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PREDICTIVE MODELING FOR AN INDUSTRIAL NAPHTHA REFORMING PLANT USING ARTIFICIAL NEURAL NETWORK WITH RECURRENT LAYERS

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ABSTRACT

In this research, a layered-recurrent artificial neural network (ANN) using the back-propagation method was developed for simulation of a fixed-bed industrial catalytic reforming unit called Platformer. Ninety-seven data points were gathered from the industrial catalytic naphtha reforming plant during the complete life cycle of the catalytic bed (about 919 days). Ultimately, 80% of them were selected as past horizontal data sets, and the others were selected as future horizontal ones. After training, testing, and validating the model with past horizontal data, the developed network was applied to predict the volume flow rate and research octane number (RON) of the future horizontal data versus days on stream. Results show that the developed ANN was capable of predicting the volume flow rate and RON of the gasoline for the future horizontal data sets with AAD% (average absolute deviation) of 0.238% and 0.813%, respectively. Moreover, the AAD% of the predicted octane barrel levels against the actual values was 1.447%, which shows the excellent capability of the model to simulate the behavior of the target catalytic reforming plant.

Keywords: Artificial neural network; Catalytic naphtha reforming; Lifecycle; Modeling; Simulation

1. INTRODUCTION

The need for transportation fuels, especially gasoline, steadily grows in the future, thus contributing to the demand for related petroleum processes. Catalytic naphtha reforming is an important process for producing high octane gasoline, aromatic feedstock, and hydrogen in the petroleum refining and petrochemical industries (Hu et al., 2002). The catalytic naphtha reforming unit uses naphtha as feedstock to produce a high octane value liquid with main by-products of hydrogen (H2) and liquefied petroleum gas (LPG) (Liang et al., 2005). To design new plants and to optimize existing ones, an appropriate mathematical model for simulating the industrial catalytic reforming process is needed (Weifeng et al., 2006).

Besides kinetic-based models that are classified as deterministic or first principal models, the use of an artificial neural network (ANN)—a "black box" model—can be beneficial, especially when the former approach cannot describe a system appropriately. In particular, neural networks are nonlinear, and they learn (or train) by examples. The user of a neural network gathers representative data and subsequently invokes training algorithms to learn the structure of data (Chaturvedi, 2010). ANN has been applied previously for modeling of various refinery processes, such as hydrodesulfurization, hydrocracking, delayed coking, and thermal cracking of naphtha (Bellos et al., 2005; Arce-Medina & Paz-Paredes, 2009; Sadighi et al., 2010; Zahedi et al., 2009; Niaei et al., 2007).

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Due to its ability to model complex and nonlinear problems, ANN can be a useful approach for modeling the complex behavior between input and output in catalytic processes, such as catalytic-dielectric barrier discharge plasma reactors (Istadi & Amin, 2006; Istadi & Amin, 2007a; Istadi & Amin, 2007b). In modeling the catalytic reforming plant using ANN, Manamalli et al. (2006) developed an ANN model to maximize the aromatics yield, subject to constraints in inlet temperatures of the reactors. Two neural networks, one in the forward path and the other in the feedback path, were trained to give set points for temperature control. Zahedi et al. (2008) developed two ANN models using the back-propagation and radial basis function (RBF) methods for simulation of an industrial catalytic reforming unit. The proposed models predict the volume flow rate of H_2, gasoline, and LPG; outlet temperatures of reactors; gasoline specific gravity; Reid vapor pressure (RVP); and the research octane number (RON) of gasoline. In this case, 97 data sets were collected from an industrial naphtha reforming plant, and all data sets were used to train, test, and validate ANN architecture. Using the ANN model, a set of optimized operation conditions leading to a maximized volume flow rate of produced gasoline was obtained. However, there were no reports to compare the optimized volume flow rate of products estimated by the model with the actual results. Furthermore, the life of the catalyst or days on streams—crucial for a commercial scale fixed-bed reactor—was not included in the model.

The present study was aimed at investigating the predictability of ANN models for an industrial naphtha reforming unit called the Platformer. This investigation discusses the use of mathematical models to describe behavior of the Platformer (i.e., yield and RON of the product) from the existing data. This work could be significant for predicting vital outputs of the plant according to the life of the catalyst and days on stream.

2. PROCESS DESCRIPTION

A catalytic naphtha reforming unit with a nominal capacity of 16,500 barrels per day, licensed by Chevron Corporation, was chosen for this case study. Protocol involves submitting the feed of the plant to a hydrodesulfurization (HDS) reaction in the hydrotreating unit prior to entering the catalytic reformer. Then, the produced naphtha, called Platcharge, can be introduced to the catalytic reforming process. The most commonly used types of catalytic reforming units have three or four reactors, and each reactor has a fixed catalytic bed. For such a unit, the activity of the catalyst is reduced during operations due to deposits of coke and loss of chloride. Generally, the catalyst is regenerated or restored periodically using in situ high temperature oxidation of the coke followed by chlorination (Weifeng et al., 2006; Chaturvedi, 2010). Therefore, the catalyst in semi-regenerative catalytic reforming is regenerated during routine shutdowns occurring once each 18 to 24 months. Normally, the catalyst can be regenerated three or four times, and then it must be returned to the manufacturer for reclamation of the valuable platinum and/or rhenium elements.

As shown in Figure 1, the Platcharge is preheated initially by the output stream of the last reactor in the effluent heat exchanger (E-1); after passing through the first furnace (H-1), it enters the first reactor (R-1) in which naphthenes are dehydrogenated to form aromatics. Then, the product stream from the first reactor passes through the second reactor (R-2) and the resulting outlet stream enters the third reactor (R-3). Similarly, the product stream from the third reactor enters the fourth reactor (R-4). Due to the endothermic nature of the naphtha reforming reaction, furnaces (i.e., H-1, H-2, H-3, and H-4) should be provided before each corresponding reforming reaction.

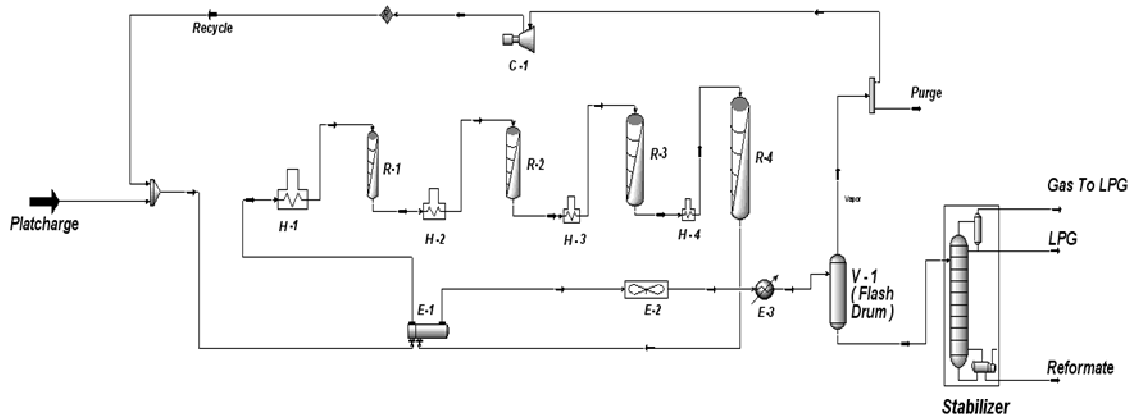

Figure 1 Block flow diagram of the catalytic reforming unit of the target oil refinery

Next, the product stream from the fourth reactor proceeding from the exchange of heat with fresh feed in heat exchanger E-1 enters a separator, V-1, wherein the hydrogen produced during the reforming process (gas stream) is recycled and mixed with the Platcharge. Finally, the liquid product leaving the separator is introduced to the gasoline stabilizer, in which the LPG and light gases are separated from the gasoline; so, the vapor pressure of the gasoline can be set according to market requirements. The final product of the stabilizer is called the Reformate.

The catalyst distribution for reactors in the industrial catalytic naphtha reforming unit is shown in Table 1. Moreover, the normal operating conditions of this unit are presented in Table 2.

Table 1 Catalyst distribution in reforming reactors

	1^{st} reactor	2^{nd} reactor	3^{rd} reactor	4^{th} reactor
Catalyst weight (kg)	5077.25	7615.87	12693.13	25386.25
Catalyst distribution (wt%)	10	15	25	50

Table 2 Operating conditions in catalytic reforming of target oil refinery

Process Variable	Value
Inlet temperature (°C)	490–515
Hydrogen/hydrocarbon ratio (mol/mol)	3–7
LHSV(h^{-1})	1–2
Yield (vol %)	70–85

3. DEVELOPMENT OF ANN MODEL

Although ANN modeling was discovered 50 years ago, only in the last two decades it has been presented to tackle practical problems. ANN is a parallel structure composed of nonlinear nodes that are connected by fixed weights and variables. ANN differs from the classic modeling approach in that it is trained to learn solutions; in other words, there is no programming of the model in the conventional way. The advantages of ANN compared to classical methods are speed, simplicity, capacity to learn from examples, and the ability to learn by experimental data.

Therefore, ANNs are more flexible and powerful than any other parametric approach (Zahedi et al., 2008).

Figure 2 shows the scheme of a typical ANN structure. A typical network consists of an input layer, at least one hidden layer, and an output layer. The most widely employed networks have only one hidden layer (Hagan et al., 1995). For a feed-forward ANN, the information propagates in only the forward direction. In this case, each node within a given layer is connected to all of the nodes of the previous layer. The node sums up the weighted inputs and a bias, and it passes the result through a linear or nonlinear function (Haykin & Hamilton, 1998).

The training of ANN is carried out by introducing it with a set of known inputs and outputs. Then, it learns the trend of the known data by manipulating the weights and biases. The ANN parameters (i.e., weights and biases) are adjusted up until the minimization criterion is reached. The most widely used criterion is the mean square error (MSE) as follows (Demuth & Beale, 2007):

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(P_{i,actual} - P_{i,\mathrm{mod}el})^2 \quad (1)$$

where N is the total number of known values; P represents the output values; actual refers to measured outputs from the plant, and model refers to the values simulated by ANN.

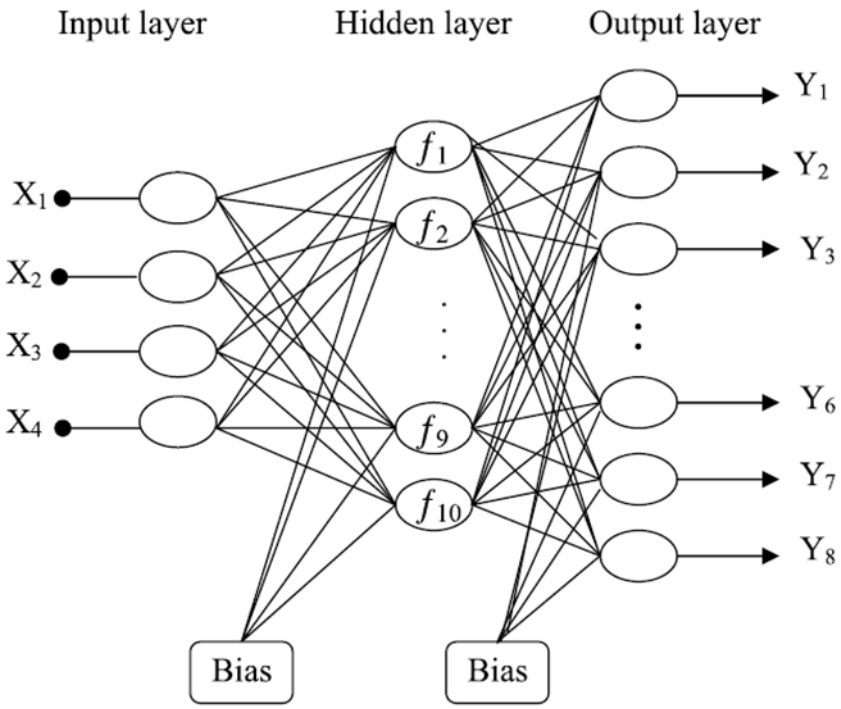

Figure 2 Schematic diagram of a typical structure layer (Niaei et al., 2007)

To create the ANN model, 110 data sets during the life cycle of the catalyst (about 919 days) were gathered from the Platformer. All data were selected under normal conditions; no abnormalities, such as tower flooding, emergency depressurization, and pump or compressor shutdown, occurred during operations. Before using these data to build the ANN model, it was necessary to validate them. If a reasonable overall mass balance (±5%) could not be calculated, the validity of the test run was compromised. According to this strategy, 97 data points were obtained. The variables and their operating ranges are presented in Table 3.

Table 3 Input variables and ranges used for building the ANN model

Variable	Ranges
Days on streams (DOS)	154–919
Naphtha feed flow rate (m^3/h)	125.76–149.18
Recycled gas flow rate (m^3/h)	112200–135100
Hydrogen to hydrocarbon molar ratio	3.52–4.963
Inlet temperature to reactor 1 (°C)	500–518
Inlet temperature to reactor 2 (°C)	500–518
Inlet temperature to reactor 3 (°C)	500–518
Inlet temperature to reactor 4 (°C)	500–518

Among 97 data points, 80 (up to the day of 800) were selected for building the ANN model. Furthermore, 48 data points were selected for training the ANN (60%); 17 data points were chosen for testing (20%); and the remaining ones were selected for validating the developed network. These data—known as past horizontal data—were supposed to show the behavior of the Platformer from start of run to day 800. The other data points (i.e., from day 800 to the end of run on day 919) were known as future horizontal data, and they were chosen to evaluate the reliability of the ANN model to predict the cycle life of the catalyst.

The ANN model of the Platformer was developed using the Neural Network Toolbox (newlrn function) presented in MATLAB 2010a. A layered-recurrent neural network consisting of seven neurons in the input layer, three neurons in the hidden layer, and two neurons in the output layer was built. The transfer or activation function used in the hidden and output nodes is the tangent sigmoid function, as identified below:

$$f(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}} = \tan sig(x) \tag{2}$$

where x is the sum of the weighted inputs to the neuron, and $f(x)$ is the output of the node (Demuth & Beale, 2007). The input neurons of the ANN model consisted of days on stream (DOS), naphtha feed flow rate, recycled gas flow rate, hydrogen to hydrocarbon molar ratio, and inlet temperatures for reactors 1 to 4. The output layer was RON and the product flow rate (i.e., Reformate). The required coefficients (i.e., weights and biases of the designed network) were limited to 80 parameters—less than the number of training data. For each data set, there were two output variables (i.e., RON and gasoline flow rate); therefore, there were 96 training data points for the ANN model. Training of ANN was carried out using the function "trainlm" which applied the Levenberg-Marquardt optimization method to estimate weights and biases. Training was performed until the minimum MSE between the simulated and actual output variables was found (i.e., all past horizontal data points). Details of the ANN model used for the naphtha catalytic reforming plant are presented in Table 4.

4. DISCUSSION

4.1. Developing the Neural Network using Past Horizontal Data

The described procedure for developing the ANN model was followed to train, test, and validate it for 80 points of past horizontal data. The MSE and AAD% obtained for RON and gasoline flow rate are presented in Table 5. Additionally, the parity plots for RON and gasoline flow rate simulated by the ANN models are presented in Figures 3 and 4. From these results, it was found that the deviation of simulated values in comparison to the measured data was acceptable for output values of past horizontal data points.

Table 4 Details of ANN algorithm built for the Platformer

Number of hidden layers	1
Number of neurons in hidden layer	3
Number of data used for training (60%) Testing (20%) and validating (20%)	80
Type of network	Layered recurrent
Number of model parameters	40
Transfer function of hidden layers	Tangent Sigmoid
Transfer function of output layer	Tangent Sigmoid
Algorithm used for training	Levenberg-Marquardt
Performance function	MSE

It is supposed that the main source of deviation was the possibility of error measurements in gathering data obtained with some faults, such as signal transmission, calibration, and power fluctuation of instruments that could not be excluded from the actual data. However, from the presented simulation results, it can be concluded that the developed simulation program was reliable enough to be applied for predicting the behavior of the target catalytic reforming unit.

Table 5 AAD% and MSE of ANN after training, testing, and validating

Variable	*AAD%*	*MSE*
RON of gasoline	0.238	0.084
Flow rate of gasoline	0.813	1.787

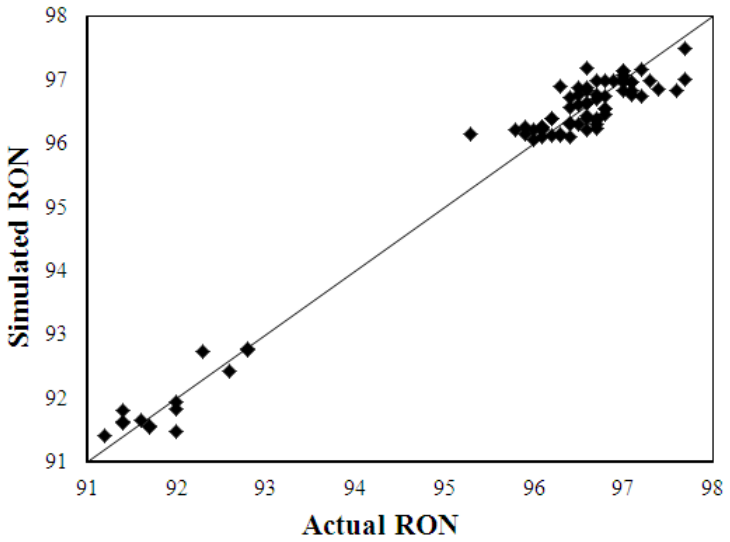

Figure 3 Parity plot for trained, tested, and validated RON simulated by ANN model

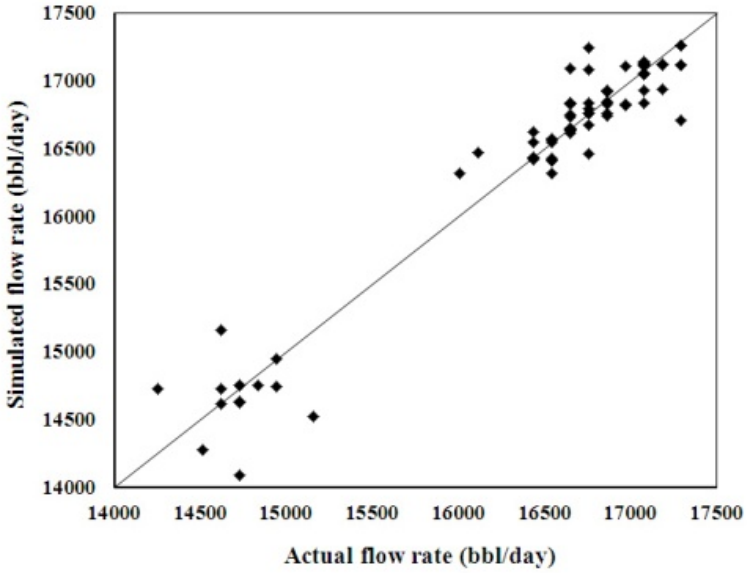

Figure 4 Parity plot for trained, tested, and validated gasoline flow rate simulated by ANN model

4.2. Predicting Future Horizontal Outputs

After building ANN, the outputs corresponding to the future horizontal data (i.e., RON and gasoline flow rate) were extrapolated. Clearly, the predicted outputs were related to DOS from day 800 to the end of run (day 919).

Figures 5 and 6 show the comparisons between RON and flow rate of the gasoline produced against the actual values. As can be seen from these figures, there are close mappings between measured and predicted (or extrapolated) output variables. It should be mentioned that the AAD% of predictions for RON and gasoline flow rate were 0.52% and 1.62%, respectively. Therefore, we concluded that the ANN-based model is good for extrapolation of the behavior of the catalytic naphtha reformer.

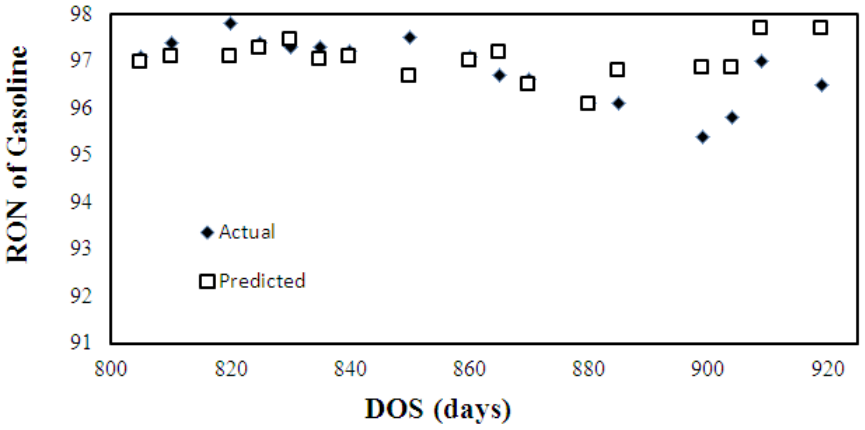

Figure 5 Actual RON of gasoline against predicted values vs. DOS

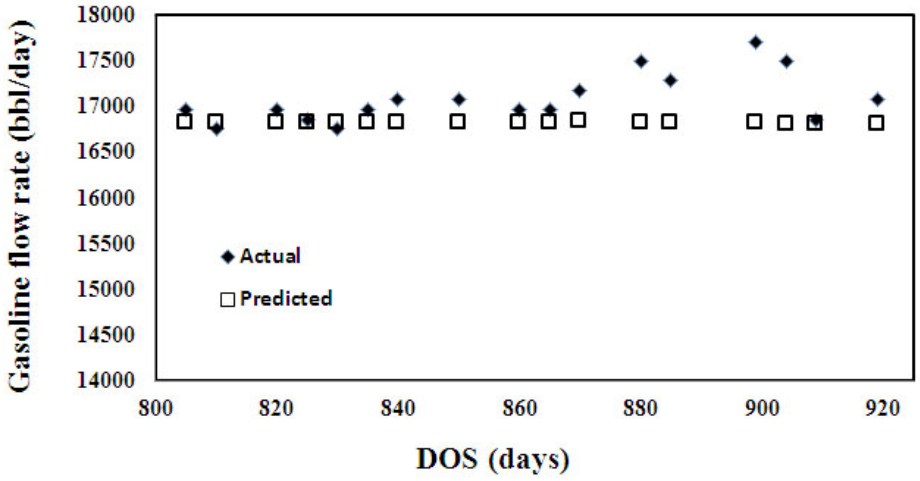

Figure 6 Actual flow rate of gasoline against predicted values vs. DOS

As an important parameter of the naphtha catalytic reforming unit, the octane barrel level of the unit (i.e., RON × gasoline flow rate) was studied using the validated ANN model. This variable is important for distinguishing the end of the life cycle, and it must be monitored at all times to estimate the catalyst life. The results showed that the AAD% of the ANN-based model against the actual octane barrel value was 1.477% for the future horizontal data.

The AAD% of the prediction for the octane barrel level at the end of run (day 919) was about 0.3%. Moreover, from Figure 7, close mappings between the measured and simulated octane barrel levels for both past and future horizontal data can be understood. These results confirm that the presented approach can be applied by refineries to monitor the operations of catalytic reforming plants, and they can be used to estimate octane levels, flow rate of gasoline, and life cycle with acceptable accuracy.

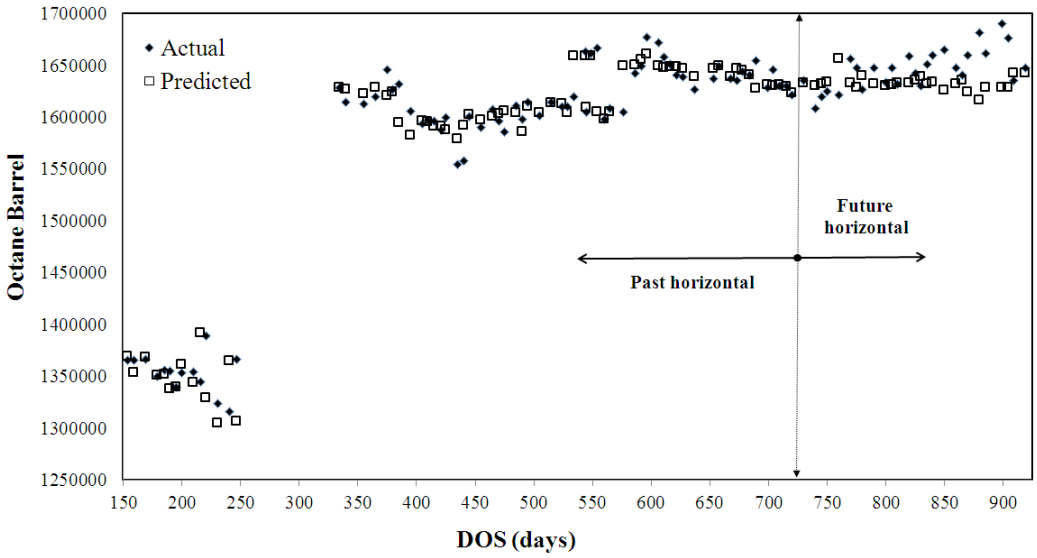

Figure 7 Octane barrel levels of past and future horizontal data against actual values vs. DOS

5. CONCLUSION

In this work, a layered-recurrent neural network model was developed for the simulation of an industrial fixed-bed catalytic naphtha reformer. The collected data from the target plant were divided into past horizontal data (80 data points from start of run to day 800), and future horizontal data (from day 800 to end of life cycle). The constructed ANN model was trained, tested, and validated on the basis of the past horizontal data. The results showed that ANN could simulate RON, flow rate of produced gasoline, and octane barrel level of past horizontal data with AAD% of 0.238%, 0.813%, and 0.853%, respectively. Finally, the developed ANN model was applied to predict RON, gasoline flow rate, and octane barrel levels of future horizontal data, which were significant for estimating the life of the catalyst. The comparison between the model predictions (extrapolations) and the future horizontal data confirmed that the developed ANN model could predict these outputs with AAD% of 0.52%, 1.62%, and 1.477%, respectively.

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