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COMPARISON BETWEEN ADAPTIVE-NEURO FUZZY INFERENCE SYSTEM (ANFIS) AND ARTIFICIAL NEURAL NETWORK (ANN) FOR PREDICTING ACTIVITY AND SELECTIVITY OF A LABORATORY SCALE ISOMERIZATION PLANT

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Abstract

This study is aimed to comparing the accuracy of the adaptive neuro-fuzzy system (ANFIS) and artificial neural network (ANN) techniques for modeling a laboratory scale n-C6 isomerization plant. The input layer of ANFIS and ANN models consist time on stream (TOS), liquid hourly space velocity (LHSV), the temperature of the catalytic bed (TR) and hydrogen to hydrocarbon molar ratio (H_2Oil). Moreover, neurons in the output layer for both models are conversion and selectivity of the isomerization product. Both proposed modeling approaches are trained and tested based on 34 data points gathered from the laboratory scale plant. From results, it is concluded that the ANN can predict the selectivity and conversion of the unseen data points with the lower absolute average deviation (AAD%); therefore, this modeling approach is more reliable to simulate output variables of the target process with the less possibility of over learning.

Keywords: Modeling; Adaptive Neuro-Fuzzy; Artificial Neural Network; Isomerization.

1. Introduction

Isomerization process is designed to produce high-octane gasoline commodity from low-octane compounds by the structural change of carbon compounds. In a commercial isomerization process, hydrogen and light naphtha mostly including normal paraffinic hydrocarbons, are introduced from the top of a fixed-bed catalytic reactor and move downward throughout the bed. Therefore, most of the normal paraffinic compounds with low octane number are transformed into the iso-paraffins with higher octane number [1]. In this process, the most important factors that affect the quality of product and yield of the process are temperature of the reactor, feed flow rate and hydrogen to feed molar ratio [2].

In order to have an effective design and perfect control over it, a model is needed to predict product yields and qualities versus variables such as space velocity and temperature [3]. To study the effect of such input variables on the performance of any isomerization process, using a process model is beneficial which can also provide a facility to investigate, implement and scale up the under study process. In this respect, many studies have been proposed to model the reactor of an isomerization process using fundamental modeling approach [4-9]. However, for developing a powerful and wide-ranging kinetic-based model an isomerization unit, the complexity of feed makes it tremendously cumbersome to describe its kinetic rate at a molecular level. 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 therefore subsequent reports become unnecessarily sophisticated [10].

Over the last years, black-box modeling methods such as adaptive-neuro fuzzy inference system (ANN) and artificial neural networks (ANFIS) have been extensively used for modeling, controlling and optimizing catalytic processes [11-23]. The former is an information processing

paradigm that is inspired by the way the biological nervous system, such as the brain, processes information [24], and the latter is a kind of artificial neural network that is based on Takagi–Sugeno fuzzy inference system in which both models complement each other [25]. This technique combines the advantages of the fuzzy system (deal with explicit knowledge which can be explained and understood), and AAN (deal with implicit knowledge which can be acquired by learning) [26]. There are many studies in which ANN and ANFIS have been utilized to model and optimize the under-study process, and based on the reported results, each method has its specific advantage, accuracy, and robustness [27-29].

To clarify this issue, the present study focuses on the comparison of ANN and ANFIS modeling techniques used to predict conversion and selectivity of a laboratory scale isomerization plant. Thus, two models are formulated and tested: the first model considers a feed-forward structure with 4 and 3 neurons in the input and hidden layers, respectively; then, Levenberg-Marquardt (LM) algorithm are used to train the model. The second one is constructed based on ANFIS technique and different fuzzy memberships. After predicting the unseen data by using developed models, the ability of ANN and ANFIS approaches for predicting the conversion and selectivity of the target process are compared.

2. Process description

All experiments were carried out in a laboratory scale reactor set-up. A schematic diagram of the experimental apparatus is indicated in Figure 1 [2]. The isomerization process was carried out in a catalytic fixed-bed reactor which was made of stainless steel. The reactor dimensions were 2.5 cm in internal diameter, 3 cm in external diameter and 60 cm in height. The middle zone of the reactor was charged with 6 g of catalyst in the form of extrudates with the diameter of 2 mm. This zone was diluted with the equal volume of inert α-alumina particles with the same size of the catalyst. Moreover, to have a better distribution of the feed through the bed, the top of the bed was charged with α-alumina particles. The temperature of this zone was 10°C lower than that of the catalytic bed. An Agilent refinery gas analyzer (model 6890N with both flame ionization and thermal conductivity detectors) was used to analyze the product gas stream. Additionally, a gas chromatograph (Tief Gostar Faraz Co. with flame ionization detector and TRB petrol column with the length of 100 meters) was used to analyze liquid products.

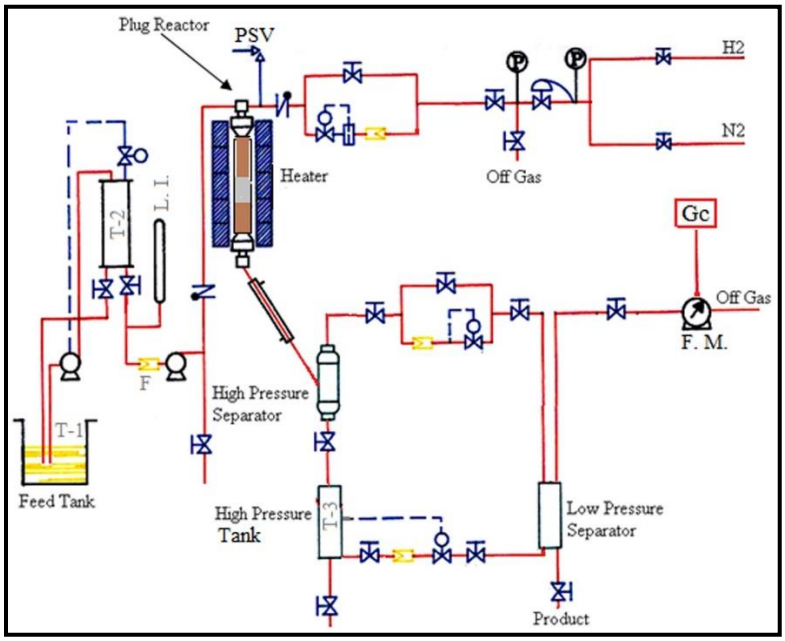

Figure 1. Flow diagram of the isomerization set up. T, storage tank; L.I., level indicator; PSV, pressure switch valve; P, pressure gauge; F, filter (mesh 40μm); GC, gas chromatography analyzer; F.M., flow meter [2]

A commercial Pt/Al_2O_3-Cl catalyst designed for light naphtha isomerization process was obtained from an industrial scale plant. It was in the form of extrudates, and its diameter and length were 3 mm and 1.5-2 mm, respectively. The catalyst was loaded into a high pressure reactor under nitrogen pressure to avoid contact with atmosphere, and activated according to the procedure provided by the refinery (i.e. reducing under a flow of hydrogen at 300ºC and chlorinating with a suitable agent).

3. Mathematical model

3.1. Artificial neural network model

A feed-forward artificial neural network model is applied to simulate the laboratory scale isomerization plant. The input layer of the ANN model consists time on stream (TOS), liquid hourly space velocity (LHSV), temperature of the catalytic bed (TR), and hydrogen to hydrocarbon molar ratio (H_2Oil) (see Figure 2). The output layer has two nodes i.e. conversion and selectivity of the isomerization product (Isomerate).

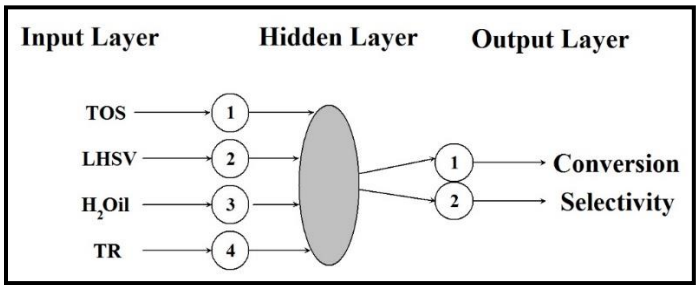

Figure 2. Simplified structure of ANN and ANFIS models developed for isomerization process

The most widely employed networks have one hidden layer only. 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 function as follows [31]:

$$a_j = \sum_{i=0}^{m} w_{ji} x_i + b_j \quad (1)$$

where w_{ji} is the weight that goes from the input (i) to the hidden neuron (j); b is the bias to the node, and x_i is the input unit of the neuron. By utilizing an activation function (f), the output of the neuron can be written as follows:

$$z_j = f(a_j) \quad (2)$$

This activation function is applied to model nonlinear behavior of the process. The activation function utilized for the hidden and output nodes is the tangent sigmoid function as follows:

$$f(a) = \frac{e^{a} - e^{-a}}{e^{a} + e^{-a}} = \tan sig(a) \quad (3)$$

In this research, ANN is programmed in the MATLAB 2013a (MathWorks, Inc.) software. Training is carried out by using Levenberg-Marquardt (LM) optimization method to estimate weights and biases until the minimum MSE (mean squared error) between the simulated and actual output variables can be obtained. Moreover, to prevent from memorizing instead of learning, only three neurons are selected for the hidden layer such that the number of coefficients is less than the number of experimental data.

3.2. Adaptive neuro-fuzzy inference system (ANFIS)

To create the ANFIS, Matlab-fuzzy logic toolbox version 2013 (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. Moreover, it applies a combination of the least-squares method and the back propagation gradient descent method for training fuzzy inference system to emulate a given training data set. The type of membership functions for the laboratory scale isomerization plant is selected from all supported types in Matlab i.e. Sigmoid, Bell, Gaussian, Trapezoidal, Π and Triangular shapes. For the proposed model, the input vector consists time on stream (TOS), liquid hourly space velocity (LHSV), hydrogen to hydrocarbon molar ratio (H_2Oil) and catalytic bed temperature (TR). The output layer is included conversion and selectivity of the process. To train the neuro-fuzzy inference system the same 34 data points as ANN network are selected, and other data are put aside as unseen data for predicting step. To train the fuzzy model, two fuzzy rules are chosen from the ANFIS toolbox, and training process is stopped whenever the designated epoch number (20) is reached.

3.3. Model evaluation

To evaluate the accuracy of the model, the absolute average deviation (AAD%) between the actual and predicted data is calculated as follows:

$$AAD\% = \frac{\sum_{n=1}^{N_t} \sqrt{\frac{(X_n^{\exp} - X_n^{model})^2}{X_n^{\exp 2}}}}{N_t} \times 100 \qquad (4)$$

where X, N_t are the output variables (i.e. conversion and selectivity) and number of data points, respectively; superscripts exp and model show the experimental data and the predicted values by the model, respectively.

4. Results and discussions

To model the n-C6 isomerization process using ANN modeling approach, actual data (42 experiments in different time on stream, levels of temperature, liquid hourly space velocity and hydrogen to hydrocarbon molar ratio), during 4472 min on stream were grouped into two categories i.e. training & testing (T&T) and predicting (PD) sets including 34 and 8 data points, respectively. As mentioned before, it was supposed that the catalyst was deactivated during the time on stream (TOS); therefore, the input layer of ANN was consisted TOS, LHSV, H_2Oil and TR. After training and testing the proposed network by using T&T data, the conversion and selectivity of unseen data (i.e. PD data) was predicted by using the developed network. As seen from Table 1, the ANN model, including 3 neurons in the hidden layer and 25 coefficients, can predict the conversion and selectivity of unseen data with the AAD% of 7.92% and 1.62%, respectively.

Table 1. AAD% of trained, tested and predicted data obtained from ANN

	Trained & Tested	Predicted
Conversion (%)	1.77	7.92
Selectivity (%)	0.044	1.62

As seen from Figure 3 and Table 1, the developed ANN model can appreciably be trained by using T&T data and simulate the output variables of the target plant. Furthermore, in Figure 4, the performance of the ANN model to predict the conversion and selectivity of isomerization process is presented. As concluded from this figure and also results given in Table 1, the developed model can acceptably predict the output variables of the laboratory scale isomerization unit.

Then, the isomerization model was trained by using ANFIS syntax in Matlab software, and output variables (i.e. conversion and selectivity of Isomer) were evaluated by applying Evalfis syntax. To train the fuzzy model, two fuzzy rules were selected from the ANFIS toolbox, and the training process was stopped whenever the designated epoch number (20) was reached. The AAD% of the trained values versus the actual ones is tabulated in Table 3. From this table, it is confirmed that the trained ANFIS model by using Triangular membership function is the best option for the target isomerization plant.

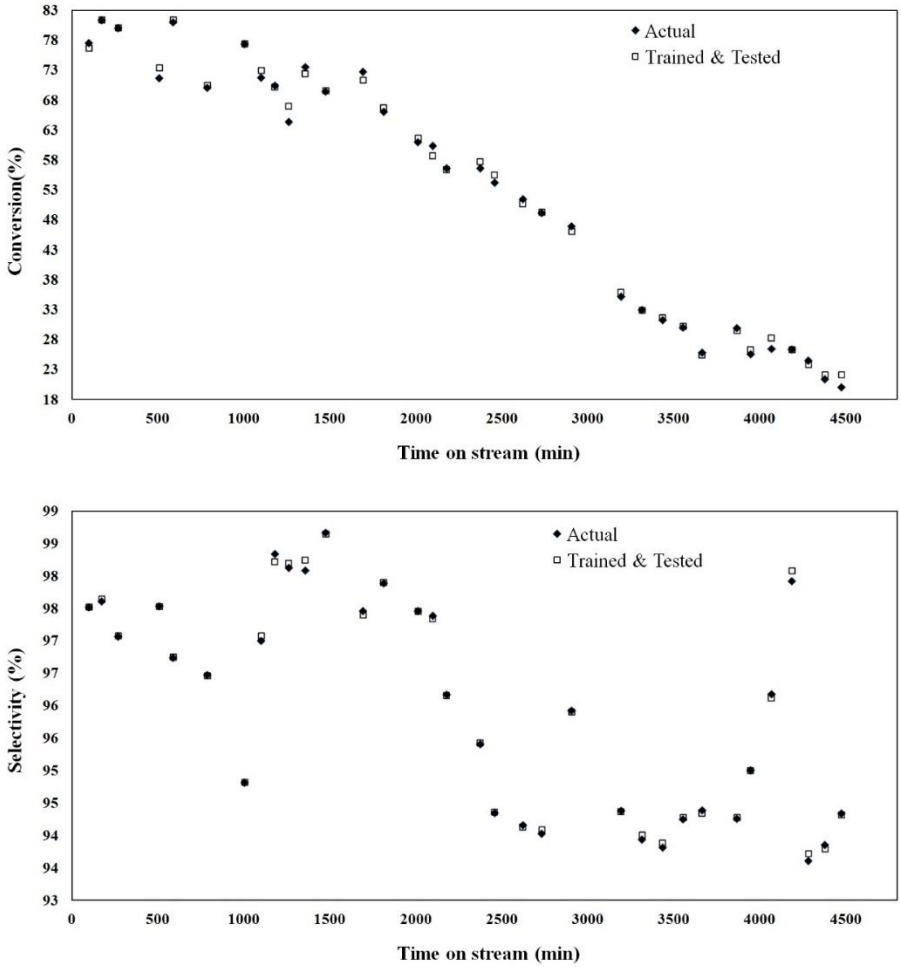

Figure 3. Comparison between actual, tested and trained values of conversion and selectivity obtained from ANN

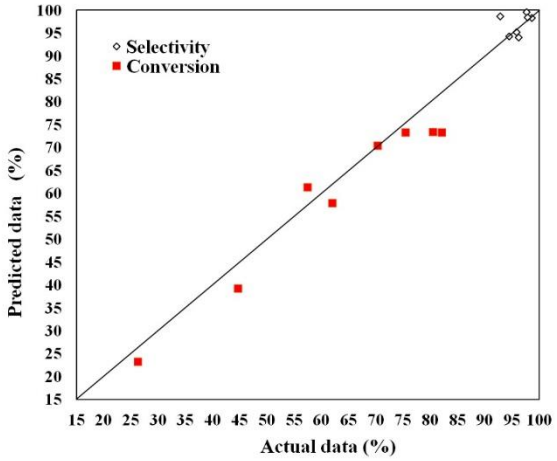

Figure 4. Comparison between actual and predicted values of conversion and selectivity obtained from ANN

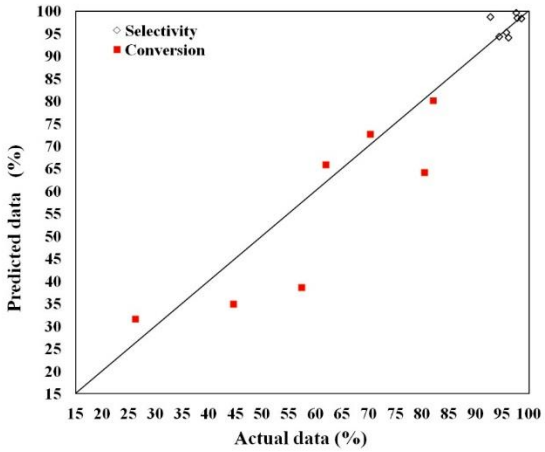

Figure 6. Comparison between actual and predicted values of conversion and selectivity obtained from ANFIS

Table 3. AAD% of different membership function for trained data by ANFIS

	Sigmoid shape	Bell shape	Gaussian shape	Trapezoidal shape	Π shape	Triangular shape
Conversion (%)	0.0117	0.0034	0.03968	0.00556	0.04877	0.00147
Selectivity (%)	0.0074	0.0013	0.04108	0.00245	0.00856	0.00039

The comparisons between the simulated conversion and selectivity versus actual ones are illustrated Figure 5 to have a better justification. As observed, such as the ANN model, ANFIS model can appreciably train these output variables with an acceptable accuracy.

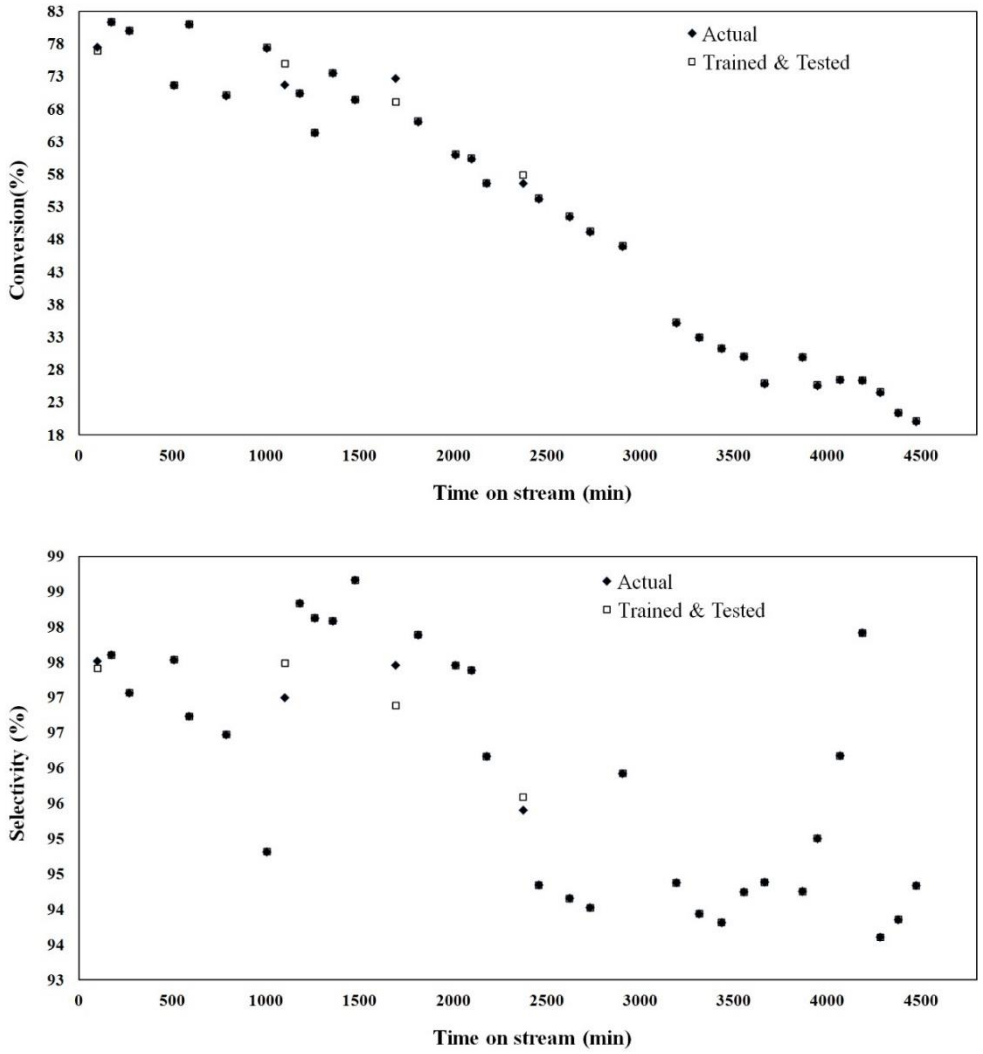

Figure 5. Comparison between actual, tested and trained values of conversion and selectivity obtained from ANFIS

Table 4. AAD% of different membership function for predicted data by ANFIS

	Sigmoid shape	Bell shape	Gaussian shape	Trapezoidal shape	Π shape	Triangular shape
Conversion (%)	123.29	86.58	79.68	53.10	82.77	18.33
Selectivity (%)	72.37	10.24	10.83	47.95	209.90	2.13

After training the laboratory scale isomerization model with ANFIS syntax, the input layer PT (unseen) data is fed to the trained ANFIS model, and output variables (i.e. conversion and selectivity) is predicted. The AAD% of the predicted values against the actual ones is presented in Table 4 for all membership functions. From this table, it is proved that the developed ANFIS models by using Triangular membership function can predict the output variables of the plant with the AAD% of 18.33% and 2.13%, respectively. The comparison between the predicted and actual values is presented in Fig. 6 to have a better justification.

As observed, the prediction of ANFIS for conversion and selectivity by all membership functions is not acceptable except for Triangular shape. In comparison to the results obtained by ANN model, it is observed that ANN has the considerably higher precision to predict desired values of the target laboratory scale isomerization plant. It is supposed that the lower accuracy of the developed ANFIS model is due to the number of coefficients of that (55 ones) which is higher than that of ANN model (25 coefficients). With regards to the number of T&T data (i.e. 34 points), the degree of freedom (DOF) of ANFIS model is negative, and therefore over learning and memorizing instead of learning is plausible for this model.

5. Conclusions

The present research discussed on the accuracy and reliability of ANN and ANFIS modeling approaches in predicting the conversion and selectivity of a laboratory scale isomerization plant. Both models were trained and validated by 42 experimental data points obtained from the under-study unit. For training and testing, 34 data points were randomly selected, and 8 points were chosen to evaluate predicting the ability of models. Both soft computing techniques (i.e. ANN and ANFIS) performed well during training and testing period such that they could simulate actual conversion and selectivity with the ADD% of 1.77% and 0.044%, and 0.00147% and 0.00039%, respectively. However, ANN modeling approach showed better performance to predict unseen data, and it could predict conversion and selectivity with the AAD% of 7.92% and 1.62%, respectively. These values were acceptable lower than those values obtained from ANFIS technique i.e. 18.33% and 2.13%, respectively. Consequently, results suggested the use of neural network based modeling technique in accurate prediction of conversion and selectivity of isomerization or other similar processes, especially when enough data is not available to train the ANFIS.

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