Artificial Intelligent Modeling and Optimizing of an Industrial Hydrocracker Plant

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Abstract

The main objective of this study is the modelling and optimization of an industrial Hydrocracker Unit (HU) by means of Adaptive Neuro Fuzzy Inference System (ANFIS) model. In this case, some data were collected from an industrial hydrocracker plant. Inputs of an ANFIS include flow rate of fresh feed and recycle hydrogen, temperature of reactors, mole percentage of H_2 and H_2S, feed flow rate and temperature of debutanizer, pressure of debutanizer receiver, top and bottom temperature and pressure of fractionator column. The network was employed to calculate the flow rate of gas oil, kerosene, Light Naphtha (LN), and Heavy Naphtha (HN).Unseen data points were used to check generalization capability of the best network. There were good adjustment between network estimations and unseen data. Finally optimization was performed to maximize the production volume percent of gas oil, kerosene, HN and LN and to identify the sets of optimum operating parameters in order to maximize yields of mentioned product. Optimum conditions were found as feed flow rate of 90.9 m^3/h, reactor temperature of 378.4 °C, hydrogen flow rate of 54.31 MSCM/h and LN (feed vol.%) of 9.34.

Keywords: Adaptive neuro fuzzy inference system, Modelling, Hydrocracker unit

Introduction

One of the major refining units in oil refineries is hydrocracker unit. Hydrocracking is a catalytic cracking process which has high conversion. Cracking conversion of a hydrocracker unit (HU) is more important than fluid catalytic cracking units and moreover hydrogen partial pressure of the unit is higher than hydrodesulphurization processes [1]. In this process, hydrogen purifies the hydrocarbon stream from sulfur and nitrogen heteroatoms. The process produces saturated hydrocarbons. The main products for HU are jet fuel and diesel, also relatively high octane rating gasoline and LPG are produced. All these products contains very low content of sulfur and other contaminants [2]. For the modeling of the HU, the First Principle Models (FPMs) are common, but the complete development of these models can be very complex. Most of the industrial chemical and petrochemical processes are typically complex in nature due to unknown reaction chemistry, nonlinear relations and numerous involved variables [3]. Heavy and time-consuming computations are sometimes drawbacks of FPMs. Sometimes, in FPMs, complex partial differential equations or complex algebraic equations appear which should be solved analytically or numerically. Also, some phenomena, for example, kinetics of HU reactions are still not well-understood to develop an accurate mathematical model [4]. ANN modeling is a good alternative to FPMs to manage the mentioned complexities since it only requires the input-output data as opposed to a detailed knowledge of a system. In addition, ANN requires less computational time and allows estimation of every continuous and nonlinear function with high precision. Because of these features, ANN is very popular for modeling, simulation, optimization and control of processes in petrochemicals and refineries [5-12]. Al-Enez and Elkamel have focused on predicting the effect of feed stock on the properties and the product yield for a Fluid Catalytic Cracking (FCC) unit. They used feed forward ANN to predict the yield of propane, butane, n-butane, iso-butane, propylene, butylene, light gas, gasoline, light cycle oil, heavy cycle oil and coke as

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well as conradson carbon number. Only four properties of feed including °API, Watson characterization factor, sulfur content and volume conversion percent of liquid were introduced to NN as inputs. Their model gave better prediction than non-linear regression and commercial simulators models [5]. An ANN hybrid model was used by Bollas et al., 2003 to scale up a FCC pilot plant into an industrial scale plant. The pilot model was able to predict the conversion weight percent and the coke yield. The hybrid model was then compared with the pilot model and the pure ANN model. The results showed that the hybrid model has better extrapolation capacity [7].The crude oil description using the near infrared spectroscopy was performed by Falla et al., 2006. This analysis was called SimDis (Simulation Distillation) and was faster than the true boiling point method. Forty oil samples with API of 1.31-36.4 were gathered. The ANN was applied, which generated the SimDis curves accurately [9]. Aminian and Shahhosseini (2008) used ANN to predict the fouling behavior of a crude oil preheat heat exchangers. They also used sensitivity analysis known as the "sequential zeroing of weights" to determine the effects of various parameters on fouling [13]. Design of the expert system for an industrial distillation column using NN and its optimization using genetic algorithm was performed by Motlaghi Jalali and Nili Ahmadabadi, 2008. They used the operating conditions and the product quality as ANN input and outputs, respectively. Then, the oil production cost function was minimized [14].This research used an ANFIS technique for modeling, and optimization of a HU process. The mentioned work began with the development of a detailed industrial ANFIS model for HU. Finally, optimization of the HU process was performed with the objective of maximizing the volume percent of gas oil, kerosene, HN and LN.

1.1. Hydrocracker unit (Isomax Unit)

Figure 1 shows process flow diagram of the Tabriz refinery HU (Arak, 2014). The unit, which is commercially known as the Isomax Unit has been designed to refine 15000 barrel/day of vacuum gas oil and to produce high quality middle-distillate products such as naphtha, kerosene and gas oil. This unit comprises of three sections: make-up compressor section, reactor section and fractionation section. In make-up compressor section, 96.5% hydrogen gas is compressed during three stages to increase the pressure of hydrogen gas from 15.5 kgf/ cm^2 to 190 kgf/cm^2. The feed is mixed with bottom recycles and hydrogen gas and then is introduced to the reactor. Reactions occur in a fixed bed reactor then after separation of light gases the products flow to the fractionation section. The fractionation section includes debutanizer tower, fractionation tower, splitter and stripper.

2. Adaptive neuro fuzzy inference system (ANFIS)

Fuzzy logic has been introduced by L. Zadeh in 1965 to deal with possibility theory (Zadeh, 1965) [15]. Concept of partial truth and some types of the uncertainty in the real are the point of L. Zadeh departure in order to introduce fuzzy logic. Fuzzy logic belongs to the uncertainty theory actually. Also artificial neural networks are introduced based on properties of biological neurons in order to efficiently use in control, estimation, classification, clustering, classify and other area of artificial intelligence. In the field of artificial intelligence, neuro-fuzzy refers to combinations of artificial neural networks and fuzzy logic. Neuro-fuzzy was proposed by Jang et al. (1997) [16]. Neuro-fuzzy hybridization results in a hybrid intelligent system that synergizes these two techniques through combining the human-like reasoning style of fuzzy systems with the learning and connectionist structure of neural networks. Neuro-fuzzy hybridization is widely termed as fuzzy neural network (FNN) or neuro-fuzzy system (NFS) in the literatures.

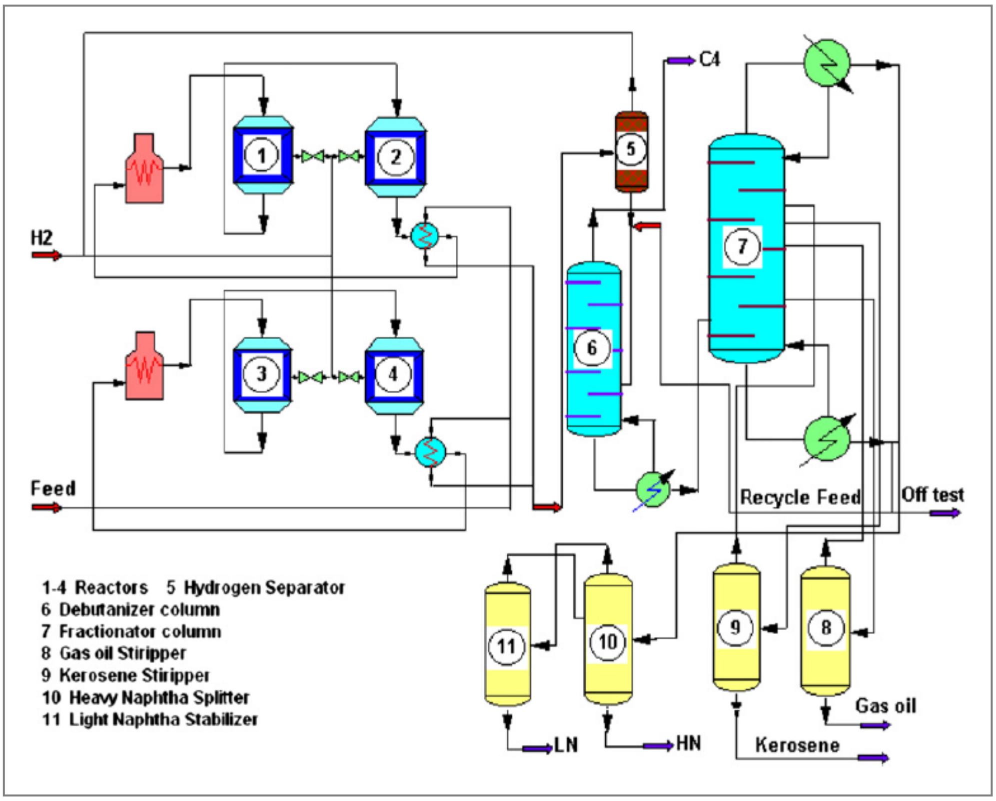

Figure 1: Process flow diagram of a hydrocracking unit (Isomax unit)

Fuzzy systems and neural networks are both very popular techniques that have seen increasing interest in recent decades. At a first glance, they seem to be totally different areas with merely marginal connections. However, both methodologies belong to the soft computing area. Soft computing includes approaches to human reasoning and learning that try to make use of the human tolerance for incompleteness, uncertainty, imprecision and fuzziness in decision-making processes. Many different structures for fuzzy neural networks (FNNs) have been proposed previously (Zhou et al. 2002) [17]. Among them ANFIS is a neural-network based on fuzzy approach, in which the learning procedures are performed by interleaving the optimization of parameters of the antecedent and conclusion parts (Aliyari et al. 2009) [18]. ANFIS uses a feed forward network to search for fuzzy decision rules that perform well on a given task. Using a given input-output dataset, ANFIS creates a FIS whose membership function parameters are adjusted using a back-propagation algorithm alone or a combination of a back-propagation algorithm with a least squares method. This allows the fuzzy systems to learn from the data being modeled. Consider a first order Takagie-Sugeno fuzzy model with a two input, one output system having two membership functions for each input. Then, the functioning of ANFIS is a five-layered feed-forward neural structure, and the functionality of the nodes in these layers can be summarized as:

$$O_i^1 = \mu_{A_i}(x) \qquad (1)$$
$$O_i^1 = \mu_{B_{i-2}}(y)$$

Where x or y is the input to the node, A_i or B_{i-2} is a fuzzy set associated with this node. At the first layer, for each input, the membership grades in the corresponding fuzzy sets are estimated. At the second layer, all potential rules between the inputs are formulated by applying fuzzy intersection (AND). The product operation is used to estimate the firing strength of each rule.

$$O_i^2 = \omega_i = \mu_{A_i}(x) \times \mu_{B_i}(y) \quad (2)$$

i=1,2

The third layer is used for estimation of the ratio of the ith rule's firing strength to the sum of all rule's firing strengths.

$$O_i^3 = \varpi_i = \frac{\omega_i}{\sum_{i=1}^{i=N} \omega_i} \quad \text{i=1,2} \quad (3)$$

$$O_i^4 = \varpi_i f_i = \varpi_i (p_i x + q_i y + r_i) \quad (4)$$

i=1,2

Where ω_i is the output of layer 3 and $\{p_i, q_i, r_i\}$ is the parameter set. Parameters in this layer will be referred to as consequent parameters. The final layer computes the overall output as the summation of all incoming signals from layer 4.

$$O_i^5 = \sum_i \varpi_i f_i = \frac{\sum_i \omega_i f_i}{\sum_i \omega_i} \quad (5)$$

Optimizing the values of the adaptive parameters is of vital importance for the performance of the adaptive system. Jang et al. (1997) [16] developed a hybrid learning algorithm for ANFIS which is faster than the classical back-propagation method to approximate the precise value of the model parameters. The hybrid learning algorithm of ANFIS consists of two alternating phases: (1) gradient descend which computes error signals recursively from the output layer backward to the input nodes, and (2) least squares method, which finds a feasible set of consequent parameters. We observe that, given fixed values of elements of premise parameters, the overall output can be expressed as a linear combination of the consequent parameters.

There are different advanced fuzzy inference techniques. In this study, we have used one kind of them that generates a Sugeno-type FIS structure using subtractive clustering and requires separate sets of input and output data as input arguments. When there is only one output, it may be used to generate an initial FIS for ANFIS training. It accomplishes this by extracting a set of rules that model the data behavior. The rule extraction method first uses the sub-cluster function to determine the number of rules and antecedent membership functions and then uses linear least squares estimation to determine each rule's consequent equations. This function returns an FIS structure that contains a set of fuzzy rules to cover the feature space. The arguments for the advanced fuzzy inference technique are as follows:

- ✓ X_{in} is a matrix in which each row contains the input values of a data point.
- ✓ X_{out} is a matrix in which each row contains the output values of a data point.
- ✓ Radii is a vector that specifies a cluster center's range of influence in each of the data dimensions, assuming the data falls within a unit hyper box.

Membership function (MF) is a curve that defines how each point in the input space is mapped to a membership value (or degree of membership) between 0 and 1. The input space is sometimes referred to as the universe of discourse, a fancy name for a simple concept. There are different kinds of membership functions as follows:

- ✓ Triangular membership function
- ✓ Trapezoid membership function
- ✓ Gaussian membership function
- ✓ Bell membership function
- ✓ Linear membership function

The default input membership function type in this study is Gaussian, and the default output membership function type is linear. Table 1 summarizes the inference methods and their types.

A structure of ANFIS is presented in Figure 2. Tables 2 and 3 show HU variables and their operating range.

For parameter estimation, the summation of squared error, SQE, was minimized, as given below:

$$SQE = \sum_{k=1}^{N_t} \sum_{J=F}^{G} \left(Y_{k_j}^{means} - Y_{k_j}^{pred} \right)^2 \quad (6)$$

In Eq. (6), N_t, Y_{kj}^{means} and Y_{kj}^{pred} are the number of test runs, measured product yield and predicted by model, respectively.

To investigate the suitability of the fitting, the average absolute deviation of predictions (AAD%), presented in the literature [18], was calculated by Eq. (7) as below.

$$AAD\% = 100 \frac{\sum_{k=1}^{N_t} \sqrt{\frac{\left(Y_k^{means} - Y_k^{pred}\right)^2}{\left(Y_k^{means}\right)^2}}}{N_t} (\%) \tag{7}$$

Table 1: Inference methods and their types

Inference method	Type	Prod	
AND (T-norm, intersection)	Min		
OR (S-Norm, union)	Max	Probor (probabilistic OR)	
Implication	Prod (product)	Min (minimum)	
Aggregation	Max (maximum)	Sum	Probor (probabilistic OR[a])

[a]http://www.mathworks.com/help/toolbox/fuzzy/probabilisticruleagg.html.

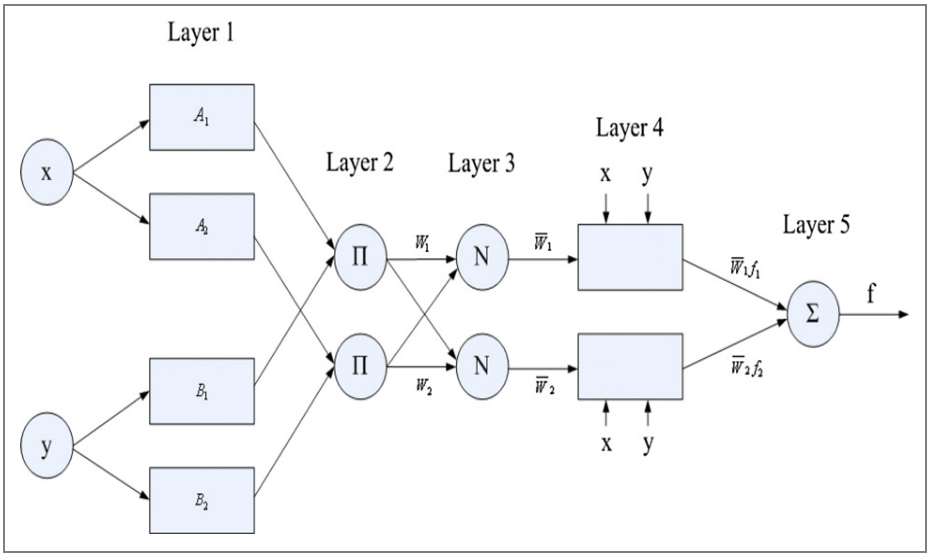

Figure 2: Adaptive Neuro-Fuzzy Inference System (ANFIS) structure

Table 2: The range of input variables of Arak HU

Variable	Range
Fresh feed flow rate (m^3/h)	0.6-100
Recycle hydrogen flow rate(KNM^3/h)	10-70
Reactors temperature (°C)	377.3-378.9
Recycle feed flow rate (m^3/h)	4.3-102.9
Fresh hydrogen flow rate (KNM^3/hr)	2.24-27.95
H_2S (% mol)	0.3-0.7
H_2 (% mol)	46-65
Debutanizer feed temperature (°C)	156-189
Debutanizer feed flow rate (m3/h)	14-134
Pressure of debutanizer receiver (kg/cm^2)	11-14
Temperature of top frctionator column (°C)	104-129
Temperature of bottom frctionator column (°C)	265-284
Pressure of frctionator column (kg/cm^2)	0.2-0.62

Table 3: The range of output variables of Arak HU

Variable	Range
Gas oil flow rate (m^3/hr)	0-63.5
Kerosene flow rate (m^3/hr)	0-61
LN flow rate (m^3/hr)	0-17.22
HN flow rate (m^3/hr)	0-35.35

Table 4: The used data for estimation and validation of model

	T (^oC)			
	378	380	382	384
RHFR[a] = $10KNm^3h^{-1}$	estimation	estimation	validation	estimation
RHFR[a]= $30KNm^3h^{-1}$	validation	estimation	estimation	estimation
RHFR[a]= $50 KNm^3h^{-1}$	estimation	estimation	estimation	validation
RHFR[a]= $70KNm^3h^{-1}$	estimation	validation	estimation	estimation

[a]Recycle Hydrogen Flow Rate

Table 5: AAD% of different membership function for data prediction by ANFIS

	Bell shape	π shape	Sigmoid shape	Triangular shape	Trapezoidal shape	Gaussian shape
Gas oil	35.67	7.79	9.96	4.34	10.22	36.16
Kerosene	22.56	7.56	5.43	13.12	5.25	14.19
L. Naphtha	31.35	10.19	6.04	4.45	4.35	33.49
H. Naphtha	49.11	12.24	15.56	19.02	15.96	53.76
Average	34.67	9.44	9.25	10.23	8.94	34.40

3. Results and discussion

To create the neuro-fuzzy inference system, Matlab-fuzzy logic toolbox version 2011a (Mathworks, Inc.) and ANFIS syntax were used. This syntax is the major training routine for Sugeno-type fuzzy inference systems. ANFIS uses a hybrid learning algorithm to identify parameters of Sugeno-type fuzzy inference systems. It applies a combination of the least-squares method and the back propagation gradient descent method for training fuzzy inference system membership function parameters to emulate a given training data set. The type of membership functions associated with hydro cracking unit was selected from all supported types in Matlab. To train the fuzzy model, three fuzzy rules were selected from the ANFIS toolbox, and the training process was stopped whenever the designated epoch number (17) was reached. For the hydrocracker unit, the input vector consists of RHFR and temperature, while the output one is the yield of products. To train the network, the Table 4 were selected and the four remained data were used to validation.

After training the neuro-fuzzy inference system with ANFIS syntax, the input data for the remaining data, simulated by trained ANFIS and yield of products, were predicted by the Evalfis syntax.

The trial with different functions showed that the prediction results with trapezoidal-shape curve resulted in better predictions than other ones, also sigmoid, π-shaped, and triangular-shaped were approximately as accurate as trapezoidal-shape. AAD% for gas oil, kerosene, light naphtha, and heavy naphtha are presented in Table 5.

As observed, the prediction of ANFIS for products by all membership functions except for Bell and Gaussian shapes were lower than 20%, which was better than other models such as kinetic base model in such a wide range of operating conditions (RHFR and temperature). Moreover, from the results presented in Table 5, it can be concluded that the best membership function for gas oil, kerosene, light and heavy naphtha were triangular, trapezoidal, trapezoidal and π-shaped, respectively. For other products, trapezoidal shape showed the best results. Therefore, a hybrid multi membership ANFIS can be the most predictive model for an industrial hydrocracker plant.

The parity plots to compare measured and predicted by the ANFIS with trapezoidal membership are shown in Figures 3–6. As it can be understood from them, these figures show the ANN outputs versus the number of unseen industrial data. These figures show good capability of both ANFIS for estimation of unseen data.

Figures 3 to 6 illustrate that the simulation of validation data for the products with uniform trend are acceptable.

Moreover, it can be seen from these parity plots that predictions have acceptable agreement with actual data, and the high value of AAD% is related to only one data point in the low yields.

Furthermore, it can be understood from Figure 6 that there is acceptable agreement between the experimental and predicted values for heavy naphtha; however, the high average absolute deviation of this lump, reported in Table 5 (15.96 with Trapezoidal membership), is because of their low experimental yields which shows a flagrant deviation when they are dominators in Eq. (7).

Figure 7 illustrates the effect of temperature on LN, HN and kerosene percent.

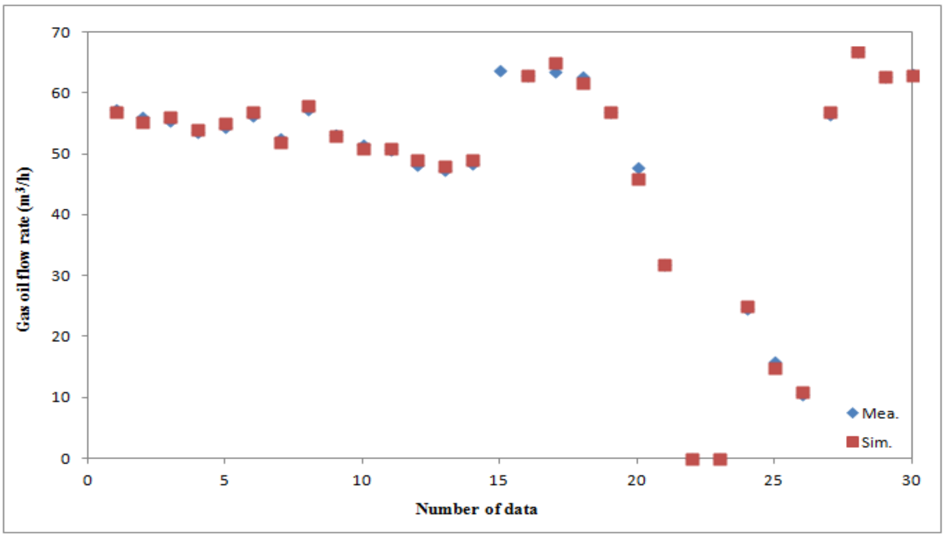

Figure 3: Comparison of measured flow rate of gas oil with values predicted by trained ANFIS

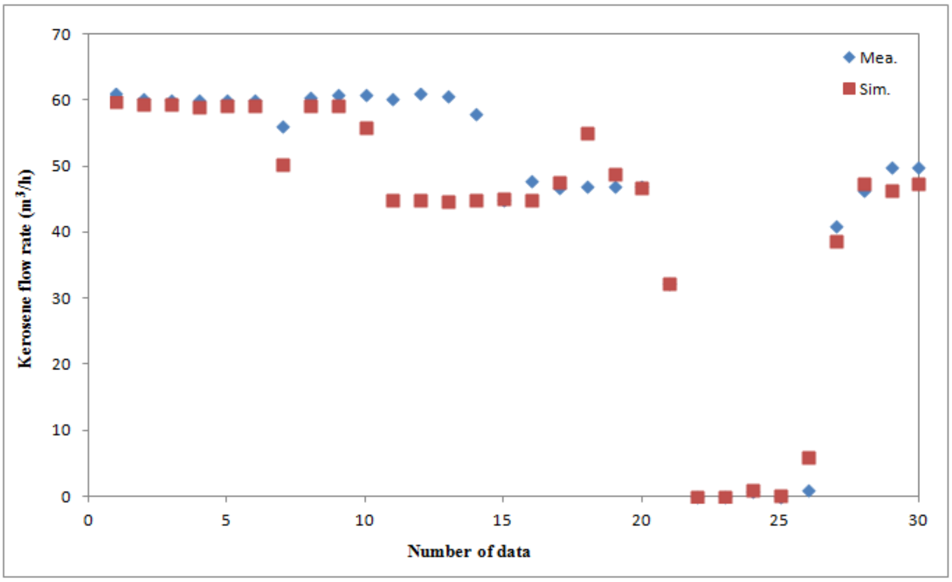

Figure 4: Comparison of measured flow rate of kerosene with values predicted by trained ANFIS

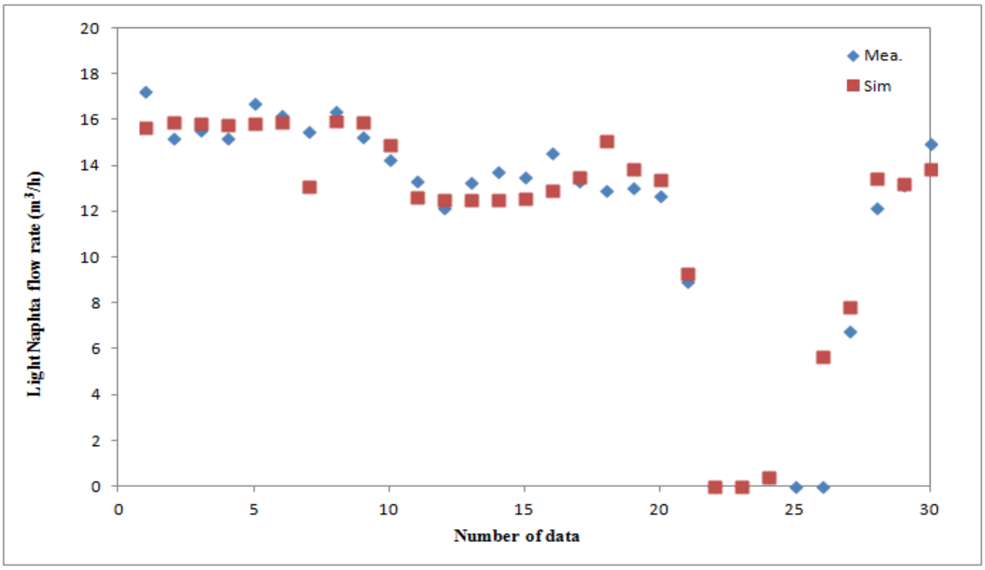

Figure 5: Comparison of measured flow rate of LN with values predicted by trained ANFIS

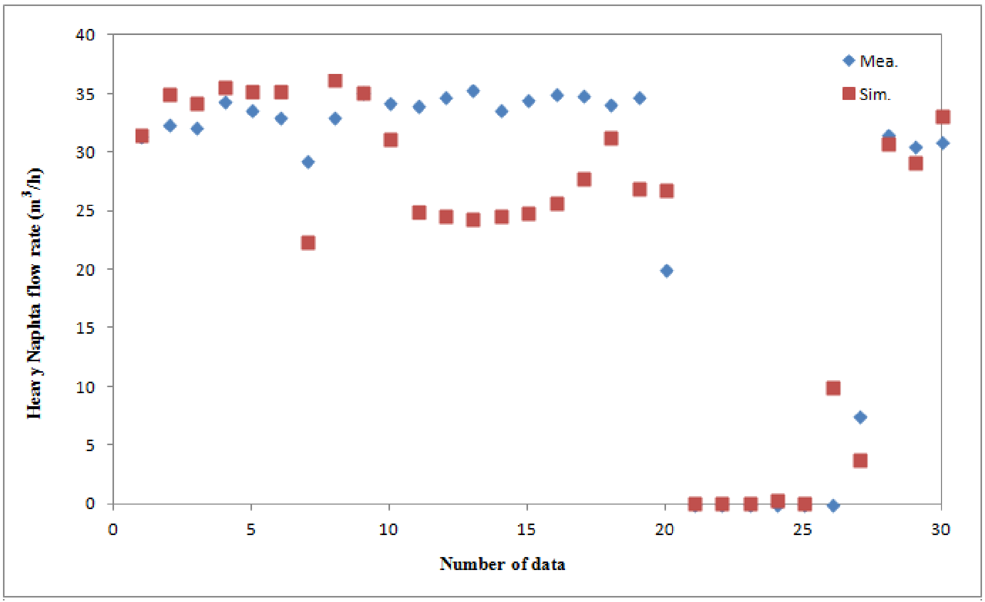

Figure 6: Comparison of measured flow rate of HN with values predicted by trained ANFIS

Figure7 illustrates the effect of temperature on the gas oil, kerosene, LN and HN percent while feed flow rate and inlet hydrogen flow rate are set in their average values. As shown in this figure, temperature is the most affective input variable. As reactor temperature changes from 377 to 379.5°C, the trend of the volume percent of gas oil, kerosene, LN and HN changes according to Figure7 (a)–(d), respectively.

Also Figures 8 and 9 illustrates the effect of total feed and recycle hydrogen flow rate on LN, HN and kerosene percent respectively.

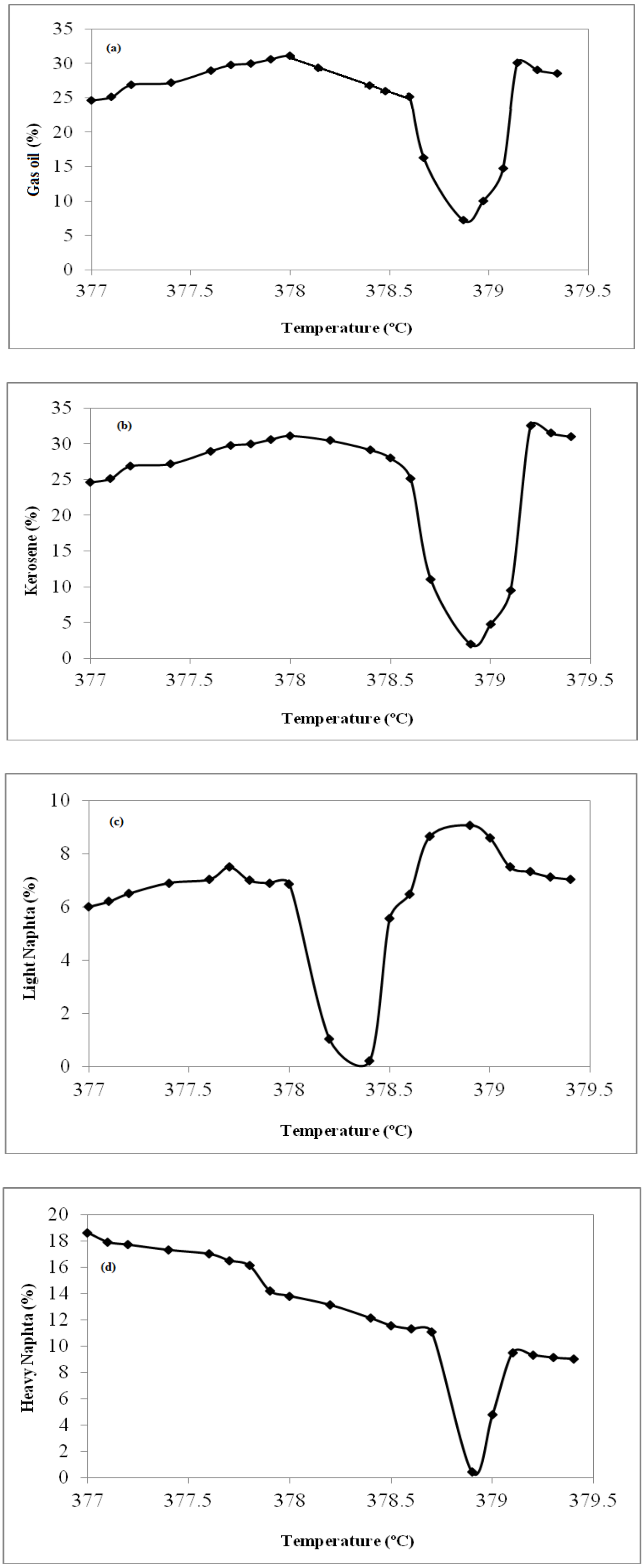

Figure 7: The effect of temperature on the volume percent of (a) gas oil, (b) kerosene, (c) LN, and (d) HN

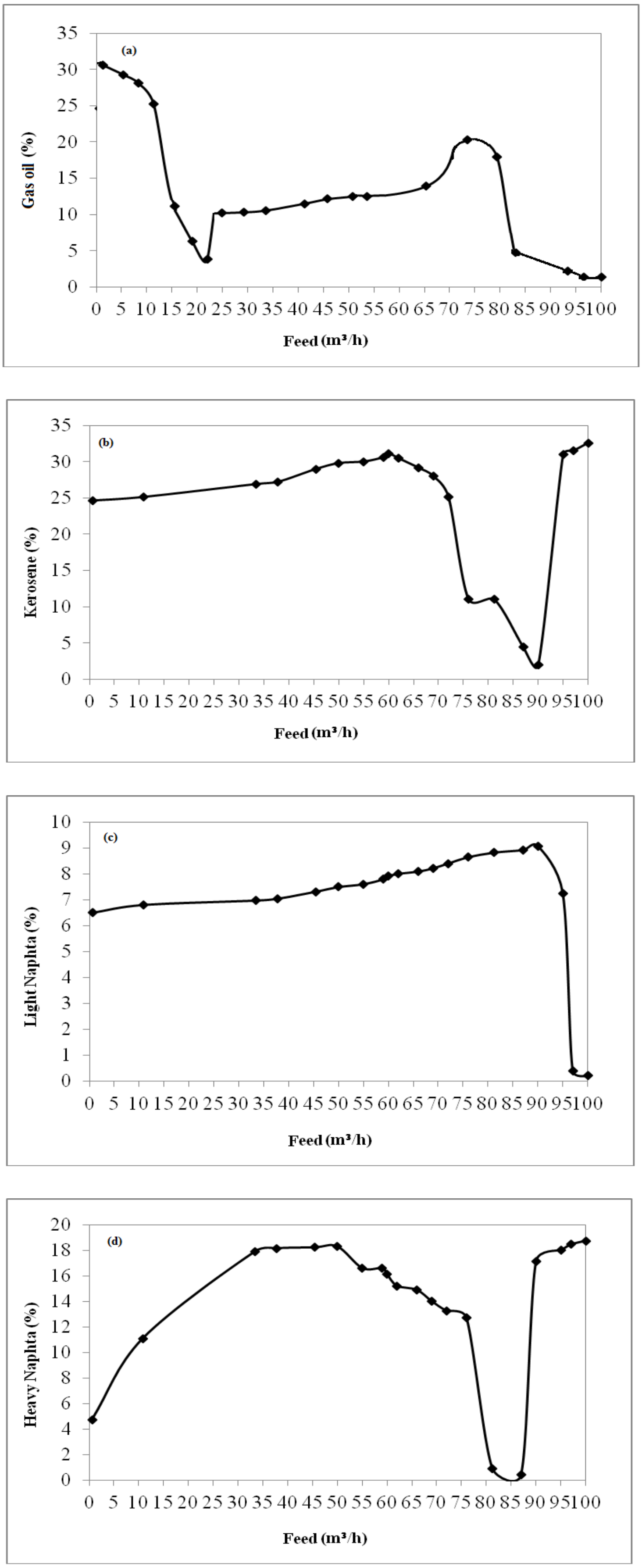

Figure 8: The effect of total feed flow rate on the volume percent of (a) gas oil, (b) kerosene, (c) LN, and (d) HN

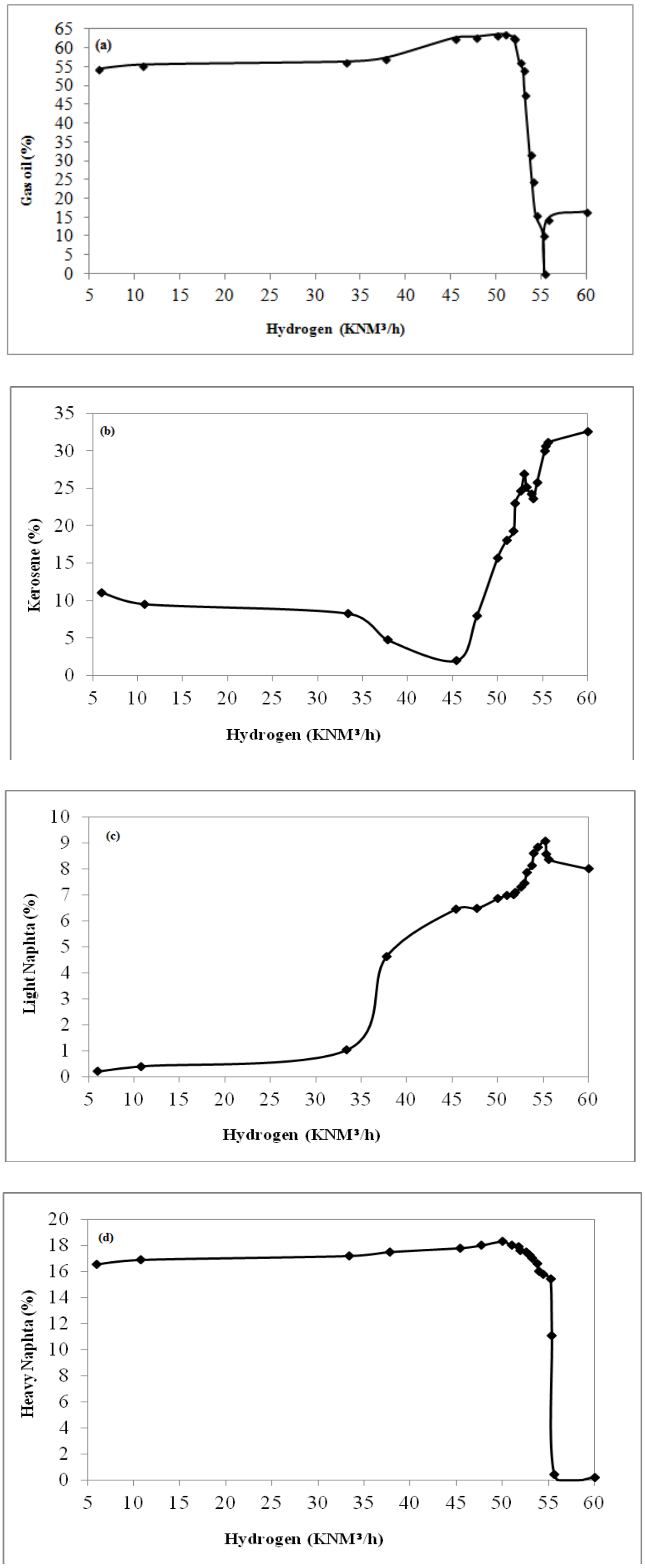

Figure 9:The effect of hydrogen flow rate on the volume percent of (a) gas oil, (b) kerosene, (c) LN, and (d) HN

Similar to temperature, the effect of total feed flow rate (make up and recycle) on the volume percent of gas oil, kerosene, HN and LN was evaluated and the obtained results are shown in Figure 8. In this figure, feed flow rate (make up and recycle) is changed from 0 to 100m^3/h, while the temperature of reactors and hydrogen inlet flow rate are set in their average values. As illustrated in Figure8, the more feed flow rate, the more production of kerosene and HN while LN and gas oil show decrease. These results will help to obtain the optimum values of these products.

Similarly, the effect of hydrogen flow rate (make up and recycle) on the volume percent of gas oil, kerosene, LN and HN are shown in Figure 9. As shown in this figure, with increasing hydrogen flow rate kerosene and LN production increases while gas oil and HN production decreases.

4. Conclusions

In this paper, the ANFIS technique was used to simulate and optimize an industrial HU. For this purpose, ANFIS model of the unit was developed based on industrial data. Finally, the obtained networks were applied to predict plant optimum operating conditions in order to maximize the volume percent of gas oil, kerosene, HN and LN as objective functions. Between all supported membership functions in the Matlab software, the trapezoidal cure was the most appropriate shape for the industrial Hydrocracker Plant. This study again emphasizes ANFIS capability to increase productions and keep plants running in more economical conditions. The ability of ANFIS in developing models for very complicated plant and analyzing the plant was confirmed. Based on current increasing fuel price the developed model easily can give us optimum operating condition of the HU while using traditional model, this is very difficult to achieve.

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