MODELING A COMMERCIAL VACUUM GAS OIL HYDROCRAKING PLANT USING ADAPTIVE-NEURO FUZZY INFERENC SYSTEM (ANFIS)

Sepehr Sadighi*, Seyed Reza Seif Mohaddecy

Research Institute of Petroleum Industry (RIPI), Catalysis Research Division, P.O. Box 14665137, Tehran, Iran

Received January 5, 2017; Accepted April 5, 2017

Abstract
In this research, an adaptive-neuro fuzzy inference system (ANFIS) to model the yield of products of vacuum gas oil (VGO) hydrocracker including light naphtha (LN), heavy naphtha (HN), kerosene (Ker), diesel (Dis) and unconverted oil (Offtest) is proposed. The input layer of the ANFIS consists of age of catalyst, feed and recycle flow rates, input temperature to the reactor and initial boiling point (IBP) of VGO. For developing the model, a set of 69 data points in different levels of temperature, pressure and LHSV (liquid hourly space velocity) are collected from the target plant (called Isomax). After training the model using 59 data points, it is confirmed that trapezoidal curve is the most suitable membership function for predicting yield of products. After applying unseen data (10 data points), results show that ANFIS can predict yields of LN, HN, Ker, Dis and Offtest with the AAD% of 1.185%, 0.758%, 0.408%, 0.593% and 2.222%, respectively.

Keywords: Neuro-Fuzzy; Modeling; Hydrocracking; Vacuum Gas Oil.

1. Introduction
Vacuum gas oil (VGO) hydrocracking process in a refinery is designed to convert VGO or similar boiling-range feedstock into the light and precious commodities. With the attention to the profit margins, hydrocracking is widely interested due to its flexibility for upgrading heavy feedstock into light precious products such as naphtha, kerosene and diesel. Moreover, it is an interested process in a refinery that upgrades the quality and the quantity of refined petroleum products, simultaneously [1]. In this process, feed reacts with hydrogen in the presence of a Ni-Mo or Ni-W type catalyst on a silica/alumina or zeolite supports [2].

In order to have an effective design and a perfect control over it, a model is needed to predict product yields and qualities versus variables such as space velocity and temperature [3]. Moreover, the model can be also used to select the suitable hydrocracking catalysts [4]. But, the complexity of hydrocracking feed makes it excessively difficult to characterize and describe its kinetic at a molecular level [5-6]. To develop a reliable fundamental model for a VGO hydrocracking process, the complexity of the VGO mixtures makes it highly cumbersome to describe its kinetic rate at a molecular level. Existing commercial simulators like Aspen plus or Hysys from Aspen Technology do not have such limitations for the number of species, and it is feasible to apply a unique set of pseudo components for petroleum assay streams; but, this approach rises the calculation time, and following reports become avoidably complicated. One approach to simplify the problem is to consider the partition of the components into a few equivalent classes called lumps or lumping technique, and then assume each class as an independent entity [7]. Developing simple kinetic models (e.g., power-law model) for complex catalytic reactions is a common approach that can give basic information for catalyst screening, reactor design and optimization [8]. This kind of modeling is proposed by several researches in which
hydrocracking process was modeled with three-lump [9-12], four-lump [4,13], five-lump [14-18], six-lump [19], seven-lump [20] and eight-lump [21] approaches.

Furthermore, over the last two decades, soft computing methods such as artificial neural networks (ANN) and fuzzy logic were widely applied for modeling, controlling and optimizing catalytic processes [22-32]. ANN is an information processing paradigm that is inspired by the way the biological nervous system, such as the brain, processes information [33]. This modeling approach has the following advantages: 1. it is highly nonlinear; therefore, its structure can be more complex and more representative than most other empirical models; 2. its structure does not have to be pre-specified; therefore, they are quite flexible models [34].

With a combination between ANN and Fuzzy logic rules, it is possible to design the fuzzy neural network model to use the both of their advantages. ANFIS (adaptive neuro-fuzzy inference system) is a kind of artificial neural network that is based on Takagi–Sugeno fuzzy inference system in which both models complement each other [35]. This technique combines the advantages of fuzzy system (deal with explicit knowledge which can be explained and understood), and AAN (deal with implicit knowledge which can be acquired by learning) [36]. The appropriate selection of model parameters such as number, parameter and type of fuzzy membership functions are significant to obtain the desired performance.

ANFIS has been applied to model various chemical processes [37-39]; but, based on our research, there is no report to apply this method for modeling an industrial scale VGO hydrocracker. In this study, by using actual data gathered from a commercial scale VGO hydrocracking unit which is called Isomax, an ANFIS model is developed for predicting the yield of hydrocracking products including light naphtha, heavy naphtha, kerosene, diesel and offtest.

2. Process description

A commercial first stage hydrocracking unit, called Isomax, licensed by Chevron research cooperation with the nominal capacity of 16,500 barrel per day is chosen as a case study. The feed of the plant is a mixture of fresh VGO and the unconverted oil. The latter is recycled from the separation section at the end of the process. The schematic diagram of the Isomax process is presented in Fig. 1. The properties of VGO fresh feed during the period of the study can vary slightly with time from the start of run (SOR) to end of run (EOR). The design pressure of this unit is 156 bar, but dependent to the feed specification, hydrogen availability and the catalyst type, operating pressure of the plant can be varied up to 165 bar during the catalyst cycle life. During the data gathering for this research, the pressure fluctuations were between the design value and 160 bar, so that the effect of pressure on hydrocracking yield is negligible.

Fig 1. The process flow diagram of the target hydrocracking unit [21]
In this process, the combined feed is mixed with hydrogen and it is heated before entering the reactor. The hydrocracking section has three similar parallel reactors each of which has four beds with the total amount of catalyst being 36600 kg. The percentage weight of loaded catalyst in Beds 1, 2, 3 and 4 is 14%, 26%, 31% and 29%, respectively.

As seen in Figure 1, there are 5 main streams, containing light dry gases (C₁ and C₂) and LPG (C₃, C₄ and C₅), which are named as HPS vent, LPS gas, sponge gas, stabilizer gas and LPG. Because all streams consist of C₁ to C₅, as well as H₂O, NH₃ and H₂S components, their flow rate and composition are separated to light gases and LPG as distinct products. It is obvious that the output products of reactors containing light gases, LPG, naphtha, kerosene, diesel and residue are separated in different separation units. The hydrocracking catalyst is a commercial dual functional amorphous type. The VGO feed, recycle stream (or offtest) and diesel samples were analyzed according to the ASTM D1160 standard procedure whilst kerosene, light and heavy naphtha samples were analyzed according to the ASTM D86 method.

### Table 1. Average specifications of vacuum gas oil feed

<table>
<thead>
<tr>
<th>Property</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density at 50°C</td>
<td>g/cm³</td>
<td>0.89</td>
</tr>
<tr>
<td>Sulfur</td>
<td>wt%</td>
<td>2.1</td>
</tr>
<tr>
<td>Total nitrogen</td>
<td>ppmwt</td>
<td>1100</td>
</tr>
<tr>
<td>Conradson carbon</td>
<td>wt%</td>
<td>0.043</td>
</tr>
<tr>
<td>Refractive index at 20°C -</td>
<td></td>
<td>1.53</td>
</tr>
<tr>
<td>Distillation analysis (ASTM D1160)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IBP</td>
<td>°C</td>
<td>372.3</td>
</tr>
<tr>
<td>Total nitrogen</td>
<td>°C</td>
<td>393.3</td>
</tr>
<tr>
<td>Conradson carbon</td>
<td>°C</td>
<td>431.9</td>
</tr>
<tr>
<td>Refractive index at 20°C -</td>
<td>°C</td>
<td>453.8</td>
</tr>
<tr>
<td>Ultimate analysis</td>
<td></td>
<td>70%</td>
</tr>
<tr>
<td>C</td>
<td>wt%</td>
<td>86</td>
</tr>
<tr>
<td>H</td>
<td>wt%</td>
<td>12.1</td>
</tr>
<tr>
<td>FBP</td>
<td>°C</td>
<td>528.4</td>
</tr>
</tbody>
</table>

### 3. Mathematical model

In this study, 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. It applies a combination of the least-squares method and the backpropagation gradient descent method for training fuzzy inference system to emulate a given training data set. The type of membership functions for the Isomax unit is selected from all supported types in Matlab i.e. Sigmoid, Bell, Gaussian, Trapezoidal, Π and Triangular shapes.

For the Isomax plant, the input vector consists age of catalyst (Age), volume flow rates of VGO fresh feed (Ff) and unconverted oil as recycle feed stream (Rf), initial and final boiling points (IBP and FBP) of VGO, and inlet temperature of catalytic beds (Tb1, Tb2, Tb3 and Tb4). The output layer is included yield of products i.e. light and heavy naphtha, kerosene, diesel, and offtest. To train the neuro-fuzzy inference system, 59 data points (see Table 3) are chosen, and 10 unseen data points are remained for validating step.

To train the fuzzy model, two fuzzy rules are selected from the ANFIS toolbox, and training process is stopped whenever the designated epoch number (20) is reached. To evaluate the accuracy of the model, the absolute average deviation (AAD%) between the experimental and predicted data is calculated as follows:

\[
AAD\% = \frac{100}{N_t} \sum_{n=1}^{N_t} \left( \frac{(X_{n}^{\text{exp}} - X_{n}^{\text{model}})^2}{X_{n}^{\text{exp}}} \right) \times 100
\]  

(1)

where X, N_t are the output variables (i.e. yield of LN, HN, Ker, Dis and Offset) 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

In Table 2, the AAD% of trained data versus the experimental values is presented. As seen from this table, trials with different membership functions of the neuro-fuzzy model indicate that the trapezoidal shape curve is the best choice for simulating the yield of the hydrocracking products. By using this fruition, the yield of LN, HN, kerosene, diesel and offtest can be simulated with the AAD% of 1.221%, 0.687%, 0.261%, 0.622% and 2.13%, respectively.

Table 2. AAD% of different membership function for data training by ANFIS

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Sigmoid shape</th>
<th>Bell shape</th>
<th>Gaussian shape</th>
<th>Trapezoidal shape</th>
<th>Π shape</th>
<th>Triangular shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>LN (%)</td>
<td>1.301</td>
<td>8.270</td>
<td>6.836</td>
<td>1.221</td>
<td>2.179</td>
<td>1.432</td>
</tr>
<tr>
<td>HN (%)</td>
<td>10.532</td>
<td>13.839</td>
<td>2.624</td>
<td>0.687</td>
<td>0.861</td>
<td>3.160</td>
</tr>
<tr>
<td>Kerosene (%)</td>
<td>0.346</td>
<td>8.018</td>
<td>4.986</td>
<td>0.261</td>
<td>0.254</td>
<td>1.926</td>
</tr>
<tr>
<td>Diesel (%)</td>
<td>23.064</td>
<td>22.992</td>
<td>7.784</td>
<td>0.622</td>
<td>0.548</td>
<td>2.942</td>
</tr>
<tr>
<td>Offtest (%)</td>
<td>23.825</td>
<td>21.198</td>
<td>18.770</td>
<td>2.130</td>
<td>3.064</td>
<td>6.283</td>
</tr>
</tbody>
</table>

After training the Isomax model with ANFIS syntax, the input layer of the unseen data (Age, Ff, Rf, IBP, FBP, Tb1, Tb2, Tb3 and Tb4) are fed to the trained Anfis model, and output variables (i.e. LN, HN, Ker, Dis, Offtest) are evaluated by using Evalfis syntax. The AAD% of the predicted values versus the experimental ones is presented in Table 3. From this table, it is confirmed that that the developed ANFIS model is reliable enough to be applied for predicting the yield of products of Isomax plant.

Table 3. AAD% of prediction using the trained ANFIS model

<table>
<thead>
<tr>
<th>Fraction</th>
<th>AAD%</th>
</tr>
</thead>
<tbody>
<tr>
<td>LN (%)</td>
<td>1.185</td>
</tr>
<tr>
<td>HN (%)</td>
<td>0.758</td>
</tr>
<tr>
<td>Kerosene (%)</td>
<td>0.408</td>
</tr>
<tr>
<td>Diesel</td>
<td>0.593</td>
</tr>
<tr>
<td>Offtest</td>
<td>2.222</td>
</tr>
<tr>
<td>Average (%)</td>
<td>1.033</td>
</tr>
</tbody>
</table>

To have a better justification, comparisons between the simulated yields (training and predicting data) and actual yields of light naphtha, heavy naphtha, kerosene, diesel and offtest are presented in Figs 2 to 6, respectively. As observed, ANFIS model can appreciably predict yields of hydrocracking product with a high accuracy. Additionally, from these figures, it is observed that yields of light products i.e. naphtha and kerosene decrease versus operation time or age of the catalyst whereas that of diesel and offtest increases. The main reason for these variations is deactivation of the catalyst which is indispensable for an industrial scale catalytic fixed-bed reactor. This unit has been designed to operate at least for 3 years without any regeneration process. As seen, the developed ANFIS model can appreciably distinguish the deactivation of the catalyst, and predicts yields of hydrocracking products versus cycle time.

Fig. 2. The comparison between trained and predicted values of light naphtha yield vs. age of catalyst
Fig. 3. The comparison between trained and predicted values of heavy naphtha yield vs. age of catalyst

Fig. 4. The comparison between trained and predicted values of kerosene yield vs. age of catalyst

Fig. 5. The comparison between trained and predicted values of diesel yield vs. age of catalyst
Fig. 6. The comparison between trained and predicted values of offtest yield vs. age of catalyst

5. Conclusions

In this study, an adaptive-neuro fuzzy inference system (ANFIS) was proposed for modeling an industrial scale vacuum gas oil hydrocracking plant with the commercial name of Isomax. This model was trained and validated on the basis of 69 experimental data points obtained from the target plant.

For training ANFIS, 59 data points were randomly selected, and the remained ones were put aside for validating the model. It was observed that among all supported membership functions in the Matlab software, trapezoidal shape curve was the most appropriate membership function for simulating yields of Isomax.

Results showed that the average AAD% of the trained yields of hydrocracking products was less than 0.984%. Moreover, by using the validation data, it was confirmed that the proposed ANFIS model could predict yields of light naphtha, heavy naphtha, kerosene, diesel and offtest with the AAD% of 1.185%, 0.758%, 0.408%, 0.593% and 2.222%, respectively. Achievements of this work are momentous for simulating industrial scale hydrocracking plants, and also making the best decision to select the optimized operating conditions from start of run (SOR) to the end of run (EOR).

Acknowledgements

The authors thank to Research Institute of Petroleum Industry (RIPI) for supporting this project (Project No: 11480696).

References


To whom correspondence should be addressed. E-mail: Sadighis@ripi.ir