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Boosting the Research Octane Number (RON) of an Industrial Scale Light Naphtha Isomerization Unit by Using Adaptive Neuro-Fuzzy Inference System (ANFIS)

Sepehr Sadighi[1,], Seyed Reza Seif Mohaddecy[1], Mahdi Talebbeigi[2]*

[1] *Catalysis Development Technologies Division, Research Institute of Petroleum Industry (RIPI), Tehran, Iran*
[2] *Engineering Department, Imam Khomeini Oil Refinery, Arak, Iran*

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Abstract

In this work, an optimization approach is proposed to increase the research octane number (RON) of a commercial scale light naphtha isomerization unit. To represent the isomerization plant, an adaptive nuero-fuzzy inference system (ANFIS) is developed. The input layer of the network includes days on stream, temperature of the deisopentanizer condenser, light naphtha feed flowrate, inlet temperature of the isomerization reactor, hydrogen to hydrocarbon molar ratio, flow rate of n-hexane recycle, and temperatures of the de-pentanizer, de-isohexanizer and de-isopentanizer reboilers. The output variable of ANFIS is the RON of the product (i.e. isomerate). At first, it is confirmed that by using the Gaussian membership function, the model is capable of predicting the RON of isomerate with the AAD% of 0.913, confirming the reliability of the ANFIS model. Then, the actual RON of isomerate is boosted by manipulating the significant variables of the plant i.e. temperatures of de-isopentanizer condenser and reboiler, inlet temperature of the isomerization reactor, hydrogen to hydrocarbon molar ratio, and temperatures of the depentanizer and deisohexanizer reboilers. During 280 days of study and considering all operational constraints, results confirm that the optimized decision variables can increase the RON of isomerate close to the designed value (about 86) which is the main concern of the target isomerization plant.

Keywords: *Isomerization; Light Naphtha; Adaptive Neuro-fuzzy Inference System (ANFIS); Optimization; Research Octane Number (RON).*

1. Introduction

Due to limitations on olefins, benzene and aromatic contents of motor fuel gasoline, crude oil refineries are enhanced with stringent environmental policies. Therefore, refineries need a process with the ability of substituting aromatic and olefin components with other species, and following Euro-4 and Euro-5 standards. The light naphtha isomerization unit in a refinery is a simple and cost-effective process that upgrades the research octane number (RON) of light naphtha, and also simultaneously reduces benzene and aromatic content by saturating these fractions [1]. In a typical isomerization process, hydrogen and light naphtha, mainly including straight chain (normal) paraffinic hydrocarbons (nP), are fed from the top of a fixed-bed catalytic reactor, and move downward throughout the bed, and the catalyst normally used in this process is platinum on chlorinated alumina or zeolite-based catalysts in the form of beads or as extrudate [2]. The RON increase in an isomerization unit is significant that determines the quality of the product. Typically, an isomerization unit can boost RON of light naphtha from 70 to 84.

For any refining and petrochemical process, optimal operation is desired to guarantee the quality of product and profitability of the plant, and therefore using process models is unavoidable [3]. Furthermore, a reliable model provides a theoretical foundation for the investigation, implementation of automatic control, and scaling up of the process [4]. In this respect, many studies have been accomplished to model the reactor of the light naphtha isomerization

process using first principal (kinetic-based) modeling approach [5-10]. However, to develop a robust and comprehensive kinetic-based model for an industrial scale isomerization plant, the complexity of light naphtha mixture makes it significantly difficult to describe its kinetic rate at a molecular level. Moreover, for predicting the RON of the gasoline for a real light naphtha isomerization unit, a plant-wide model is needed in which all process equipment including heaters, distillation columns, separation vessels and recycle pumps are considered. Modern day rigorous simulators such as Aspen plus or Hysys from Aspen Technology do not have such restrictive limits on the total number of components, but this approach increases the calculation time, and characterization of the streams and subsequent reports become unnecessarily sophisticated [11].

On the other hand, soft computing methods such as artificial neural networks (ANN) and fuzzy logic were widely applied for modeling, controlling and optimizing catalytic processes [12-25]. These intelligent systems are quick, accurate, and cheap methods for extracting the underlying dependency of a set of input/output data [26]. ANN is an information-processing paradigm that is inspired by the way the biological nervous system, such as the brain, processes information [27]. Additionally, a fuzzy model is a system description with fuzzy quantities which are expressed in terms of fuzzy numbers or fuzzy sets [28]. However, these methods have several limitations resulting from possibly getting trapped in a local minimum, the choice of model architecture and difficult to design and adjust automatically [29]. But, with a combination between ANN and Fuzzy logic rules, a model can be obtained that inherit the advantages of both methods [30]. In this respect, ANFIS (adaptive neuro-fuzzy inference system) is a kind of ANN based on Takagi–Sugeno fuzzy inference systemin which both ANN and Fuzzy models complement each other. ANFIS represents a useful neural network approach for the solution of function approximation problems, and it has been successfully applied to model different chemical engineering processes [31-35].

In what follows, an industrial scale isomerization unit is studied. The main concern in this plant is the RON of the isomerization gasoline (called isomerate) which is lower than the designed value (about 86). To overcome this problem, at first an ANFIS model is trained and validated for predicting RON of isomerate by using actual data collected from the plant during days on stream. Then, the significant decision variables of this commercial scale unit are manipulated such that the RON of gasoline can meet the desired value. Based on our knowledge, there is no report for applying ANFIS for modeling and optimizing an industrial scale light naphtha isomerization plant.

2. Process description

The target isomerization plant has the capacity of 8,500 BPSD of light naphtha (mostly contains pentanes and hexanes) which is received from upstream naphtha hydrotreating unit. The plant should increase the RON of the light naphtha (about 86) to meet the new gasoline specifications (high octane, sulfur-free, aromatic-free and olefins-free).

To perform the isomerization process, feed (contains 9.83 mole% of isopentane) enters the deisopentanizer tower (see Fig. 1) where iC5 is separated, and sent to the isomerate pool (with the purity of 98.3 mole %). The balance of the feed is sent to the isomerization reactor, and H_2 is added to reactor feed to encourage the desired reactions and minimize the coke formation on the catalyst. After passing through the reactor (loaded with 54000 kg of a commercial Pt/zeolite catalyst at operating pressure of 26 bar), the stream enters a H_2 separation unit where H_2 is removed and recycled to the reactor. Then, the output stream is sent to a stabilizer tower that eliminates light hydrocarbons (mostly C_1 to C_4) formed during the isomerization reactions. These compounds are consumed as the fuel gas in the refinery. The product stream from the bottom of the stabilizer tower is fed to a C5/C6 depentanizer column where C5 species are separated and recycled to the de-isopentanizer, and heavier components are sent to de-isohexanizer column. In this tower, iC6 is separated and recycled to the reactor whilst heavier components leave the bottom of the de-isohexanizer, and are sent to the isomerate pool.

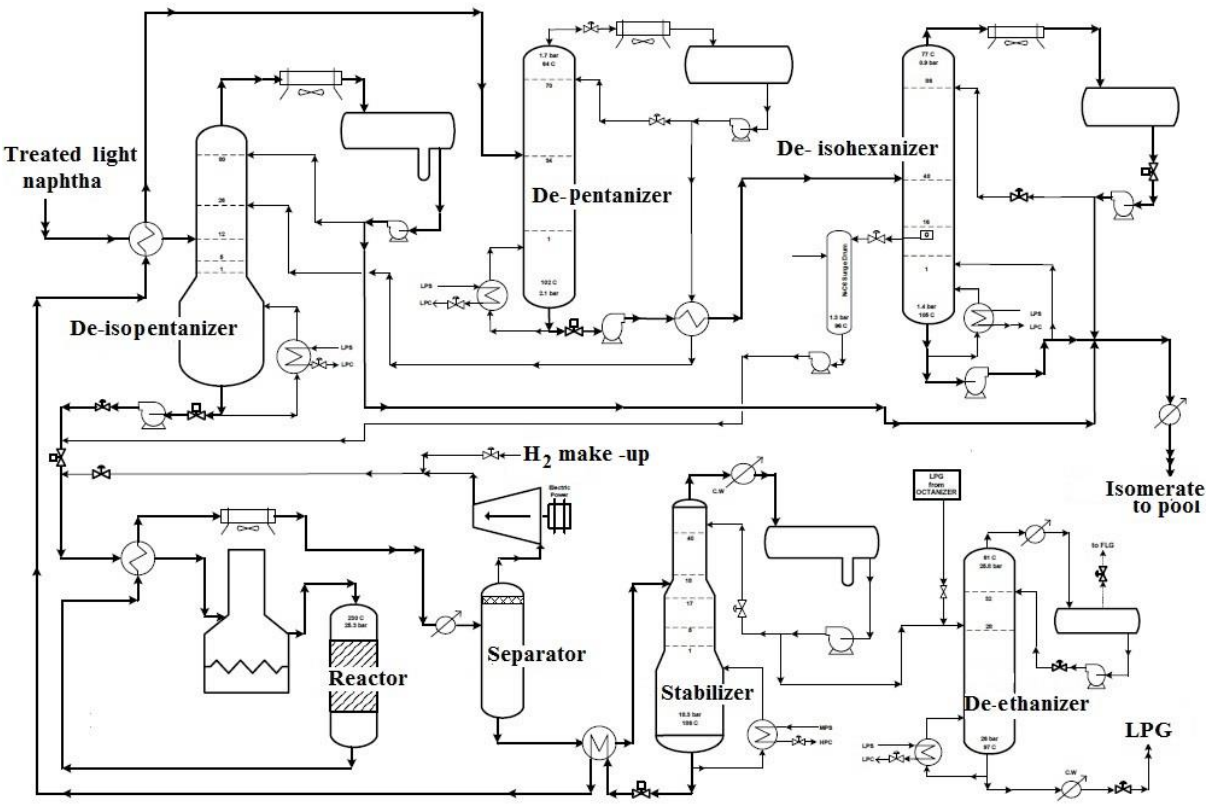

Figure 1. Block flow diagram of the light naphtha isomerization plant

3. Model formulation and optimization

The success in developing a reliable and robust artificial network strongly depends on the choice of process variables involved, as well as the available sets of data and the domain used for training purposes [36]. Therefore, it is essential to include all significant variables, affecting the RON of product (i.e. isomerate) in the input layer of the ANFIS model. According to Fig.1, momentous input variables of the ANFIS consist of days on stream (DOS), temperature of the deisopentanizer condenser (TconiC5), temperature of the de-isopentanizer reboiler (TrebiC5), light naphtha feed flowrate (F_{in}), inlet temperature of the isomerization reactor (TiR), hydrogen to hydrocarbon molar ratio (H2Oil), flow rate of n-C6 recycle (RC6), temperature of the de-pentanizer reboiler (TrebC5) and temperature of the de-isohexanizer reboiler (TrebiC6). The output variable of ANFIS is the RON of the isomerate.

To create the ANFIS, Matlab-fuzzy logic toolbox version 2013 (Mathworks, Inc.) and ANFIS syntax are 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 systems. It applies a combination of the least-squares and back propagation gradient descent methods for training membership parameters of fuzzy inference system to emulate a given training data set.

In this study, the type of membership functions used for developing light naphtha isomerization model is selected from all supported types in Matlab. To train the neuro-fuzzy model, two fuzzy rules are chosen from the ANFIS toolbox, and the process is stopped whenever the designated epoch number (20) is ended. Then, to evaluate the accuracy of the model, the absolute average deviation (AAD%) between the experimental and simulated data is reported as follows:

$$AAD\% = \frac{\sum_{n=1}^{N_t \Sigma} \sqrt{\frac{(X_n^{exp_n^{model}})^2}{X_n^{exp^2}}}}{N_t} \quad (1)$$

where X, N_t are the RON and number of data points, respectively; superscripts $exp$and model show the experimental data and the simulated values by the model, respectively.

In the target plant, the main concern is the deviation of the RON from the designed value (about 86). According to monitoring data obtained from the isomerization plant, the momentous variables that affect the RON of the isomerate product are: 1. temperature of the de-isopentanizer condenser, 2. temperature of the de-isopentanizer reboiler, 3. inlet temperature of the isomerization reactor, 4. hydrogen to hydrocarbon molar ratio, 5.temperature of the de-pentanizer reboiler and the temperature of the de-isohexanizer reboiler. Due to some operational problems in the hydrotreating plant installed at the upstream of isomerization plant and lack of storage tank, increasing or decreasing the flow rate of light naphtha feed is impossible. Moreover, the recycle flow rate cannot be changed due to the limitations in de-isohexanizer column. Therefore, light naphtha feed flowrate (F_{in}) and flow rate of n-C6 recycle (RC6) are not considered as the manipulated variables for the optimization program. Hence, the objective function is expressed as follows:

$$Objective function = Abs(RON - 86) \quad (2)$$

Subject to:

$$\begin{bmatrix} abs(TconiC5^{opt} - TconiC5^{act}) \le 2^{\circ}C & (a) \\ abs(TrebiC5^{opt} - TrebiC5^{act}) \le 2^{\circ}C & (b) \\ abs(TrebC5^{opt} - TrebC5^{act}) \le 2^{\circ}C & (c) \\ abs(TrebiC6^{opt} - TrebiC6^{act}) \le 2^{\circ}C & (d) \\ abs(TiR5^{opt} - TiR5^{act}) \le 2^{\circ}C & \rightleftarrows (e) \\ 0.98 \times H2Oil^{actual} \le H2Oil^{opt} \le 1.02 \times H2Oil^{actual} & (f) \end{bmatrix} \quad (3)$$

where superscripts act and opt show actual and optimized input variables of the target isomerization plant, respectively.

It should be noted that because of some restrictions in the temperatures of re-boilers and condensers, they have to be changed by only 2°C within the actual value. Thus, constraints 3(a) to 3(d) are considered. Moreover, due to the low capacity of hydrogen compressor and lack of hydrogen make up, H2Oil can be manipulated by only 2% of actual value (constraint 3f).

Although, there are many numerical methods proposed to perform an optimization problem, in this research the genetic algorithm (GA) is chosen to optimize the target light naphtha isomerization plant. GA is a part of soft computing science that deals with exploring the search space, selecting the best solution, and working for global optimization [37]. GA operates on a population of potential solutions, using the principle of survival of the fittest to produce successively better solutions to a problem, and it has advantages over the other traditional optimization methods. In particular, GAs can deal with discrete optimum design problems, do not need derivatives of objective functions, and also have the capability of identifying global optimal values.

Thus, by combining neuro-fuzzy network with GA optimization method, advantages of both approaches are utilized to produce a robust and fast methodology. To minimize the objective function (Eq. 2), the genetic algorithm function ('ga') of Matlab 2013a is applied.

4. Results and discussions

For the target isomerization plant, the input vector consists of DOS, TconiC5, TrebiC5, F_{in}, TiR, H2Oil, RC6, TrebC5 and TrebiC6. The output variable of ANFIS is the RON of the isomerate. To train the ANFIS, 43 data points were chosen, and 8 unseen ones were remained for validating the model.

In Table 1, the AAD% of trained data versus the experimental values is presented. As seen, trials with different membership functions indicate that the Gaussian function is the most suitable membership for simulating the RON of isomerate, but its accuracy should be evaluated in predicting step.

Table 1 AAD% of different membership function for training and prediction RON by ANFIS

	Training (%)	Predicting (%)
Sigmoid shape	8.30×10-4	4.708
Bell shape	6.21×10-5	1.182
Gaussian shape	2.68×10-5	0.913
Trapezoidal shape	1.08×10-4	3.334
Π shape	2.17×10-4	7.310
Triangular shape	3.95×10-4	0.916

After training the system with ANFIS syntax, the input layer of unseen data is fed to the trained ANFIS model, and output variable (i.e. RON of isomerate) is predicted by using Evalfis syntax. The AAD% of the predicted values versus the experimental ones is presented in Table 1. It is confirmed that the developed ANFIS with Gaussian membership function is reliable enough (AAD%<0.92%) to be applied for predicting the RON of isomerate as the object of the isomeration process. To have a better justification, a comparison between the trained and predicted data points against actual values is presented in Fig. 2. As observed, the ANFIS model can reliably predict the RON of isomerization product.

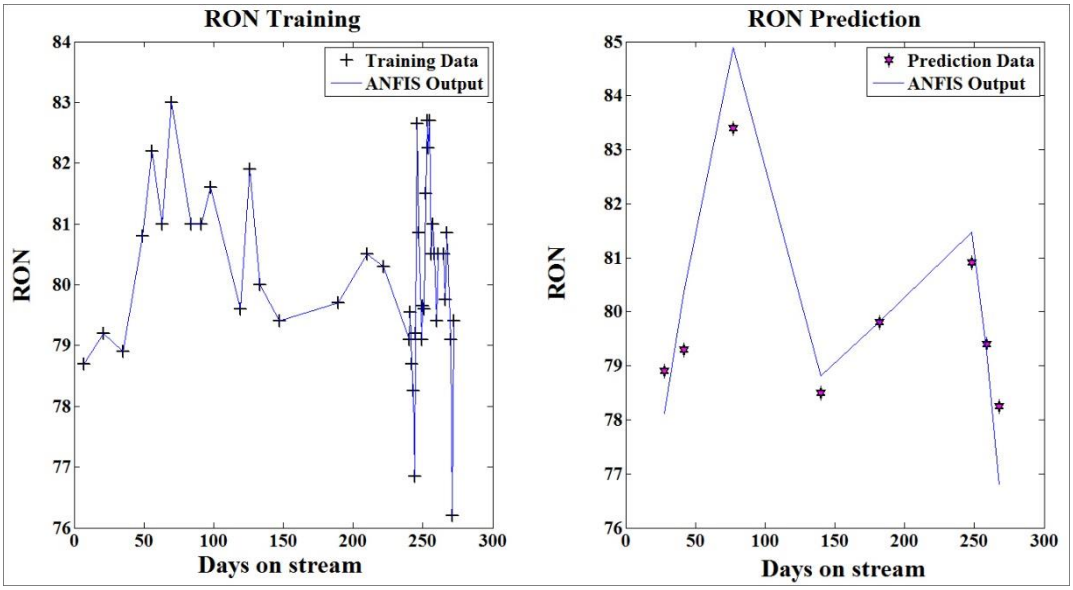

Figure 2. Comparing trained and predicted RON of the isomerate against actual data

After validating the isomerization ANFIS model, it is now ready to be used for maximizing the RON of isomerate. Therefore, the optimized operating conditions of the process, including temperature of the de-isopentanizer condenser (TconiC5), temperature of the de-isopentanizer reboiler (TrebiC5), inlet temperature of the isomerization reactor (TiR), hydrogen to hydrocarbon molar ratio (H2Oil), temperature of the de-pentanizer reboiler (TrebC5) and the temperature of the de-isohexanizer reboiler (TrebiC6), are calculated for all 53 data points. For each case, the optimized decision variables subject to the process constraints (Eq. 3) are obtained to maximize the RON of product (Eq. 2).

Plot in Fig. 3 show the comparison between the actual RON of isomerate and the corresponding value after applying the optimal operating conditions versus DOS. From this plot, it is obvious that the RON of product is considerably improved for the optimized cases such that for most points it can meet the desired value (i.e. 86). Consequently, the main concern of the

plant which is producing the gasoline below the market requirement is considerably mitigated. As seen, for some points, the RON of product has not increased to the desired value. It is supposed that for these points, the RON of light naphtha feed received from naphtha splitter in naphtha hydrotreater unit is lower than the expected value (about 73), and therefore the RON of product cannot meet the desired value.

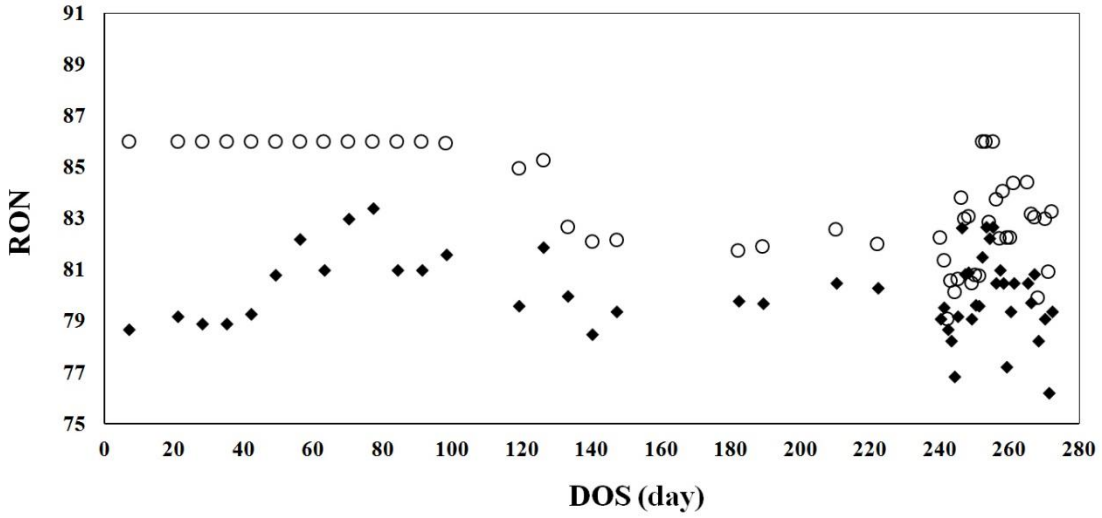

Figure 3. Comparison of the maximized (○) and actual (◆) RON of the target isomerization plant

Figs. 4 and 5 present the temperature of the condenser and reboiler of de-isopentanizer column in real mode and after optimization. As seen, the optimizer proposes the lower temperatures for the reboiler and condenser of this tower. It can be concluded that by reducing the condenser temperature, the purity of iso-pentane (RON=90.3) leaving the condenser increases as close as to the designed value (about 98.3 vol %), resulting in increasing RON of isomerate that leaves the pool (see Fig. 1). On the other hand, decreasing the reboiler temperature reduces the entry of normal pentane (RON=62) to the top of de-isopentanizer column in consequence with improving the RON of the final product.

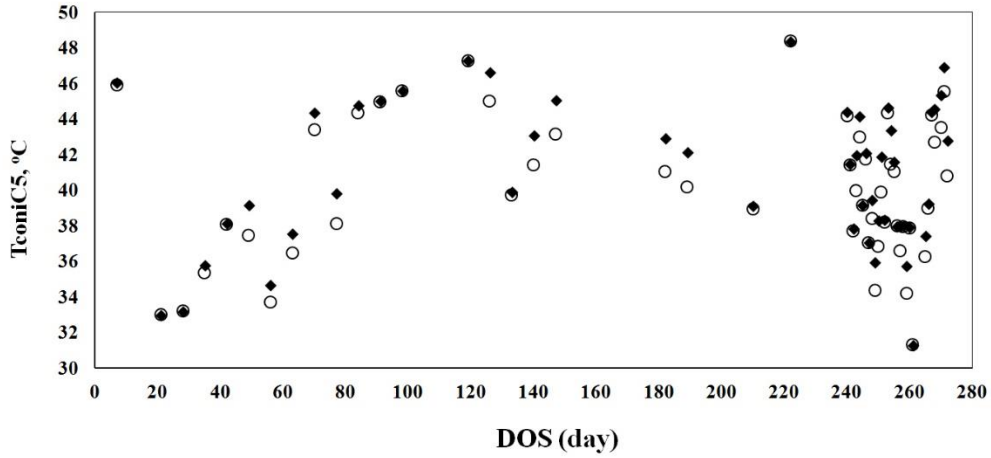

Figure 4. Comparison of the optimum (○) and actual (◆) de-isopentanizer condenser vs. DOS

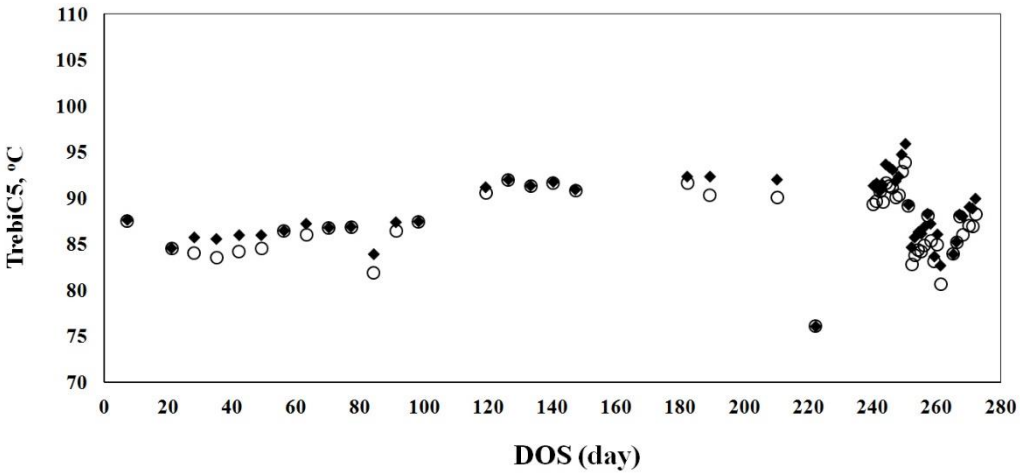

Figure 5. Comparison of the optimum (○) and actual (◆) temperature of de-isopentanizer reboiler vs. DOS

Fig. 6 shows that increasing the temperature of the isomerization reactor increases the RON of product. It is supposed that increasing this temperature promotes the conversion of normal to iso-C5/C6, and therefore the RON of isomerate significantly enhances. It should be mentioned that increasing this variable can accelerate the hydrocracking of heavy hydrocarbons (with high RON) to the compounds such as methyl pentanes, n-hexane and n-pentane and gaseous products, and conversely, decreases the RON of product. Thus, increasing the RON of isomerate by increasing the temperature should be meticulously carried out during days on stream (Constraint 3e) based on the program proposed by the catalyst manufacturer to compensate the deactivation of catalyst.

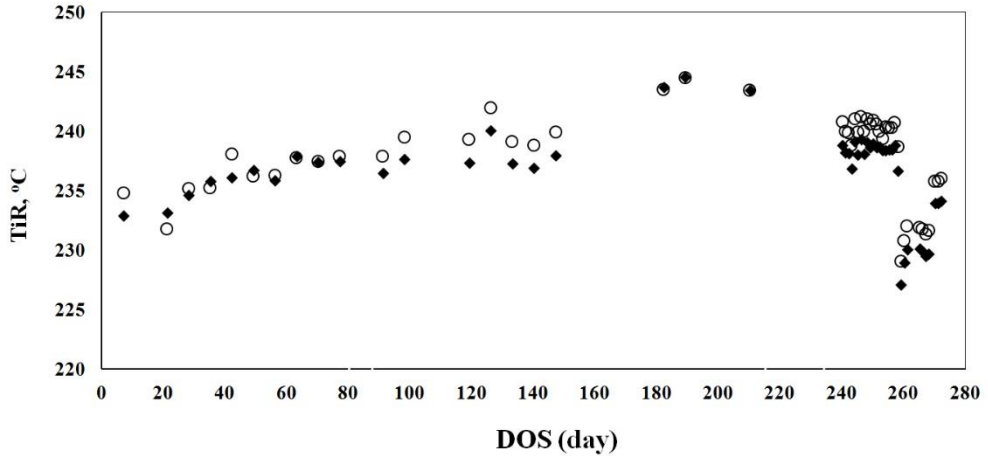

Figure 6. Comparison of the optimum (○) and actual (◆) isomerization reactor (TiR) vs. DOS

In Fig.7, the actual H2Oil of the isomerization plant is compared to the optimized values versus DOS. From this figure, it can be concluded that for all cases, the optimized H2Oil is a little higher than the real condition. Therefore, to provide the optimal point, this variable should be raised to reach the optimum RON. Furthermore, at high hydrogen partial pressure, less coke formation takes place on the catalyst surface; however, it should not be switched to higher values due to preventing from reactant dilution, and decreasing RON of isomerate. It seems than considering constraint (3f) can satisfy this condition.

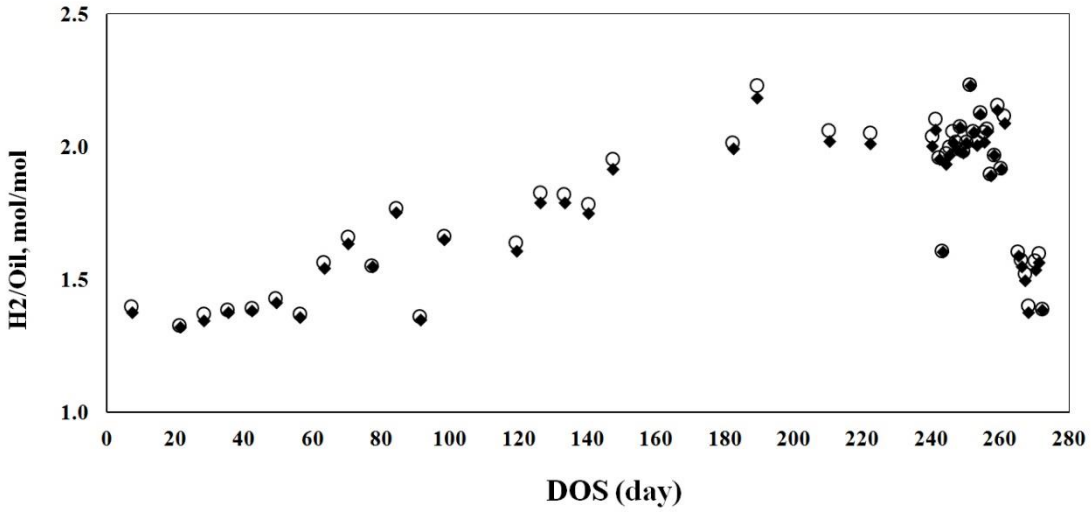

Figure 7. Comparison of the optimum (○) and actual (◆) hydrogen to hydrocarbon molar ratio vs. DOS

The relevant optimal temperatures for de-pentanizer and de-isohexanizer reboilers in comparison to the actual ones are presented in plots of Fig. 8 and Fig. 9, respectively. From Fig. 8, it is clear that excessive reboiler temperature of de-pentanizer can transfer heavy compounds with high octane number to the top of the tower, and recycle them to the beginning of the process; therefore, the RON of isomerate reduces. But, a reverse situation exists for the de-isohexanizer column where a side stream from tray No.16 (mainly consisting nC6) is recycled to the reactor. This stream is combined with iso-pentane stream separated from light naphtha in de-isopentanizer column (see Fig.1). As seen in Fig. 9, by working at lower temperatures than the optimum temperature in the reboiler of de-isohexanizer column, the recycle rate of n-hexane decreases; therefore, this compound enters into the product, and RON of isomerate decreases.

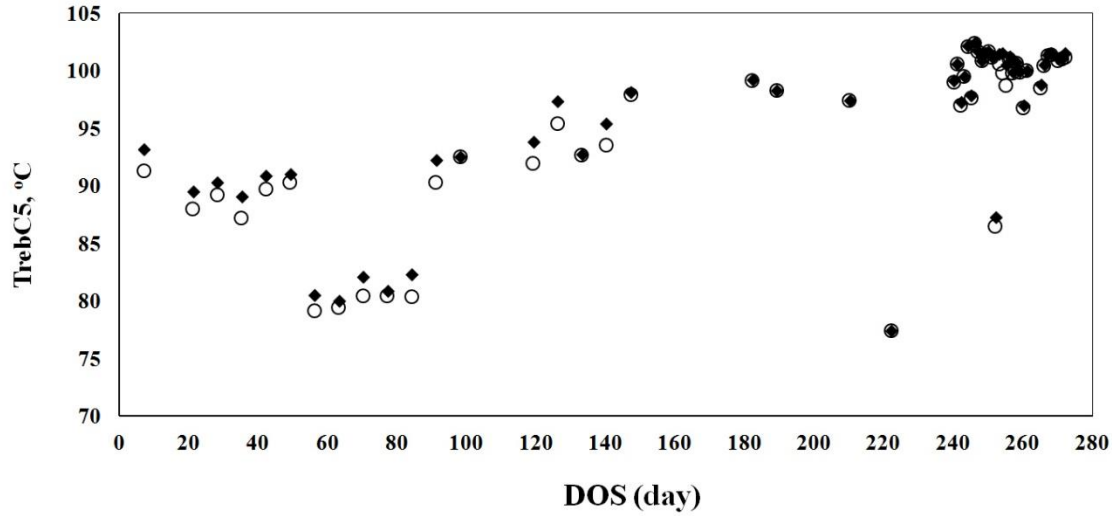

Figure 8. Comparison of the optimum (○) and actual (◆) temperature of the de-pentanizer reboiler vs. DOS

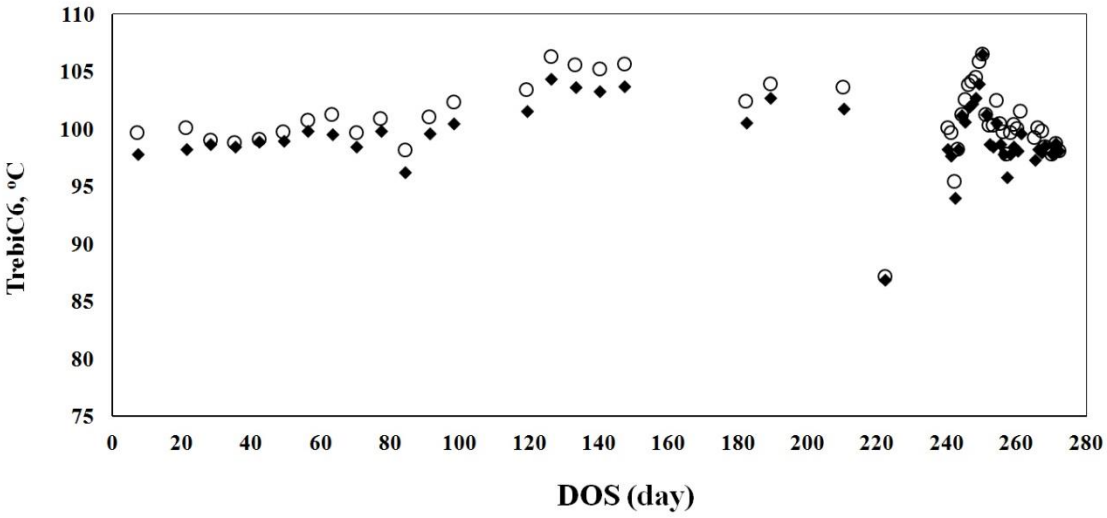

Figure 9. Comparison of the optimum (○) and actual (◆) temperature of de-isohexanizer reboiler vs. DOS

5. Conclusion

In this research, by using ANFIS and genetic algorithm, the RON of an industrial scale light naphtha isomerization plant increased to meet the designed value (86). Reliability of the model was validated by comparing its predictions with actual values obtained during 280 days of operation. It was concluded that the Gaussian membership function was the most appropriate option to simulate the RON of the target isomerization plant such that it could predict the RON of isomerate with the AAD% of 0.913.

After validating ANFIS, the decision variables of the process including temperatures of condenser and reboiler of de-isopentanizer column, inlet temperature of the isomerization reactor, hydrogen to hydrocarbon molar ratio, and temperatures of the de-pentanizer and de-isohexanizer reboilers were adjusted such that the RON of isomerate could reach to 86. The prediction results indicated that by setting the decision variables on the optimized values, the RON of isomerate increased to meet the expectation of the market. It was concluded that the presented method provided an appropriate approach for developing a plant-wide model for simulating and optimizing the commercial light naphtha isomerization process subject to operating constraints and process limitations.

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To whom correspondence should be addressed: Dr. Sepehr Sadighi, Catalysis Development Technologies Division, Research Institute of Petroleum Industry (RIPI), P.O. Box 14665137, Tehran, Iran,
E-mail: ssadighis@ripi.ir