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Development of Artificial Neural Network Model of Crude Oil Distillation Column

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ABSTRACT

Artificial neural network in MATLAB simulator is used to model Baiji crude oil distillation unit based on data generated from aspen-HYSYS simulator. Thirteen inputs, six outputs and over 1487 data set are used to model the actual unit. Nonlinear autoregressive network with exogenous inputs (NARX) and back propagation algorithm are used for training. Seventy percent of data are used for training the network while the remaining thirty percent are used for testing and validating the network to determine its prediction accuracy. One hidden layer and 34 hidden neurons are used for the proposed network with MSE of 0.25 is obtained. The number of neuron are selected based on less MSE for the network. The model founded to predict the optimal operating conditions for different objective functions within the training limit since ANN models are poor extrapolators. They are usually only reliable within the range of data that they had been trained for.

Keywords: Artificial Neural Network Model, Crude Oil Distillation Unit, MATLAB, Aspen-HYSYS.

تطوير موديل بواسطة الشبكة العصبية الصناعية لوحدة التقطير الجوي للنفط الخام

الخلاصة

استخدمت الشبكة العصبية الصناعية في برنامج ماتلاب لعمل موديل لوحدة التقطير الجوي لمصفى بيجي بالاعتماد على المعلومات التي تم توليدها للحالة الديناميكية للوحدة في برنامج محاكاة اسبن-هايسز. ثلاثة عشر مدخل ,ستة مخارج, و1486 من البيانات استخدمت لعمل موديل للوحدة الفعلية.الارتداد الأوتوماتيكي الغير خطي ولوغاريتم الارتداد الخلفي وقد تم استخدام الارتداد الخلفي او التراجعي للتدريب. سبعون بالمائة من البيانات استخدمت لتدريب الشبكة بينما ثلاثون بالمائة المتبقية من البيانات تم استخدامها للصلاحية والتأكد من فعالية الشبكة ودقة التخمين لها. طبقة مخفية واحدة وثلاث وأربعون عصبون مخفي استخدم لهيكلية الشبكة مع قيمة لمربع الخطأ مقدارها 0.25 ,تم اختيار عدد العصبونات بالاعتماد على اقل قيمة لمربع الخطأ للشبكة.وجد بان الموديل الذي تم إنشائه له القابلية على تخمين الظروف التشغيلية المثالية ولمختلف الظروف شرط ان تكون ضمن نطاق تدريب الشبكة لكون موديل الشبكة العصبية ضعيفة في ايجاد القيم التي تقع خارج المدى.

الكلمات الدالة:موديل الشبكة العصبية الصناعية, وحدة التقطير الجوي,ماتلاب, اسبن-هايسز

Nomenclatures

E	Error criteria for network convergence	α	Momentum rate
t	Time,(min)	η	Learning rate
T	Temperature,(^oC)	b	Bias
Wij	Weight value between input and hidden layer	y	Output of neuron
X	Input of neuron	Δ	Difference

Introduction

The petroleum refining processes are highly complex and integrated especially in the crude oil distillation unit (CDU because it produces a wide range of products [1].The mechanism of separation in the fractionating columns is based primarily on the difference in the boiling points of the components. Thus, when this vapor is cooled and condensed, the condensate will contain the more volatile components which have lower boiling points [2]. Crude oil distillation unit today are facing new challenges in order to meet the requirements with respect to improving fuel properties, product quality and increasing the yields of the distillate products**.** A lot of crude units currently operate with different feed slates to their original feed specifications, satisfying the demands of the market [3]. Most petroleum distillates, especially those from atmospheric distillation tower, have different physical properties depending on the characteristics of the crude oil [4].

In multivariable processes such crude oil distillation column, unknown models structures and high correlation between process variables are examples of problems that are faced daily. On the other hand, artificial neural networks (ANN)have been successfully used for a number of chemical engineering application[5]. An artificial neural network (ANN) is an information processing paradigm that is inspired by the way biological nervous systems (such as the brain) process information. It is composed of a large number of highly interconnected processing elements (neurons) working in unison to solve specific problems [6]. Among these methodologies, the back propagation algorithm, gradient descent supervised learning has an enormous influence in research on neural network. Neural networks have been used as an alternative to the traditional mathematical models to simulate complex and nonlinear patterns. Basically, the design of a neural network only requires a relatively large set of data to adjust the parameters in the net. The great disadvantage of neural networks is their limited capability to predict situations not considered in their design.

Khairiyah[7]developed and simulate a model constructed in ANN for CDU under MATLAB environment. Training and testing data for the network model were generated using steady state process models simulated in the aspen plus, the ANN models were developed using back propagation training algorithm. Ali and Khalid [8] introduced a mathematical model for large scale crude fractionators by the implementation of NN models using back propagation algorithm based on. Collection of real-time data operation, the proposed neural network architectures can accurately predict the properties online. The inputs of NN consist of plant data such as temperature, flow rate and pressure where the output is the predicted inferred process stream property for naphtha. The neural network model achieved the desired sum squared error goal of 0.01 in 3180 iterations. Khairiyah et al.[9] studied the development of connectionist of ANN models for a crude oil distillation column that can be utilized for real time optimization(RTO). The RBFN models were found to yield better and more consistent predictions with shorter training times than MLP models. Khairiyah et al.[10]discusses the artificial neural network (ANN) models for a crude oil distillation column, the multivariable models were developed for real time optimization (RTO).The results obtained showed that RBFN is suitable for modeling the crude oil distillation column. The root mean square error for the prediction is less than 1%.

Pavel et al.[11]present a empirical model for atmospheric column of crude unit by implementing neural network model. It has been estimated that the lab data has an average error with standard deviation of approximately 2ºc.Motlaghi et al.[12]establish the neural network model database of a crude oil distillation column by MATLAB. The neural networks model is well established and can represent and describe the distillation process for the input (system operation) and output (product quality) relations. Chang et al.[13]develop a bootstrap aggregated neural networks model to estimate the product quality. The developed technique gives better classification accuracy for kerosene dry point estimation with varying crudes than a single neural network, the accuracy of the models are higher than those of other models. Lekan et al.[6]proposed ANN models by MATLAB, fuzzy logic and genetic algorithm approach had been found is best and effective ways to model complex processes such as crude oil distillation column. They serve as substitutes for dynamic mathematical models as they are time independent. The accuracies obtained for the model were high. Chau-Kuang[14]investigated the maximizing oil production rate under the required oil product qualities of crude oil distillation unit (CDU) by the help of an ANN toolbox developed by MATLAB. The model founded to predict the optimal operating conditions for different objective functions.

The purpose of this study is to build a model for crude oil distillation unit of Baiji refinery. This model can be consider as a reference for optimal a predicted operation condition for the unit, also further to apply advance control strategies in the future for this model to study the controllability for crude distillation column.

Modeling Procedure by Artificial Neural Network

ANN, a connectionist-based black box model, consists of layers of nodes with non-linear basis functions and weighted connections that link the nodes. Using the nodes and weights, the inputs are mapped to the outputs after trained with a set of data known as training data. Multilayer feed forward ANNs have been mathematically proven to be a universal approximate, However, since ANNs are data driven, the resulting mode1 can only be as good as s the data provided to the network for testing and training[15]. Each neuron receives a signal from the neurons in the previous layer, and each of those signals is multiplied by a separate weight value.

The weighted inputs are summed, and passed through a limiting function which scales the output to a fixed range of values. The output of the limiter is then broadcast to all of the neurons in the next layer. So, to use the network to solve a problem, we apply the input values to the inputs of the first layer, allow the signals to propagate through the network, and read the output values [16].Figure (1) shows a ANN, which is for crude oil distillation unit and consist of these parts: The first is inputs and output this is the synapse or connections from or to other nodes. Inputs to the node, xi, may also come from data that have been normalized. The node manipulates the inputs to yield the output. yj, which may then be sent to more than one node. The second is the connection weights, determine the influence of the input on the output of the node. In this work, the first subscript of the weight, i. refers to the input while the second subscript, j, refers to the node. Weight factors can be inhibitory (if the value is negative) or excitatory (if the value is positive). A weight factor that is close to zero will have a negligible effect. The third is activation function, summation of the weighted inputs is passed through an activation function (also called squashing function or transfer function). This function units the amplitude range of the output. The most commonly used functions are the sigmoid function.

$$f(x) = l/(l + e^{-xj(t)}) \quad (1)$$

Where the f(x) is the sigmoidal transfer function and limits the output of all nodes in the network to be between -1 and 1.The neuron input, xi, is multiplied by the corresponding weight factor, wi , before being sent to the neuron. This is followed by performing summation of all input in the neuron body. An internal bias, b is also introduced to enhance performance of the network. The result is passed through a nonlinear activation transfer function to obtain the output y (Hunt,1992).

$$y = f(net) = f\left(\sum_{i-1}^{i=n} X_i W_i + b\right) \quad (2)$$

Back propagation learning algorithm is used to update the network weights and biases during training in order to improve the network performance by minimizing an error function between the desired (target) output(s) and the network output(s). The general rule used to update the weight can be written as:

$$\Delta Wij = -\eta \frac{\partial E}{\partial Wij} \quad (3)$$

Where wij is the weight on the connection between nodes i and j and η is the learning rate which is multiplied by the negative of the gradient to determine the changes to the weights and biases. The larger the learning rate, the bigger the step. If the learning rate is made too large, the algorithm becomes unstable. If the learning rate is set too small, the algorithm takes a long time to converge. Therefore careful choice of η is vital to increase the convergence time without affecting algorithm stability. It is not practical to determine the optimal setting for the learning rate before training, and, in fact, the optimal learning rate changes during the training process, as the algorithm moves across the performance surface. The new weight can be updated as follow:

$$Wij(k) = Wij(k-1) + \Delta Wij(k) \quad (4)$$

In order to accelerate the convergence of the network, some algorithms may introduce the previous weight change into the updating equation as:

$$Wij(k) = Wij(k-1) + \Delta Wij(k) + \alpha\, \Delta Wij(k-1) \quad (5)$$

Where α is called the momentum rate which can be any number between 0 and 1. When the momentum constant is 0, a weight change is based only on the gradient. When the momentum constant is 1, the new weight change is set to equal the last weight change and the gradient is simply ignored [17]. The back propagation algorithm stated was used as part of the implementation procedure for building the artificial neural network (ANN) for the crude distillation column. The coefficients of the model were discovered by training the neural network program using back propagation algorithms. The neural network program was trained by adjusting the weight coefficients until the difference between the predicted product quality and the measured product quality was within acceptable limits. When the coefficients had been determined, they would be tested by comparing the predicted quality to the measured quality for data sets which were not used in finding the coefficients. The major steps involved in implementing the ANN predictor [6].In this work we used trainlm function to updates weight and bias according to the Levenberg-Marquardt optimization. It is often the fastest back propagation algorithm in the toolbox and is highly recommended as a first choice supervised algorithm although it does require more memory than other algorithms. Trainlm implements the Levenberg-Marquardt algorithm, which works in such a way that performance function will always be reduced at each iteration of the algorithm. This feature makes trainlm the fastest training algorithm for networks of moderate size. Similar to trainbfg, trainlm suffers from the memory and computation overhead caused by the calculation of the approximated Hessian matrix and the gradient[18].

The System

The unit consists of the main atmospheric distillation column, side strippers, condenser ,heat exchanger, furnace , pumparounds , as the main process. Usually, five products are generated from the crude distillation (naphtha, kerosene, light gas oil, heavy gas oil and reduced crude). Crude distillation unit involves complex stream interactions with various sections of the main column which includes 52 trays of valve cap type,7 meter inside diameter,61 meter high, that is supplemented with secondary columns. The crude oil is pumped from storage with 850 m^3/h as a volumetric flowrate and is heated using a heat exchanger network (HEN).

The HEN enables the crude to achieve a temperature of about 200 - 250 ^oC, then the crude oil enters a furnace and is heated to a temperature 345 ^oC that will vaporize distillate products in the crude tower. Column normal pressure is 157kN/m^2, the heated crude then enters the fractionation tower in a lower section called flash zone at tray 47 the un vaporized portion of the crude oil leaves the bottom of the tower via a stream stripper section. The operating conditions and input specification for crude oil used for the simulation representation are in the Table (1). Three pump around top, intermediate and bottom pump arounds are involved to remove a hot side stream to cool it and then return it back to the column at a section above the draw off tray. The pump around is an internal condenser that takes out heat of that section and ensures reflux below that section.

Side stream distillate products are kerosene, light gas oil and heavy gas oil. These are stripped free of entrained light ends in separate stripping towers (called secondary columns). Four trays are required in these secondary columns. The purpose of secondary columns is to strip the side stream distillate products from entrained light ends. In these columns, steam is injected below the bottom tray which moves up the tower and leaves at the secondary column top along with light ends stripped out. The stripped steam (with light ends) is allowed to enter the main column just above the side stream draw off tray. A conceptual diagram of the CDU is presented in Figure (1).

Steam injected at the bottom of the main column used to stripped free of light ends, it enables the flashing of the streams at a reduced partial pressure and therefore contributes significantly for the removal of light ends throughout the main and secondary column.

Simulation Work

The neural network architecture for the design of the crude oil distillation column (CODC) is thirteen inputs with one hidden layer consist of nine nodes and six outputs (13-9-6) making a total of 34 nodes distributed over the three layers. The inputs to the network are(feed specific gravity, feed temperature, feed volumetric flowrate, top pumparounds volumetric flowrate, intermediate pumparounds volumetric flowrate, bottom pumparounds volumetric flowrate, top temperature, top pressure, and steam, reflux, naphtha, kerosene, LGO volumetric flow rate). The outputs from the NN architecture are (naphtha, kerosene, LGO D86 95% and top, intermediate, bottom pump arounds temperatures). The back propagation algorithm is used for the ANN of crude oil distillation unit. Figure (2) is the neural network architecture for the design of crude oil distillation column. The number of the hidden neurons is an important design issue. On the one hand, having more hidden neurons allows the network to approximate functions of greater complexity. But, as a result of network's high degree of freedom, it may over fit the training data while the unseen data will be poorly fit to the desired function.

Aspen-HYSYS simulator as shown in Figure (3) are used to build the dynamic state for the crude oil distillation unit of Baiji refinery. Out of 1487 records for inputs and outputs set are collected from the designed unit in aspen-HYSYS simulator, these data are collected by making step changed in the manipulated variables for dynamic case as shown in Table(2). The response is recorded for each input and output mentioned earlier in aspen-HYSYS simulator and converted to Excel spreadsheet, The range of the data used is shown in Table(3), these data are used in MATLAB simulator to build NN model for CDU. Nonlinear autoregressive network with exogenous inputs (NARX) are used for the ANN model in MATLAB. Since the aim of the case is to study the dynamic behavior and control of crude oil distillation unit. Input and output data are loaded to the workspace from excel spreadsheet. 70 % of the data are selected for training and 15 %, 15% are used for validation and testing.

The simulator normalized the training data between (-1,1). The final step is by converting the CDU model to SIMULINK window as shown in Figure (4).

Result and Discussion

The simulated work and actual refinery data obtained from Baiji oil refinery for the products quality, temperature and pressure profile are compared, to check the validity of the unit modeling with Aspen-HYSYS simulator for steady state case. Mean overall deviation (MOD) is used for all the trends to compare actual and simulated curves which is:

$$\%\mathrm{MOD} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{M_{Actual} - M_{Simulater}}{M_{Actual}}\right| * 100 \quad (6)$$

The temperature gradient through the tower is important for separating the various fractions based on the vapor pressure and the average boiling point. Figure (5) shows that the temperature profile for crude oil distillation column increases with the number of trays from top down. The streams leaving the top tray of the fractionation tower at (135 ^oC) and maximum value of the temperature occurs at the flash zone when the mixed flow rate of crude oil is fed to the main column at tray 47 with temperature of (345 ^oC) .As shown, the temperature profile trend after tray number 26 toward the top column which decreases sharply due to the heat removed by pump rounds effect. The MOD of (2.5532%) between two curves shows a good agreement.

For pressure profile Figure (6) shows the comparison between pressure profile for Baiji oil refinery column and Aspen- HYSYS simulator. Simulator pressure profile is almost increased linearly with the number of trays from top down while the actual data has small curvature due to trays level and pipes pressure drop which are not counted in the simulator. The maximum value of the pressure occurs at the flash zone when the mixed flowrate of crude oil is feed to the flash zone with 350 kN/m^2. The streams leave the top tray of the fractionation tower at 157.9 kN/m^2.As we can see, a good agreement between two cases are established. The MOD % for these curves is 0.8933 reflect the good results obtained from the simulator.

ASTM D86 test for naphtha, kerosene and gasoline is used since this test is daily assessment test in the refinery also which is, simpler ,less expensive , required only one-tenth of the time and it is performed under atmospheric pressure. It is used for determining the boiling point distribution of light petroleum fractions, such as naphtha, kerosene, diesel, and light gas oil. In Baiji oil refinery the analysis of the naphtha, kerosene, light gasoil are based on the ASTM D86 so we preferred to compare between actual and simulated ASTM. We see very good agreement between both form 20% to 90%

distillate as shown. The MOD% for curves of naphtha ASTM D86 is 0.17144 which is very small value and give a good impression.

Figure (8) shows the comparison between the actual ASTM of Baiji refinery and the Aspen-HYSYS simulator for kerosene, and we can see clearly the matching in the two cases that indicate the program simulator can represent the unit in a good way. Also, the simulator can give us an indication of the maximum amount for specific products. The MOD for curves is (0.03054%) which is less than MOD for naphtha.

Figure (9) shows the comparison between ASTM of LGO for the actual Baiji oil refinery and the Aspen- HYSYS program. As a result, we can see the matching between two curves and that gives us an impression about good representation for the real unit with Aspen- HYSYS simulator. The mean overall deviation MOD for both curves is (0.021422%). It is the smallest value among naphtha and kerosene.

In MATLAB simulator for ANN the optimum number of neurons in the hidden layer is predicted by plotting the number of neurons versus the mean square error. As shown in Figure (10). the increasing number of neurons in the hidden layer above thirty four does not achieve an observed improvement in the performance of the system as shown.

To obtain sufficiently excited data that cover the entire range of operating conditions, well-planned step tests on the plant are required. It must be done carefully as the quality of data generated determines the validity of the resulting estimation model. In this work, the tests were conducted on simulation basis. The step test experiments were conducted by changing selected inputs according to some step size. The data collected and exported to Excel.

For step change in feed temperature from 325 to 345 ^{o}C we get increasing of the vapor pressure of feed and the bottom liquid which means more vapor climbing up the column, this results in higher trays temperature correspondingly as well as the top tray temperature. While the step change in the column top pressure from 157 to 127 kN/m^2, column pressure upsets has a direct effect on the vapor pressure of the components decreasing in the column pressure with allowable limits is energy saving but can significantly affect product compositions, decreasing in the column pressure are effected on increasing the response of products and pump arounds temperature. Also the step change in steam volumetric flow rate from 4 to 5 m^3/hr, As increased in steam volumetric flow rate the response for products D86 95% and pump arounds temperature increased.

For step change in naphtha volumetric flow rate draw from 186 to 176 m^3/hr. As decreased in naphtha volumetric flow rate the response for products, pump rounds and top temperature decreased. Finally the step change in reflux flow rate from 114 to 124 m^3/hr. As decreased in reflux volumetric flow rate the response for products D86 95%, pump rounds and top temperature also decreased. Neural network training performance as we can see from this Table have the value of 0.25MSE for the performance also it tells us about the iteration time for the program which is 18 iterations. The neural network validation performance which is 23.34 at epoch 12(time steps for adaption). Neural network training regression for training and validation are 0.99996 and 0.99844 respectively as we can see in Table (4). This model has been tested with different step changes in input variables and we get satisfied result for the output but the step changes should be in the training limits.

Conclusions

Crude oil distillation model in MATLAB neural network toolbox is built with high performance. From what we get we conclude that neural network model is a good way to handle the nonlinear interacted model and consider as a reference to predict and optimize the operating conditions for the unit. Also ANN model gives the ability to predict and expect the future manner for certain circumstances. Finally NN controller can be applied to this model to control product quality and column pump arounds temperature. The great disadvantage of neural networks is their limited capability to predict situations not considered in their design. Advantages of NN based model are that they can take care of a nonlinear model of the process.

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Table 1: Operating parameter for crude oil column.

Item	Value
Feed flowrate,(m^3/hr)	848
Feed temperature,(^oC)	343
Feed pressure to the column,(kN/m^2)	380
Number of trays	52
Number of pumparounds	3
Number of side strippers	3
Column inside diameter,(m)	7
Feed location	Tray 47
Top tray temperature,(^oC)	135.42
Top pressure, (kN/m^2)	157.9
Bottom temperature,(^oC)	342
Top pumparounds draw and return	4-1
Top pumparounds return temperature,(^oC)	68
Top pumparounds Volumetric flow,(m^3/hr)	730
Intermediate pumparounds draw and return	13-11
Intermediate pumparounds return temperature,(^oC)	180
Intermediate pumparounds Volumetric flow,(m^3/hr)	530
Bottom pumparounds draw and return	24-22
Bottom pumparounds return temperature,(^oC)	230
Bottom pumparounds Volumetric flow,(m^3/hr)	320
Naphtha Product rate,(m^3/hr)	175
Kerosene draw and return	10-9
Kerosene Product rate,(m^3/hr)	105
Light gas oil draw and return	21-19
Light gas oil Product rate,(m^3/hr)	160
Heavy gas oil draw and return	41-39
Heavy gas oil Product rate,(m^3/hr)	30
Steam temperature,(^oC)	195
Steam volumetric flow,(m^3/hr)	3.807

Table 2 : Simulation runs for dynamic systems in aspen-HYSYS dynamic.

Run No.	Type of Disturbance	Value of Disturbance
1	Step change in feed temperature,(^oC)	328 - 348
2	Step change in top column pressure,(kN/m^2)	157 - 127
3	Step change in stram volumetric flowrate,(m^3/hr)	4 – 5
4	Step change in naphtha draw volumetric flowrate,(m^3/hr)	186 – 176
5	Step change in reflux volumetric flowrate,(m^3/hr)	114 – 124

Table 3 : Input and output training values range.

Variable name of input	**Range of data**
Feed specific gravity	0.8807-0.8332
Feed temperature,(^oC)	328.22-349
Feed volumetric flowrate,(m^3/hr)	800- 1030.
Top pump arounds volumetric flowrate,(m^3/hr)	733.2-685.13
Intermediate pump arounds volumetric flow rate,(m^3/hr)	533.7-560
Bottom pumparounds volumetric flowrate,(m^3/hr)	225.5-320
Top temperature,(^oC)	135.3-170
Top pressure,(kN/m^2)	127-157
Steam volumetric flowrate,(m^3/hr)	4.31-4.97
Reflux volumetric flowrate,(m^3/hr)	113.2-302.39
Naphtha volumetric flowrate,(m^3/hr)	176.4-180.27
Kerosene volumetric flowrate,(m^3/hr)	115-150
LGO volumetric flowrate,(m^3/hr)	100-180
Variable name of output	Range of data
Naphtha D86 95%,(^oC)	150-183
Kerosene D86 95%,(^oC)	224-309
LGO D86 95%,(^oC)	325-393
Top pump arounds temperature,(^oC)	60-138
Intermediate pump arounds temperature,(^oC)	175-214
Bottom pump arounds temperature,(^oC)	184-255

Table 4: Neural network model results.

	value
performance	0.25
Gradient	46.6
Number of iterations	18
Validation checks	6
Training regression	0.99996
Validation regression	0.99844
Test regression	0.99521
Overall regression	0.999

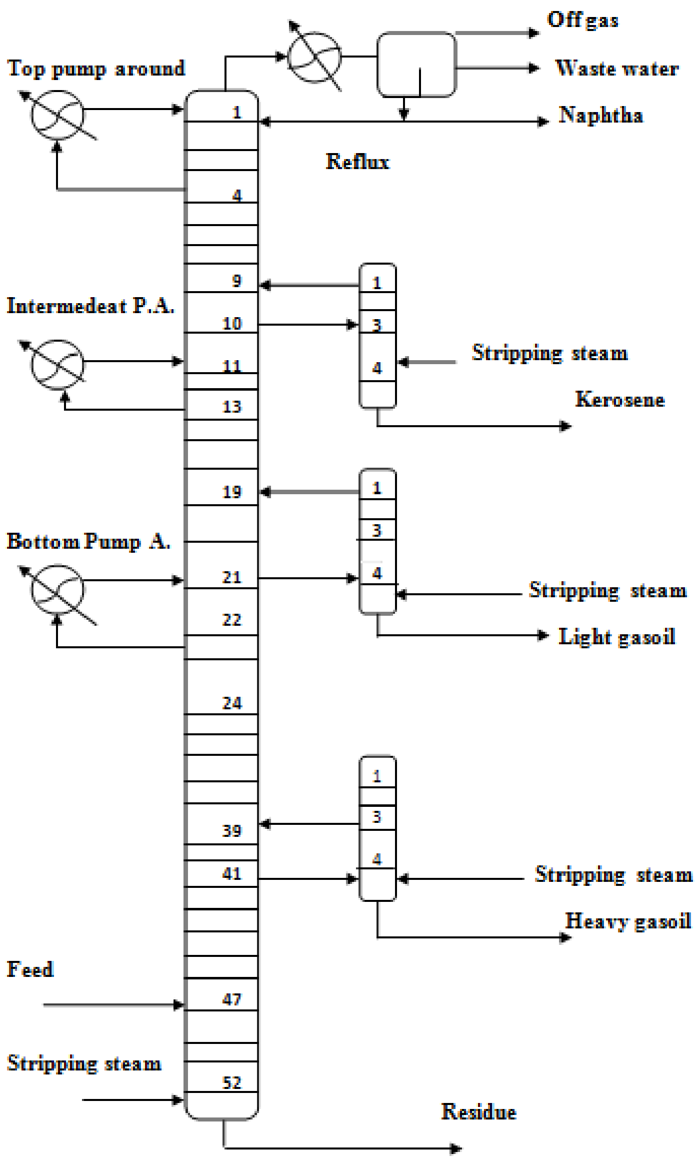

Fig.1 Crude oil distillation column diagram.

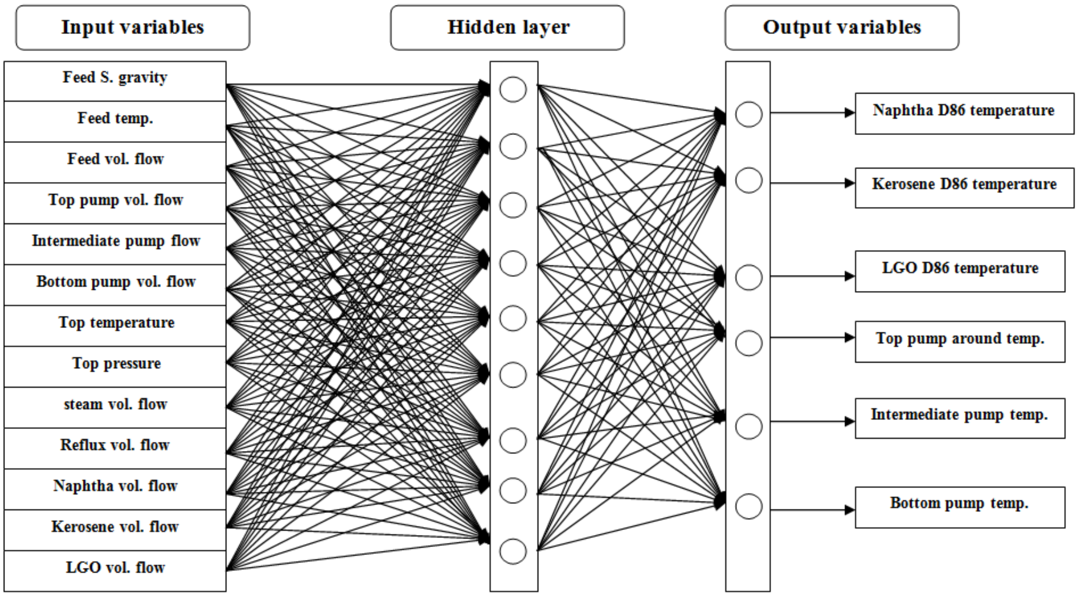

Fig. 2 Artificial neural network structure.

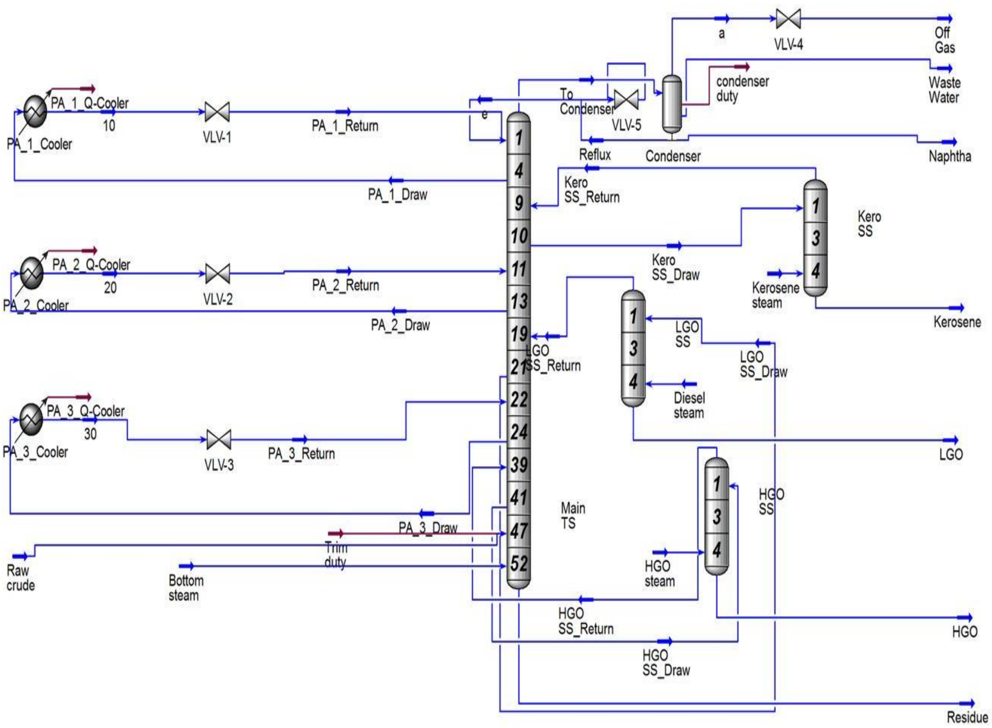

Fig. 3 Scheme of the dynamic crude distillation column.

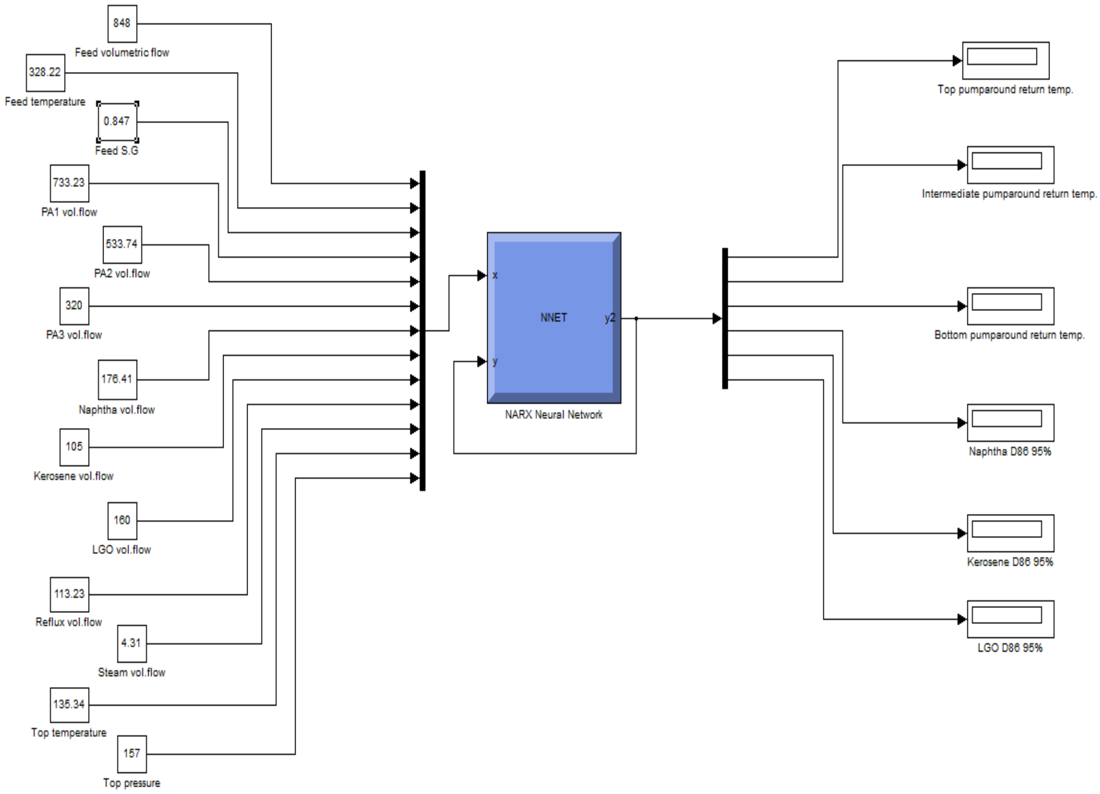

Fig. 4 : Simulation work of ANN model for crude oil distillation column.

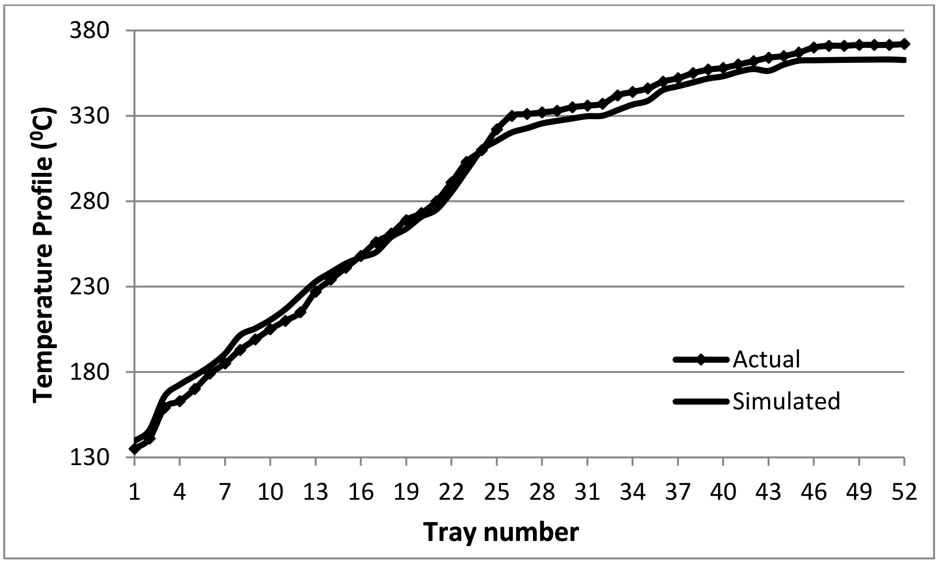

Fig. 5: Comparison of simulation and actual temperature profile along the main distillation column.

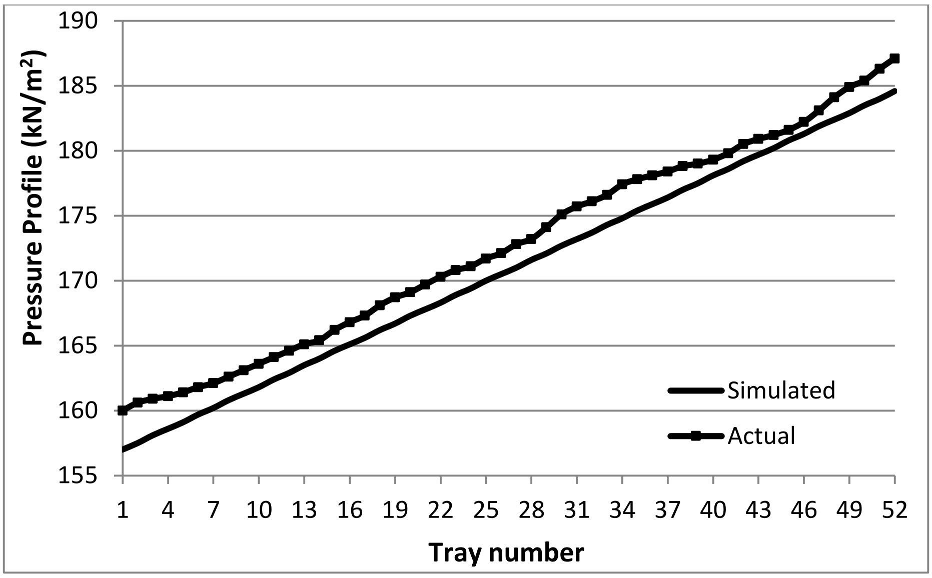

Fig.6: Comparison of simulation and actual pressure profile along the main distillation column.

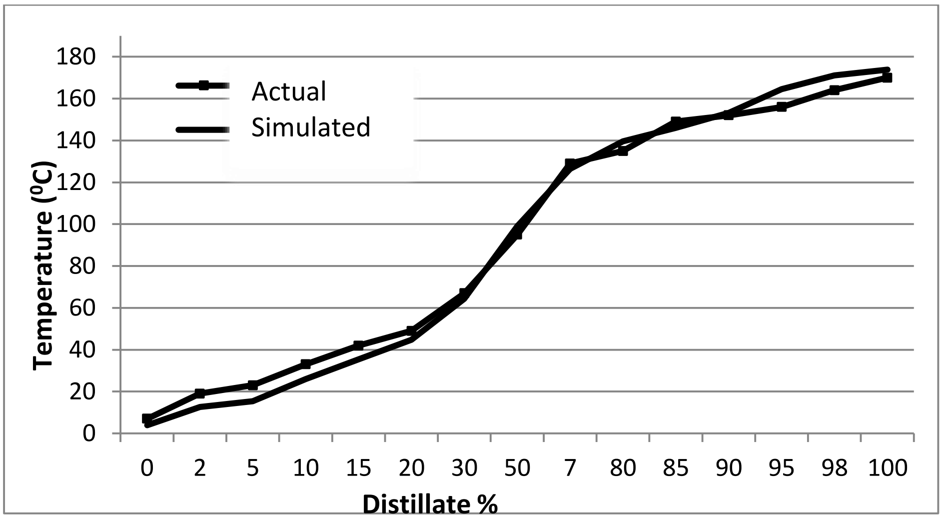

Fig. 7: Comparison of simulation and actual naphtha D86 distillate.

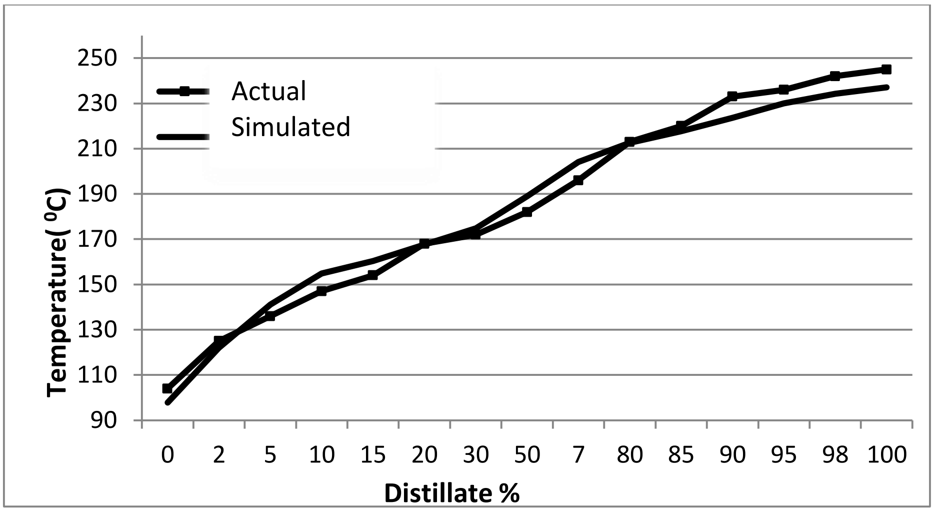

Fig.8: Comparison of simulation and actual kerosene D86 distillate.

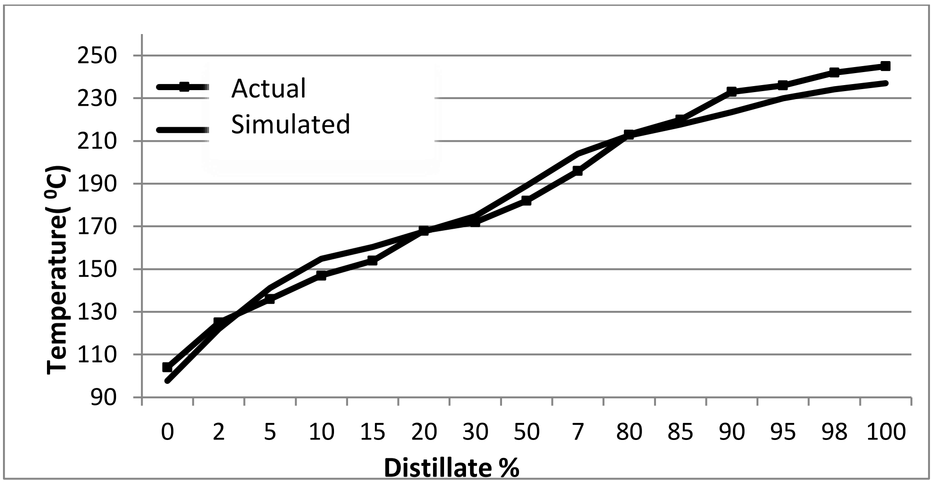

Fig. 9: Comparison of simulation and actual LGO D86 distillate.

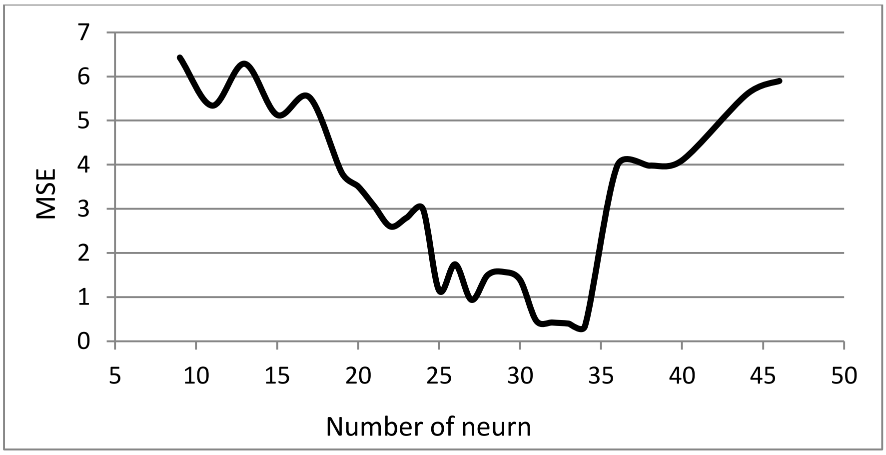

Fig.10: Comparison between number of neuron and MSE.