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Artificial Neural Network Modeling Applied for Predicting Reformate Yield and Research Octane Number in the Reforming Process

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Abstract: The prediction model of the continuous catalytic regeneration reforming process was developed for expecting the reformate yield and research octane number using an Artificial Neural Network technique (ANN) to improve the process performance. The proposed model includes temperatures, pressures, and hydrogen to hydrocarbon molar ratio as input parameters while the output of the process represents reformate yield and research octane number. The ANN model was carried out to estimate the process behavior based on the Levenberg-Marquardt Algorithm, which included the nine input parameters, two hidden layers (10-5 neurons), and two parameters as network outputs. The results obtained were that the prediction error for the reformate test was 0.0027 with a regression of 0.9995, while the research octane number was 0.0026 with a regression of 0.9979. The proposed model showed the ability of Artificial Intelligence to predict either the yield & octane number or simulate the behavior of the process with more accurate.

Keywords: Artificial Neural Network; CCRRP; Modeling; Reformate Yield; Research Octane Number; Simulation

1. Introduction:

Catalytic naphtha reforming is a very important process in oil refining that aims for research octane improvement and besides the aromatic compounds as feedstock for petrochemical industries. Naphtha continuous catalytic reforming (CCR) is one of the greatest beneficial processes in any refineries whose duty is increasing RON [1]. Catalytic reforming processes are commonly classified into three types based on the regeneration systems of the catalyst, namely (i) semi-regenerative catalytic reformer process (SRCRP), (ii) cyclic regenerative catalytic reformer process (CRCRP) and (iii) continuous catalytic regeneration reformer process (CCRRP). The major difference among the three processes is the requirement to shut down for catalyst regeneration. The mechanism for the regeneration steps could be classified into fixed-bed catalyst system; fixed-bed catalyst combined a swing reactor and a move-bed catalyst with special regenerator of SRCRP, CRCRP or CCRRP type, respectively [2].

Technical neural networks represent computational modeling tools that have found wide acceptance in many majors for modeling complicated real-world problems. Artificial neural networks can be defined as structures consisting of violently interconnected, adaptive simple processing elements (called artificial nodes) able of implementing vast parallel computations for data processing

and knowledge performance [3, 4]. The development of mathematical algorithms is the main goal of computing based on artificial neural networks and will enable artificial neural networks to learn by simulating information processing and knowledge procurement in the human brain. Artificial neural network-based models are empirical in nature, however they can provide practically accurate solutions to well-formulated or imprecise problems and phenomena that can only be understood through empirical data and field observations [5]. During the past 20 years, neural networks have been the focus of much interest, mostly due to their wide range of applicability and ability to handle extremely complex and non-linear problems. neural networks have been successfully applied to problems from various fields comprising commercial, medical and industrial fields [6]. Process modeling is field in which neuron network with different configurations and structures have been considered as alternative modeling techniques. Models for these units are developed by utilizing the unit data via Artificial Neural Network methods [7].

In modeling the catalytic reforming process using artificial neural network, Manamalli et al. (2006) developed a kinetic model of a catalytic reformer to extract parameters from the kinetic reactions of the reforming process. In addition, optimal control of the catalytic reformer using ANN has been implemented to maximize the aromatics yield [8]. In the latter few decades, the use of neuron network has increased to cover a wide range of fields involving the medical, economic and engineering sectors. Neuron network is reduction techniques to develop computational efficiency especially when great and complex structures are required to approximate and capture quite nonlinear models [9]. Zahedi (2008) studied simulation of catalytic reforming unit for enhancing gasoline production using artificial neural networks. They proposed model included some parameters as the volume flow rate of gasoline, hydrogen and liquid petroleum gas (LPG), and addition to output temperatures of each reactors, specific gravity of gasoline, Reid vapor pressure (RVP), and research octane number of gasoline. The various training network architectures were tested and the proper network was chosen. The gotten results show the capability of the ANN model to predict the unseen plant data. The estimated error of the ANN model is 1.07% and a maximum volume flow rate of produced gasoline were achieved by optimizing operation conditions. The gasoline production yield increases from 80 to 82.38% when optimal conditions were applied [10]. Alves (2008) fit an ANN model to the industrial data selected a mapping technique consists of fitting an ANN to the industrial data, and applying this model to create new values of the process variables with acceptable resolution. The results based on the recommended model agree with actual operating data very well in a petroleum refinery [11].Vezvaei (2011) applied Adaptive Neuro-Fuzzy Inference Systems (ANFIS) for the system of naphtha reforming. In this study, 31 actual data points were used (21 data points for training and the 10 data points used for generalization). The results displayed that, the ANFIS model show good agreements between actual data and simulated results [12]. Sadighi and Mohaddecy (2013) developed the artificial neural network model of the research octane number and the volume flow rate of the gasoline of naphtha reforming process. The results showed that the proposed ANN model has a capability to simulate the behavior of the target catalytic reforming plant. Where, the average absolute deviation (AAD%) of the estimated the research octane number and volume flow rate were 0.813% and 0.238%, respectively [13].

Recently, Dias (2020) analyses of research octane number as a key factor for gasoline quality analysis in an industrial catalytic reforming unit. Dias compared between different models and a actual industrial refinery and the accuracy succeeded with the best soft sensors open up perspectives for industrial applications and provide also relevant information about the main RON variability sources [14]. Yahya (2020) applied the artificial neural network with genetic algorithm to optimize the hydrogen production and response surface methodology of toluene steam reforming unit. They used the ANN-GA and RSM models and obtained the optimum H2 yield of 92.6% and 81.4% with predicted error equal 1.19% and 6.02% respectively. The two models are evaluated by statistical factors, including the root mean square error (RMSE) and correlation coefficient (R2). Lower RSME and higher R2 values are estimated for ANN-GA model (RMSE = 4.09, R2 = 0.95) indicating the superiority of ANN-GA in calculating the nonlinear behavior compared to RSM model (RMSE = 6.92, R2 = 0.87). These results show that ANN-GA is a more reliable and robust predictive steam reforming modelling tool for H2 production optimization compared to RSM model [15]. Al-Gathe (2021) applied Neural Network with Particle Swarm Optimization (PSONN) and Neural Network with Fuzzy (NFuzzy)) to predict oil properties with simply and accurately [16]. Al-Gathe (2022) proposed Neural Network with Fuzzy (Neuro-Fuzzy) model to predict gas compressibility factor. This study showed the superiority of Neuro-Fuzzy models in calculating gas compressibility factor [17].

This work focused on the model development of the reforming process for predicting the reformate yield and research octane number to improve the process performance. The model based on nine input parameters with two output parameters and implemented by artificial neural network (ANN) using MATLAB®.

2. Process Description:

Continuous Catalytic Regeneration Reforming Process (CCRRP) is the modern process used to produce high-octane gasoline and rich aromatic compounds. The process includes three sections namely; reaction with regenerator catalyst section, compressor with re-contacts section, and section of product separation. The products produced from this process are reformate, liquefied petroleum gas, off gas, and hydrogen rich gas. The prime target of this process is to improve the low-octane to high-octane naphtha to mix engine fuel. Figure 1 illustrates the simplified process flow diagram of CCRRP [18].

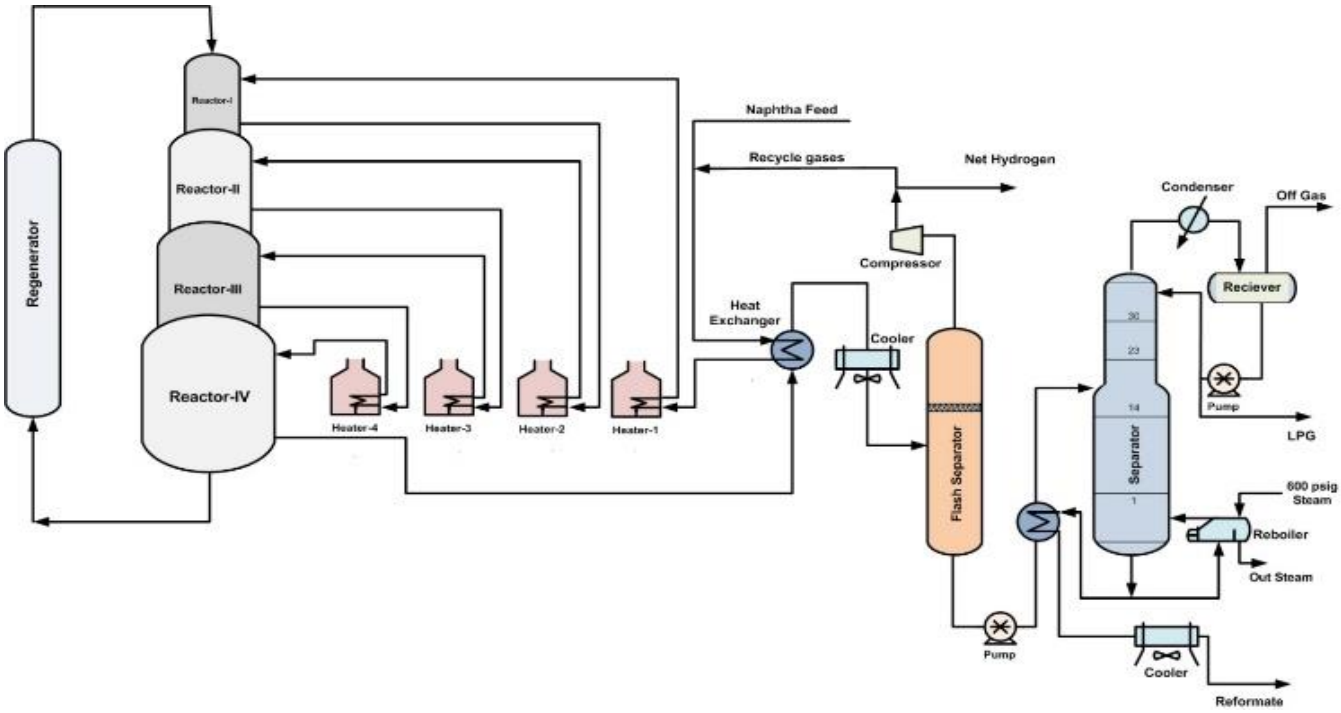

Figure 1. Simplified process flow diagram of CCRRP

3. Methodology:

The current data were collected from the actual process of continuous catalytic regeneration reforming process via process simulation [19]. The ANN technique applied to estimate the predictive modeling of output parameters. MATLAB Program was used to complete that task.

3.1 Artificial Neural Networks

The basic structure of an ANN consists of artificial neurons that are grouped into layers. The ANN is an artificial intelligence model that used to solve much industry problems. The most common ANN structure consists of a number of interconnected neurons or nodes [9, 20]. Figure (2) describes ANN model with two hidden layers. The first input layer takes data from external sources, and passes it to the network for processing. Then, the two hidden Layers will process them in a hidden way. The last output layer collects processed data and sends it out of the system [21].The number of input/output neurons of the neural network are the same as the number of desired input/output variables. The total of neurons in the hidden layer be determined by the application of the network [22].

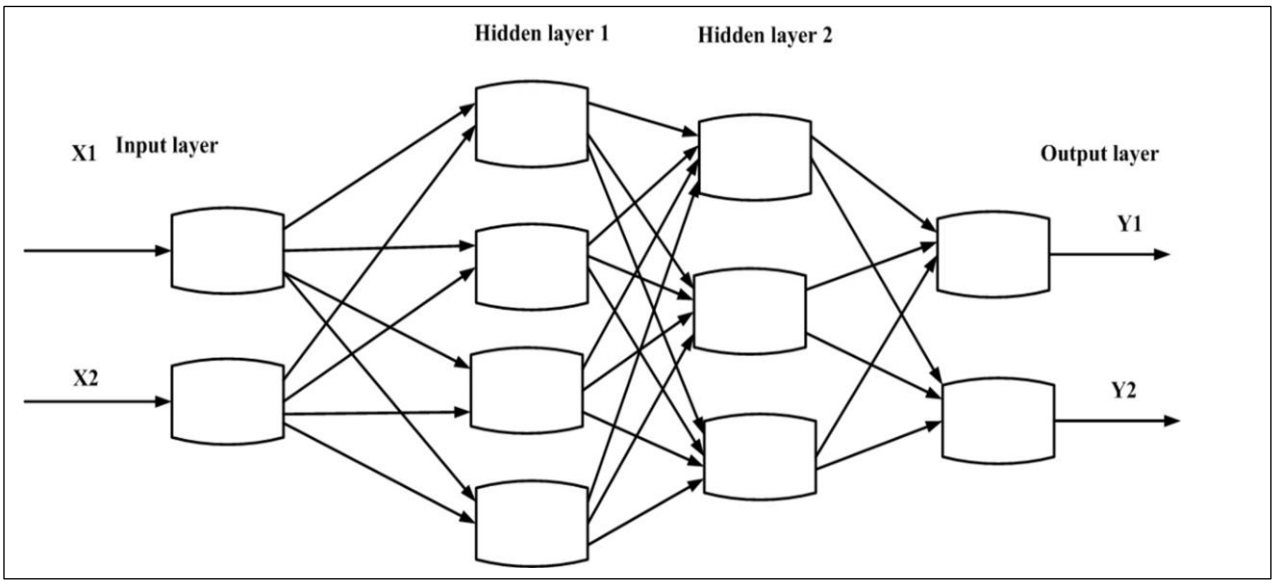

Figure 2. Basic structure of ANN model

3.2 Model of artificial neural network

Artificial Neural Networks (ANNs) are relatively new approach that have used in solving many complex real-world problems. Around 300 industrial data test cases that measured in catalytic reforming unit are used. 70% of these data used to train the neural network as training sets and 30 % of data used to test and validate the trained network. Table 1 shows the input and the output parameters with their ranges of the proposed ANN. The Structure of the algorithm for training and testing processes of the ANN can be explained as shown at flow chart in Figure 3.

Table 1. Parameters of input and output of the proposed ANN model.

Input Parameters		Output Parameters	
Inlet Reactor temperature (K)	value	Reformate yield (mol%)	value
T1	810-840		
T2	810-840	RY	90-95
T3	810-840		
T4	810-840		
Reactor Pressure (kPa)	value		
P1	339-530	Gasoline octane number	value
P2	470-482		
P3	421-430	RON	65-76
P4	362-369		
Hydrogen to hydrocarbon ratio (mol/mol)	value		
H/HC	2.42-8.24		

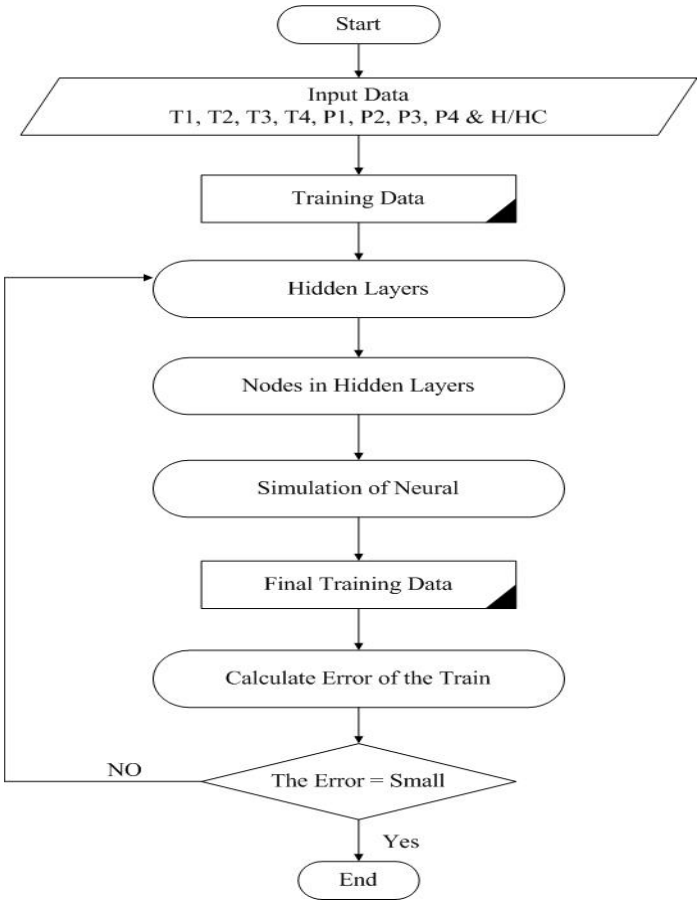

Figure 3. Flowchart of neural network algorithm

This procedure is continued to run until minimum mean square error (MSE) value is achieved:

$$MSE = \frac{1}{n}\sum_{k=1}^{n}\left(Y_{k,actual} - Y_{k,model}\right)^2 \quad (1)$$

The input parameters of the ANN model comprised of hydrogen to hydrocarbon molar ratio, inlet temperatures, and inlet pressures for reactors 1 to 4 whereas the outputs are yield reformate and RON. The Levenberg-Marquardt algorithm is applied to determine the optimal weights and biases. The training was executed until the minimum MSE was achieved between the actual and simulated values. Table 2 summarizes the most ANN model parameters.

Table 2. Model details of ANN algorithm.

Model	Details
Number of hidden layers	2
Number of neurons in hidden layer	10-5
Number of data used for training (70%) Testing (15%) and validating (15%)	300
Algorithm used for training	Levenberg-Marquardt
Performance function	MSE

4. Results and Discussion

In this work, the neural network is tested with two hidden layers configurations where the number of nodes in each hidden layers are ten and then five in ANN modeling. Training algorithm is investigated to predict the best algorithm and structure. The network during training was illustrated in Figure 4. The network was trained, tested and validated using the Neural Network Toolbox of MATLAB 2013a program.

After the ANN model was run, the following figure will appeared. Figure 5 depicts the training, validation, and testing performance versus number of each epochs (iterations) until goal error meeting. The training was ended after 8 iterations. The best validation performance is 8.43E-6 at epoch 8. The performance parameter for mean squared errors (MSE) at the final of iteration is 0.000182 that is a good value for total neural network error.

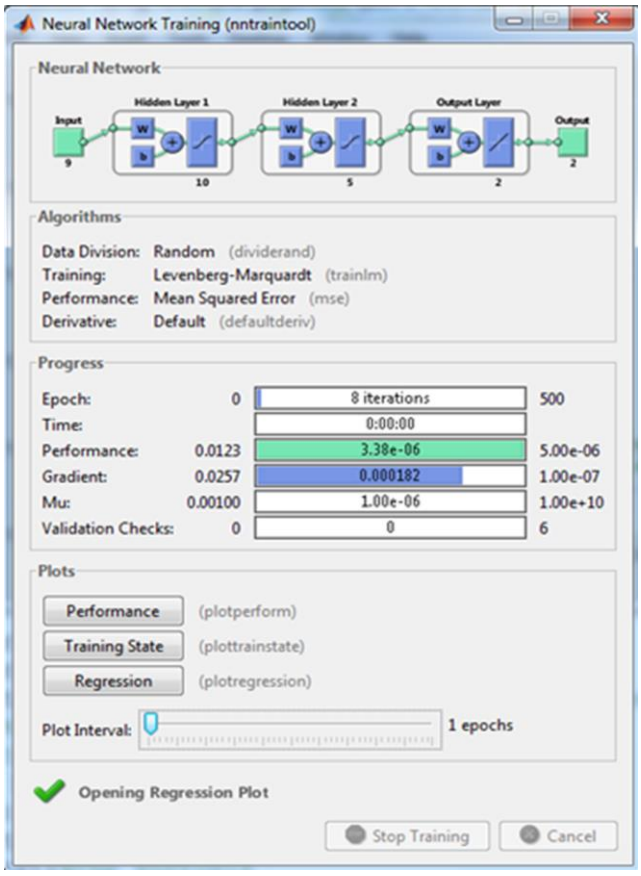

Figure 4. The network during training

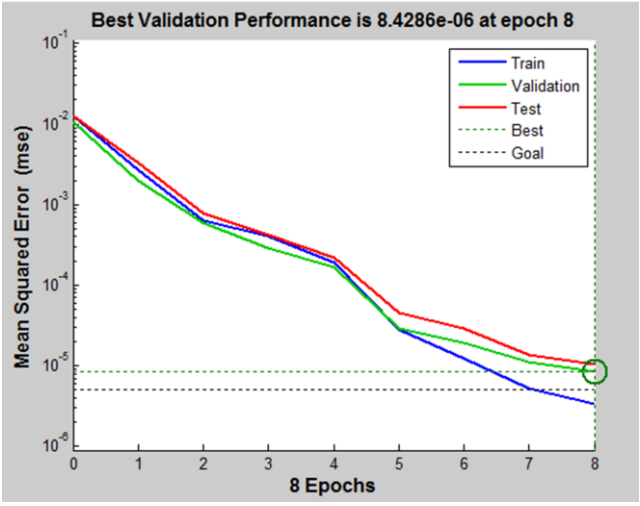

Figure 5. Mean squared errors for training, validation and testing data for hidden layers

Figure 6 shows the regression analysis between the actual reformate yield and the predicted reformate yield of the neural network whereas the regression analysis between the actual research octane and the predicted research octane of the neural network was plotted in Figure 7. In these figures, we can notice that the regression values are very close to one. The Standard deviation, RMSE, correlation factor and relative error of ANN model illustrated in Table 3.

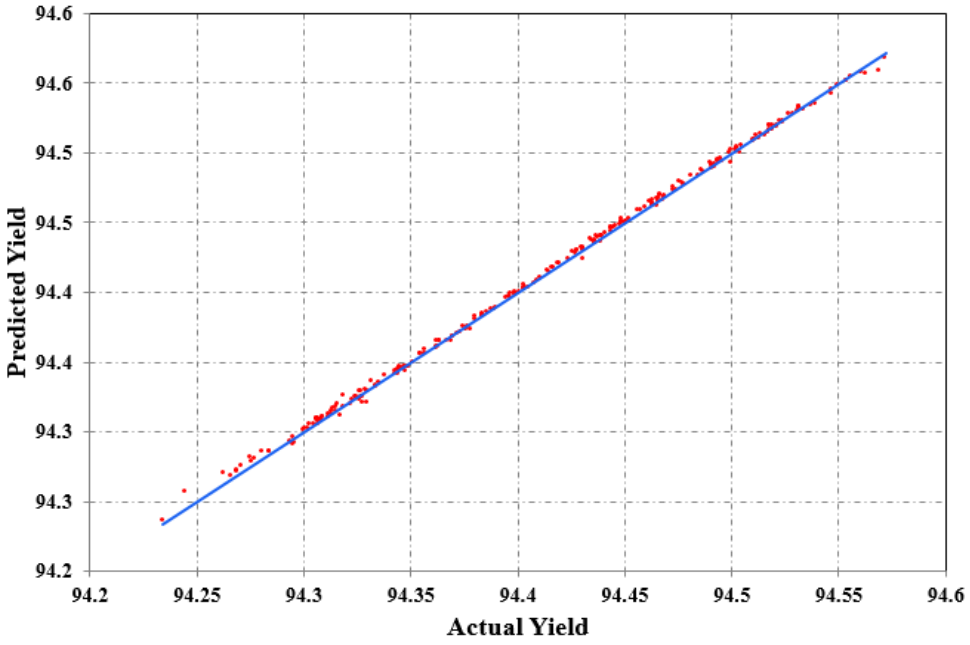

Figure 6. Regression for hidden layers of the reformate yield

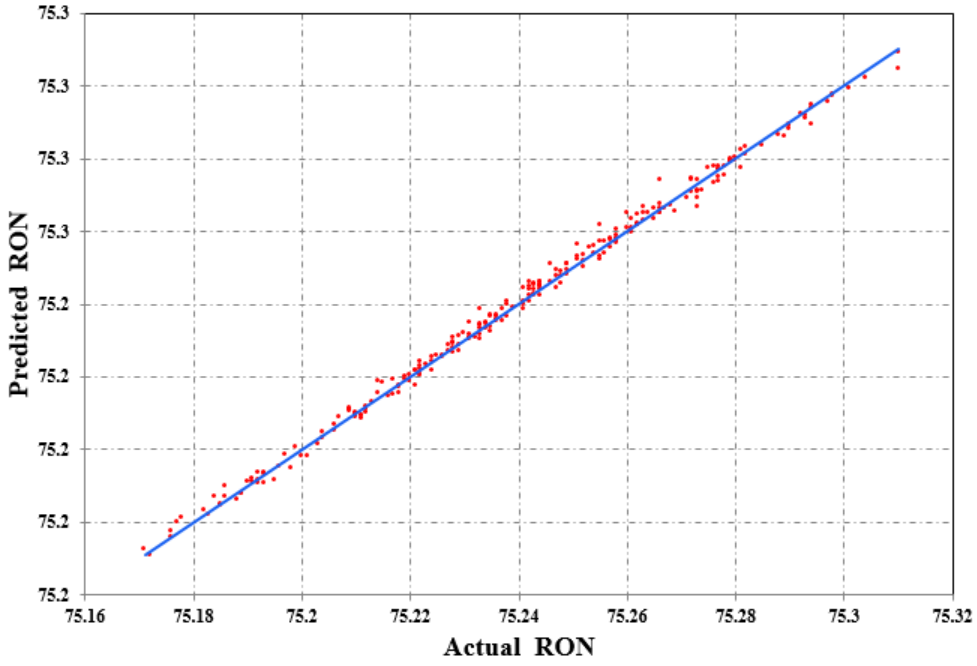

Figure 7. Regression for hidden layers of the research octane number

Table 3. Comparison summary of ANN for the hidden layer Levenberg-Marquardt Algorithm.

Variables	SD	RMSE	R^2	RE%
Reformate Yield	0.0017	0.0027	0.9995	0.0018
RON	0.0013	0.0026	0.9979	0.0017

Figures 8 and 9 display the comparisons between predicted reformate yield and predicted research octane number against the actual data values of the plant, respectively. As can be seen from these figures, there are convergence between predicted and actual values of these processes. It should be mentioned that the standard deviation (SD) was 0.0017 with root mean SQR error was 0.0027 for reformate yield, while octane number was 0.0013 as standard deviation and root mean SQR error was 0.0026. Figure 10 shows the proposed model of neural network structure which predicted of the output model data with actual operating data of the industrial unit, and these is given the convergence very well of them. Therefore, we concluded that the ANN-based model is a good for predicting of the behavior catalytic reforming.

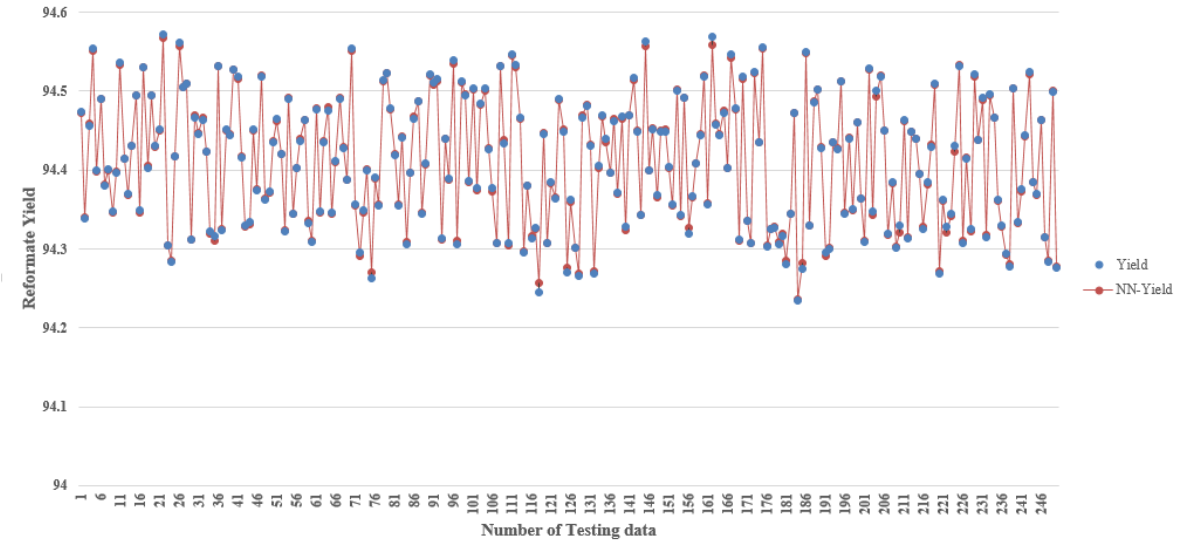

Figure 8. Prediction of proposed ANN for reformate yield (RY)

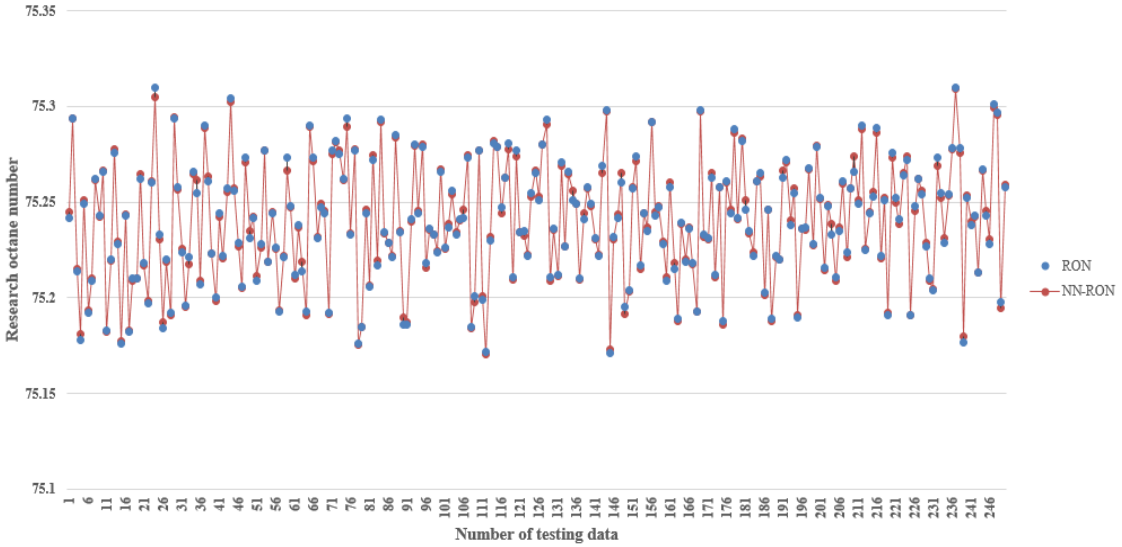

Figure 9. Prediction of proposed ANN for octane number (RON)

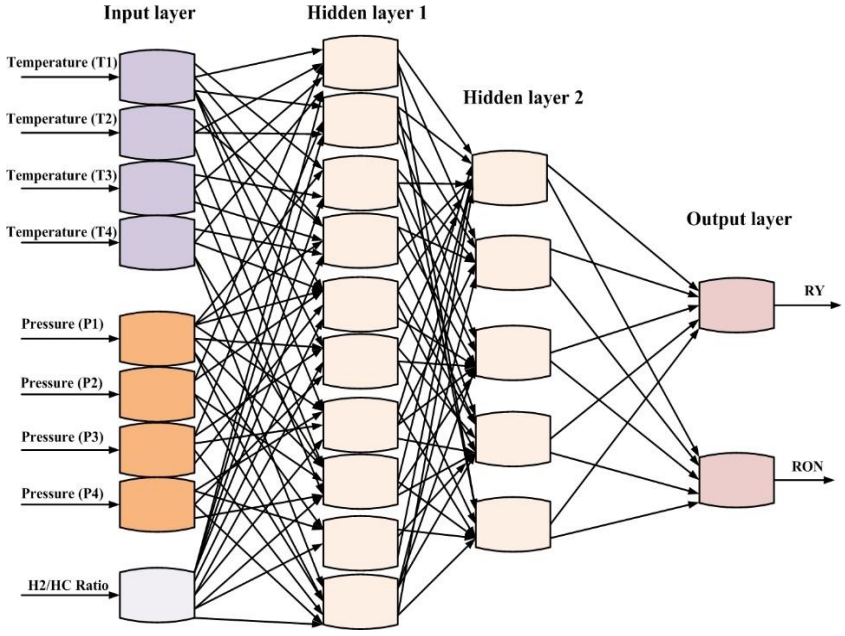

Figure 10. The proposed model of neural network structure

5. Conclusion

Industrial data of the continuous catalytic regeneration reforming process was used for expecting the reformate yield and research octane number using an artificial neural network technique. The proposed model includes temperatures, pressures, and hydrogen to hydrocarbon molar ratio as input parameters while the output of the process represents reformate yield and research octane number. The proposed network in this study was built with two hidden layers which is including ten nodes in first hidden and five nodes in the second hidden layer. Where, the values of prediction error for test of reformate yield and research octane number is excellent and that were 0.0027 and 0.0026. The implemented model showed the ability of Artificial Intelligence to predict the yield and octane number and to simulate the behavior of the process.

Abbreviations:

SD	:	Standard deviation
RMSE	:	Root mean square error
R	:	Correlation factor
RE%	:	Relative error
MSE	:	Mean square error
CCRRP	:	Continuous catalytic regeneration reforming process
ANN	:	Artificial neural network
SQR	:	Square root

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تطبيق نمذجة الشبكة العصبية الاصطناعية للتنبؤ بإنتاجية الريفورميت والرقم الأوكتاني في عملية التهذيب

بديع بابقي، عبدالرقيب القاضي، موهد تاكريف و محمد الدوح

الملخص: تم تطوير نموذج التنبؤ لعملية التهذيب ذي التجديد الحفزي المستمر لتوقع المردود المعاد تشكيله، وبحث رقم الأوكتان باستخدام تقنية الشبكة العصبية الاصطناعية (ANN) لتحسين أداء العملية. يتضمن النموذج المقترح درجات الحرارة والضغوط ونسبة الهيدروجين إلى الهيدروكربون المولية كمعلمات مدخلات بينما يمثل مخرجات العملية إعادة صياغة العائد والبحث عن رقم الأوكتان. تم تنفيذ نموذج ANN لتقدير سلوك العملية بناءً على خوارزمية ليفينبرج – ماركوارت، التي تضمنت معلمات الإدخال التسعة، اثنتان طبقات مخفية (5–10 خلايا عصبية)، ومعلمتان كمخرجات للشبكة. وكانت النتائج التي تم الحصول عليها أن الخطأ المتوقع لاختبار إعادة الفورمات كان 0.0027 مع انحدار قدره 0.9995 أمَّا رقم الأوكتان البحثي فكان 0.0026 مع تراجع 0.9979. النموذج المقترح أظهر قدرة الذكاء الاصطناعية للتنبؤ إما بالإنتاجية ورقم الأوكتان أو محاكاة سلوك العملية بالمزيد من الدقة.