaded cell in **Table 2** has explained that the networks with (*tansig*, *tansig*) arrangement will be able to give the best performance and regression. In other hand, for two hidden layers network, different types and arrangements of activation function for hidden and output layers are considered to estimate the optimal arrangement. Finally, the shaded cell in **Table 3**, refer to that the networks with activation function arrangement as (*tansig*, *tansig*, *purelin*), give the best values for both performance and regression. Moreover, **Figure 10** and **Table 4** shows a comparison between the performances (MSE) for testing data of those network arrangements.

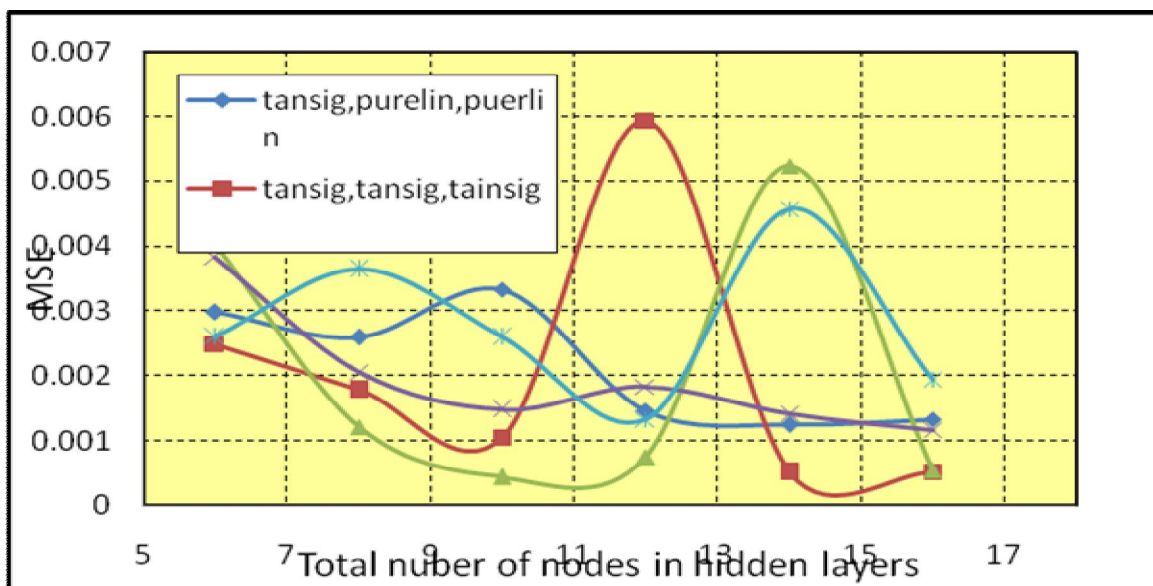


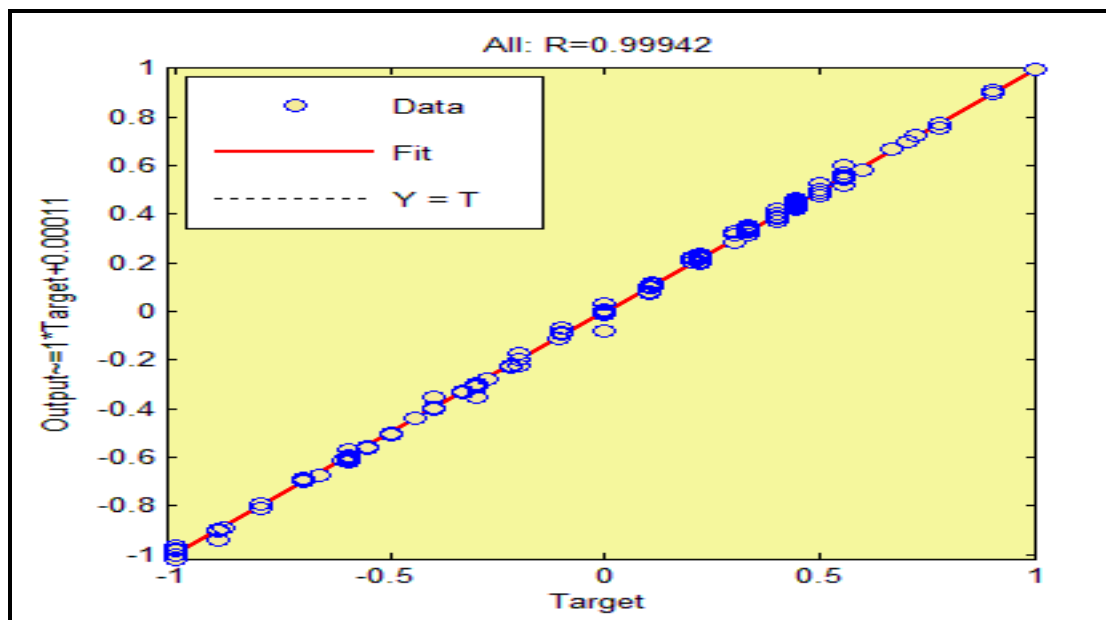
Figure 10: Comparisons various activation function arrangements of two hidden layer

Table 4: Comparison between one and two hidden layer networks

Item	Nodes Numbers	R	MSE	Activation function arrangement
One hidden layer	19	0.99871	0.00067	<i>tansig- tansig</i>
Two hidden layer	7-7	0.99935	0.000431	<i>tansig- tansig-purelin</i>

As the processing of one hidden layer network, the regression analysis between the output of neural network and the corresponding target was implemented as shown in **Figure 11**. In this figure, the outputs are plotted versus the targets as open circles. The solid line indicates the best linear fit and the broken line indicates the perfect fit (output equals targets). The regression value is very near to 1. Also, the performance parameter for the proposed network is a good value as shown in **Figure 12**.

Finally, **Figure (13)** and **Figure (14)** gives comparisons between the prediction data from neural network and the industrial data information from Basrah refinery. The first figure has explained the prediction values for the produced gasoline (yield %) from the catalytic reforming unit. While, the second figure related with the prediction of gasoline octane number. Both figures have shown that the predicted data based on the proposed model of ANN are agreed very well with actual operating data of the industrial unit.

**Figure 11:** Training regression for two hidden layer

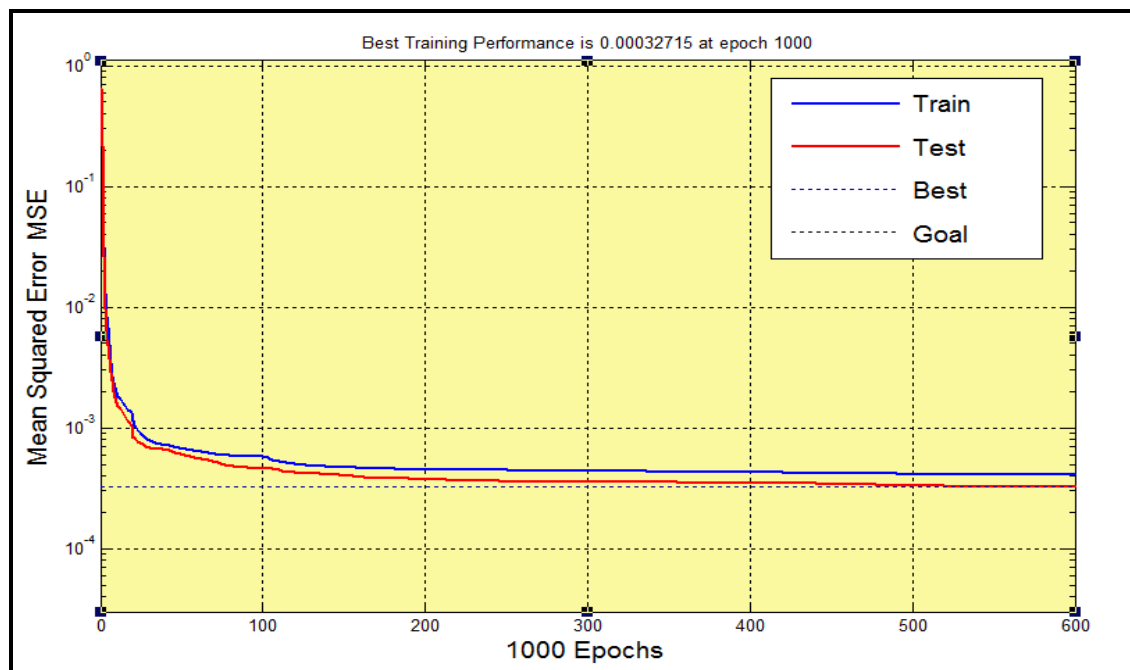


Figure 12: MSE for both training and testing data for two hidden layer.

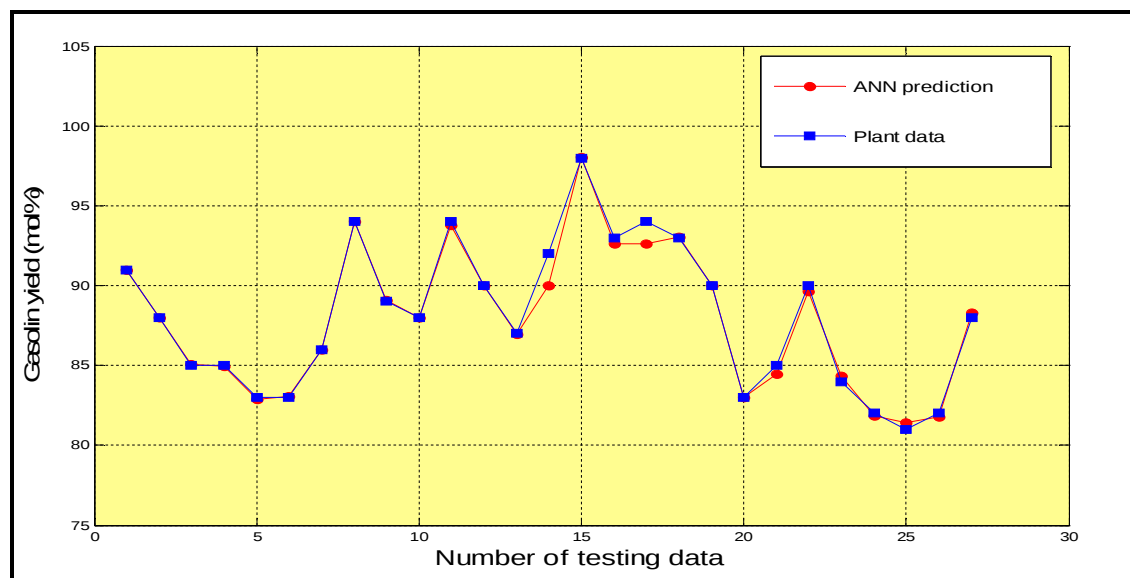


Figure 13: Prediction of proposed ANN for gasoline yield.

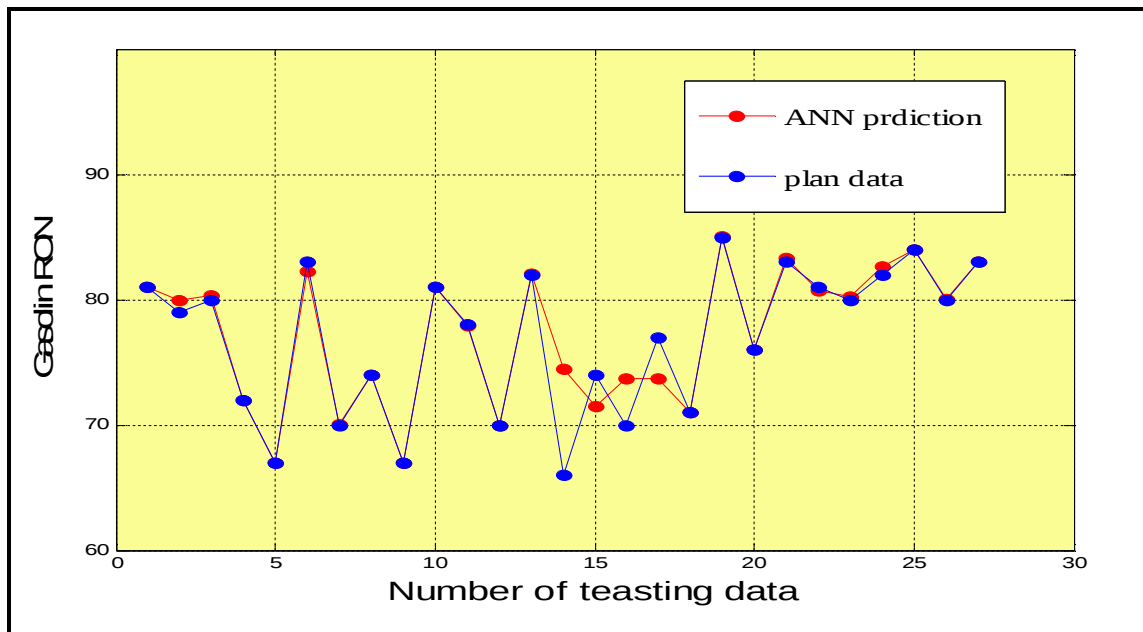


Figure14: Prediction of proposed ANN for gasoline octane number (RON).

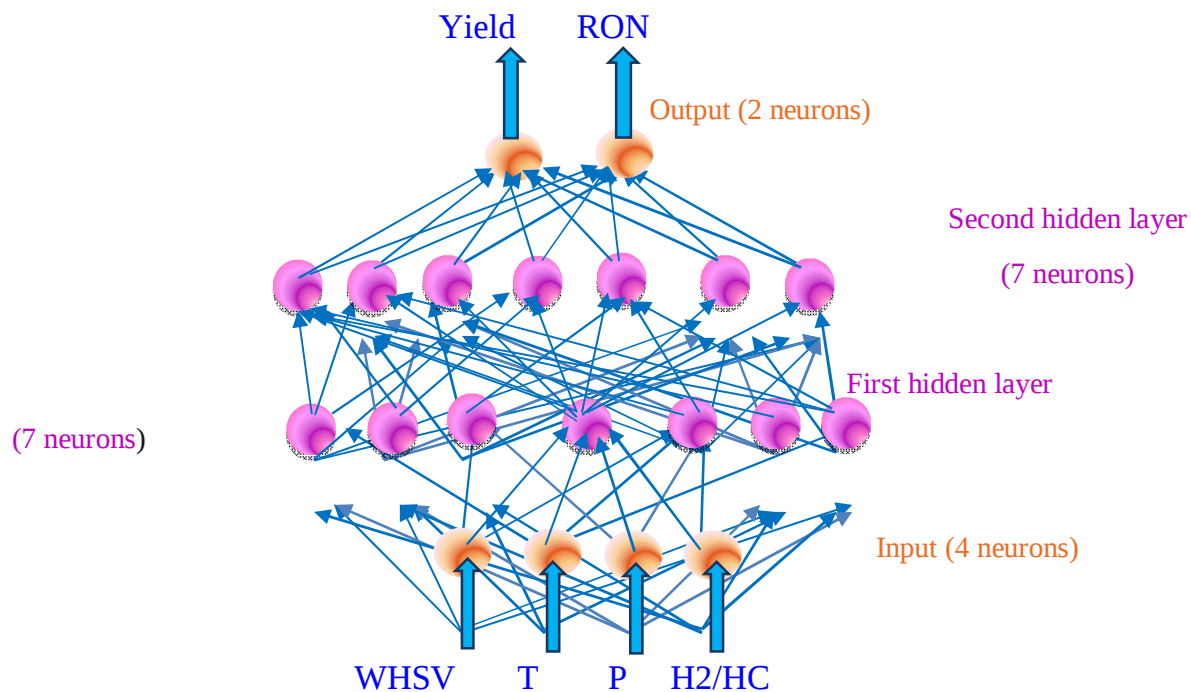


Figure 15: the proposed neural network structure.

CONCLUSION

In this study, industrial data from reforming plant in Al-Basrah refinery are used for the simulation of prediction model. The input parameters of the model consist of inlet reactors temperature, operating pressure, weight hour space velocity, and hydrogen to hydrocarbon molar ratio. The outputs of the

network model include property parameters namely; yield and research octane number (RON) of the gasoline.

Multilayered feed forward back propagation neural networks are used for this research. The performances of the six training algorithms are compared to select the most suitable training algorithm for naphtha reforming model. The results show that Levenberg-Marquardt Algorithm (trainlm) can give the desired results as compare with other algorithms. Moreover, the network with two hidden layers (7 nodes in both the first and the second hidden layer) is significantly better than that with one hidden layer. Also, by using various networks with different types and arrangements of activation functions it can be seen that (trainlm) training function with (*tansig*, *tansig*, *purelin*) as activation functions for the two hidden layers and output layer will be able to produce the best mean square error and correlation coefficient for both training and testing. Therefore, this network will be selected as a proposed network for the present study. In this study, the network with two hidden layers which is including 7 nodes in first hidden and 7 nodes in the second hidden layer is the proposed network. Where, the values of *MSE* and *R* are desirable, these values indicate that the mapping of neural network for the training and testing data is very good. In addition, the following table shows the proprieties of the best one and two hidden layer(s) network which are discussed in this study.

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