

# Hydrocracker Reactor Catalyst Activity Model Using Artificial Neural Network

Ibrahim H.. Alhajri and Abdolreza R. Moghadassi

**Abstract**— Hydrocracking technology plays an important role in petroleum refining industry. This work developed an artificial neural network (ANN) model to estimate the catalyst activity based on the weighted average bed temperature (WABT) and the normalized time of operation (BPP) in the hydrocracker reactor. ANN was designed to define the relations between WABT and BPP, and the catalyst activity was subsequently calculated using the experimental data of the WABT and a theoretical equation for activity in terms of WABT. In three different cycles of catalyst operation, a perceptron ANN model with two hidden layers was consequently used to estimate WABT and catalyst activity. In conclusion, an empirical model was developed and the results demonstrated good agreement between experimental data and ANN predictions.

**Index Terms**— Catalyst activity, hydrocracker reactor, weighted average bed temperature (WABT), normalized time (BBP), perceptron ANN model.

## I. INTRODUCTION

Artificial neural networks (ANN) are extensively used in different aspects of science and technology. An ANN can be considered to be a black box that accepts a series of input data and produces one or more outputs. The transformation of the data is done through several basic processing units, called artificial neurons, which perform identical tasks. The neurons are connected into networks through synapses or connecting links. The programs carried out by ANNs may be quite varied; one of the most important programs is modeling—namely, the search for an analytical function or procedure that gives a specified n-variable output for any m-variable input. The ANN does not require the knowledge of mathematical functions and relations like any standard modeling techniques: The nonlinearity of a single unit transformation and a sufficiently large number of variable parameters (e.g., weights and biases) ensure enough “freedom” to adapt the neural network to any relation between input and output data [1].

In modeling a chemical process, all phenomena present in the process have to be identified and properly described.

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The mathematical description of the process usually involves conservation laws, and processes are expressed using a set of deterministic (algebraic, differential, or integral) equations. However, a neural model includes two general methods in modeling: a global neural model (GNM), in which the whole model is represented with a single ANN, and a hybrid neural model (HNM), in which only the unknown part of the model is replaced by the ANN. Since its introduction in the early 1990s [2].

Hydrocracking technology is an important conversion technology for producing high-value naphtha or middle-distillate products from a wide range of a refinery's heavy feedstocks. Various technologies, such as fixed-bed, moving-bed, or ebullated-bed reactors, are available for hydroprocessing heavy oil fractions. The major selection criterion between each type of technology is based on the catalyst deactivation rate [3]. Among all the commercially proven technologies for heavy fraction hydroprocessing, those using fixed-bed reactors in a series loaded with catalysts with different functionalities are the most commonly used process configurations [4]. The main disadvantage of fixed-bed reactors is the loss of catalyst activity over time as a result of premature catalyst deactivation, which drastically reduces the length of operation [3].

In the current work, an HNM was used to model the catalyst activity of the hydrocracker reactor. All of the experimental results and correlations were obtained under limited conditions in the hydrocracker unit, making it very difficult to extrapolate the correlations to a wide range of operating conditions. Hence, it is important to develop a general correlation for predicting temperature increases under different operating conditions.

## II. MATHEMATICAL MODEL FOR CATALYST DEACTIVATION

A good catalyst is defined according to three characteristics: activity, selectivity, and life. Catalysts have a highly active surface, and a layer of the reactants are adsorbed on the active sites that lead to decreases in the activation energy of the reaction or to increases in the reaction rate. The efficiency of entire catalytic systems decreases gradually, making it necessary to monitor and control the catalyst activity in order to determine when catalyst regeneration and optimal conditions occur.

Two aspects of catalyst are used to observe catalyst activity: surface activity and reactor pressure drop. The activity of catalyst particles at each time is given by:

$$activity = \frac{reactionrate\ with\ catalyst}{reactionrate\ with\ fresh\ catalyst} \quad (1)$$

Kinetics can determine the key properties of a hydrocracking catalyst—namely, initial activity, selectivity, stability, and product quality. In hydrocracking, activity is defined as the temperature required to obtain fixed conversion under conditions associated with certain processes.

Equation 2 defines a simple reaction, such as ( $A \rightarrow Product$ ), and an n-order reaction rate:

$$-r_A = K.C_A^n.a = K_0 e^{-E/RT}.C_A^n.a \quad (2)$$

where  $C_A$  is the feed concentration in the reactor effluents. Since the  $K.a$  is constant, the conversion can be maintained at the same level, if the temperature increases as the catalyst activity gradually decreases.

At the initiation of operations (when the catalyst is fresh), the activity is considered equal to 1 and temperature is  $T_0$ .

$$K.a = K_0 e^{-E/RT_0}.1 = cte \quad (3)$$

After time  $t$ , the temperature (WABT) is  $T$ , and catalyst activity is  $a$ ; meanwhile, the  $K.a$  remains constant. Thus:

$$K.a = K_0 e^{-E/RT}.a = cte \quad (4)$$

Based on (3) and (4), a final relation for activity is obtained in terms of weighted average bed temperature ( $T$ ) as

follows:

$$a = e^{\left[ -E / R \left( \frac{1}{T_0} - \frac{1}{T} \right) \right]} \quad (5)$$

where  $E$  is the activation energy of the hydrocracking and  $a$  is the catalyst activity function. Equation (5) is obtained based on the assumption of constant conversion when the temperature gradually increases. The average hydrocracking activation energy for the feed of the hydrocracker unit in the Arak Refinery Company is approximately 277,545 (J/mol) [5].

The percentage of relative error in estimation of WABT was calculated using the following equation:

$$RelvError\% = \frac{(WAPT^{Exp.} - WAPT^{ANN})}{WAPT^{Exp.}} * 100 \quad (6)$$

The training process requires a proper set of data (i.e., input and target output). During training, the weights and biases of the network were iteratively adjusted to minimize the network performance function [4]. The typical performance function used for training feed-forward neural networks is the network Mean Squares Errors ( $MSE$ ). Both  $MSE$  and average absolute relative deviation ( $AARD$ ) are defined as follows:

$$MSE(u) = \frac{1}{n} * \sum_{i=1}^n (u_i^{exp} - u_i^{ANN})^2 \quad (7)$$

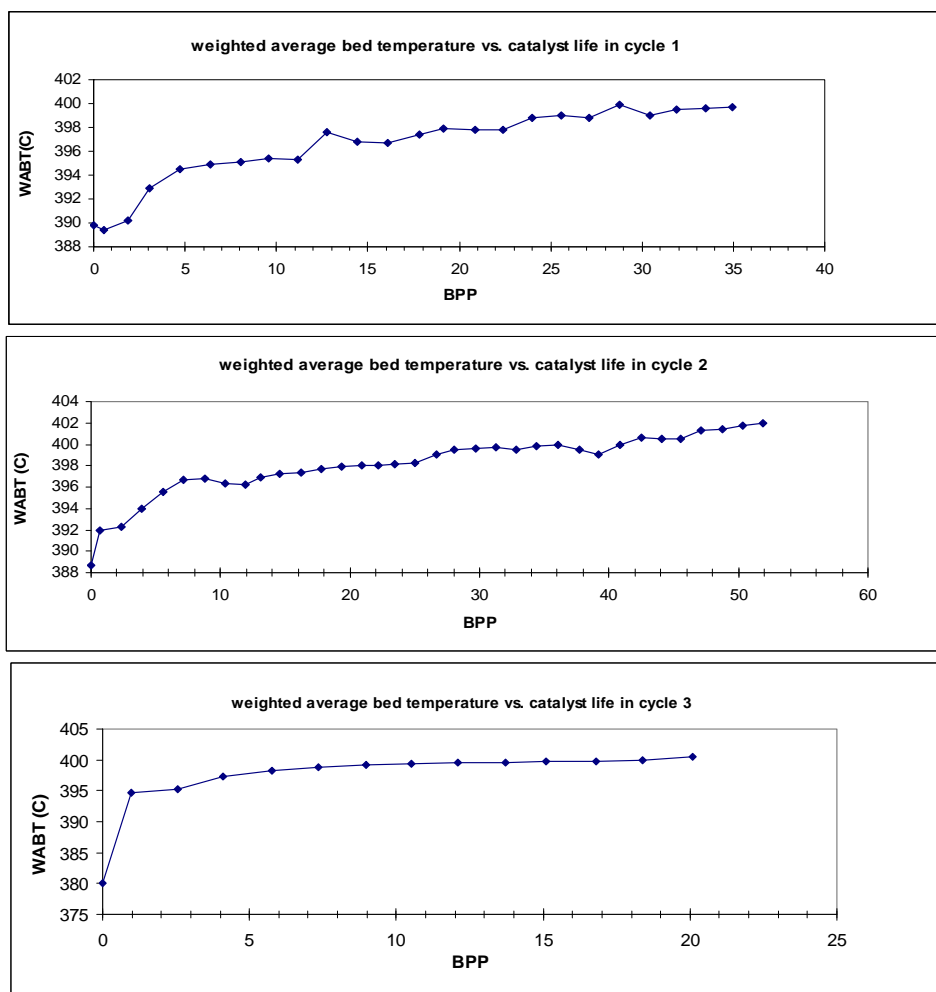


Figure 1: Weighted average bed temperature vs. normalized time

$$AARD\%(u) = \frac{100}{n} * \sum_{i=1}^n |(u_i^{\text{exp}} - u_i^{\text{ANN}}) / u_i^{\text{exp}}| \quad (8)$$

### III. RESULTS AND DISCUSSIONS

For our catalyst in the hydrocracking reactor, the WABT versus the normalized time was plotted in three cycles of catalyst operations. As evident in Fig. 1, the average bed temperature gradually increases as the catalyst is deactivated, thereby maintaining the conversion at the same level.

A study of general trends in Fig. 1 shows that changes in three cycles are constant. The following equation for defining the relation between WABT and normalized time is obtained from curve fitting:

$$T_{\text{WABT}} = a + bx + c/x^2 \quad (9)$$

where  $a$ ,  $b$ , and  $c$  are determined by curve fitting (listed in Table I) and  $x$  is the BPP. The values of  $a$ ,  $b$ , and  $c$  in Table I for all three cycles are very close to one another and indicate the accuracy of (9).

Table I: Constants of (9)

	Cycle 1	Cycle 2	Cycle 3
A	394.3487300	395.6206000	398.53994
B	0.166857500	0.120427	0.0886568
C	-16.2683080	-20.2158420	-23.60243

Several neural networks were trained using specific parts of the experimental data in these three cycles. Finally, a neural network with two hidden layers was chosen as the optimum neural network. This optimum neural network has two hidden layers with nine and six neurons, respectively. The transfer functions are tansig and logsig. The neural network structure is shown in Fig. 2.

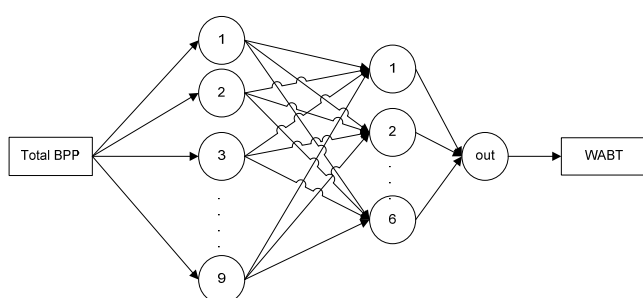


Figure 2: The schematic diagram of feed-forward Multi-layer ANN with two hidden layer.

Fig. 3 shows the deviation of ANN results against the used experimental data for these three operation cycles.

A quantitative comparison of experimental data and the neural network predictions is presented in Table II. Activity is subsequently calculated in terms of WABT based on (5). Fig. 3 depicts the comparison between experimental activity and ANN activity predictions. As evident in Fig. 4, good agreement exists between experimental and ANN model activity.

To understand the empirical relation between catalyst activity and the age of catalyst (BPP), the calculated activity from (5) was plotted versus the BPP. Fig. 5 illustrates the catalyst activity versus normalized time in the three cycles of catalyst operation.

After the end of each cycle, the catalyst activity increases by regeneration operation. At the beginning of the second cycle, the catalyst activity is about 85% of the fresh catalyst activity; at the start of the third cycle, this amount is about 69%. The trend of catalyst deactivation in these three cycles indicates that the changes in three cycles are constant while the overall function for catalyst activity and its parameters are determined from curve fitting as follows:

$$activity = a + bx + c/x^2 \quad (10)$$

where  $a$ ,  $b$ , and  $c$  are the model parameters and  $x$  is the normalized time (BPP). The parameters of (10) are summarized in Table III. Therefore, the performance of the hydrocracking catalyst can be estimated using (10), with the assumption that—except for temperature—other operation conditions affecting the catalyst activity remain constant during a cycle of catalyst operation.

Table III: Constants of (10)

	Cycle 1	Cycle 2	Cycle 3
a	0.7117811200	0.7577796700	0.76897246
b	-0.006973351	-0.0052748349	-0.00424660
c	1.0895077000	1.4325603000	1.59082020

### IV. CONCLUSION

This paper studied the catalyst activity in a hydrocracker unit by using the industrial data of three different operation cycles. It demonstrated that data normalization must be carried out in order to monitor hydrocracking operation

Table II: Deviation of ANN results and experimental data for three operation cycles.

Cycles	BPP Range	WABT Range	ANN		(9)	
			MSE	AARD%	MSE	AARD%
Cycle 1	1.89-34.96	390.2-399.7	1.76E-06	1.94E-03	1.97E-01	8.51E-02
Cycle 2	37.27-86.84	392.3-402.0	3.66E-04	3.14E-03	1.80E-01	7.75E-02
Cycle 3	89.39-106.94	395.2-400.5	3.33E-06	2.92E-04	1.84E-02	2.91E-02
Total	1.89-106.94	390.2-402.0	1.81E-04	1.66E-03	1.55E-01	7.13E-02

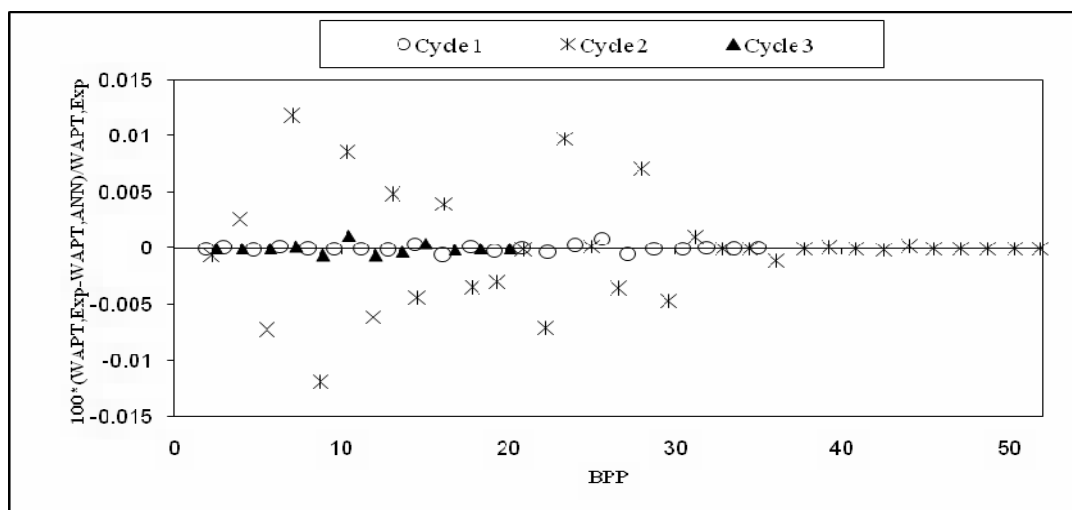


Figure 3: Percent error of ANN results against the used experimental data

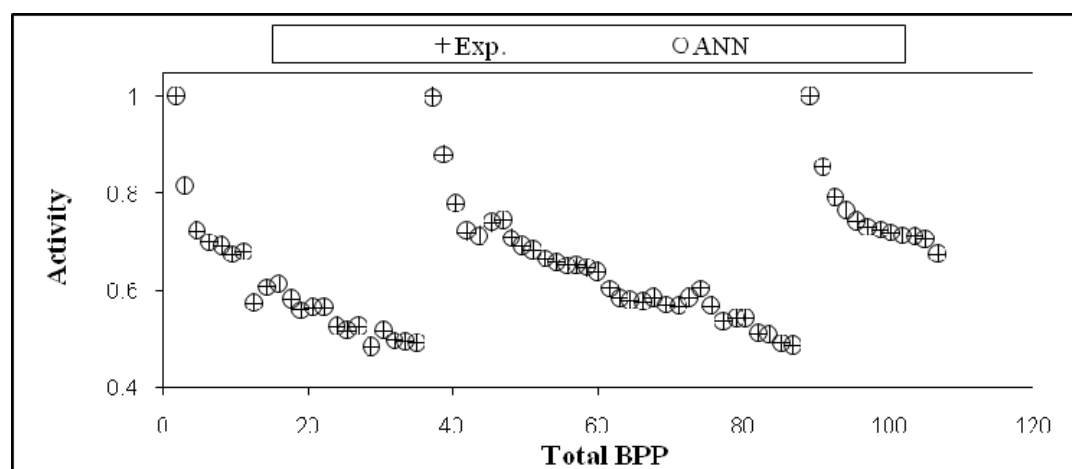


Figure 4: Comparison between the ANN activity predictions and Exp. Data

properly. To normalize the catalyst bed temperature, the WABT was used; to normalize the time of unit operation, the processed feed barrels per pound of catalyst (BPP) were used in the equations and calculations.

An ANN model was subsequently developed to predict the WABT in terms of BPP. The best ANN structure was determined by minimizing the network MSE. Finally a feed-forward back propagation ANN model with two hidden layers was chosen as the optimum neural network. Thus, BPP is the ANN model input and WABT is the output.

Two models were developed for catalyst activity: a theoretical model in terms of WABT (T) and an empirical model in terms of catalyst age (BPP). The result of theoretical catalyst activity model was compared with the ANN model predictions of activity, indicating very good agreement between ANN predictions and experimental data.

This work has clearly demonstrated the ability of ANN in calculating the weighted average bed temperature and catalyst activity based on the experimental data and theoretical model.

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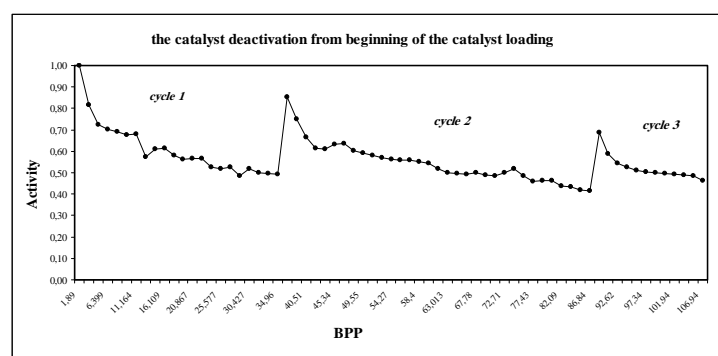


Figure 5: catalyst deactivation vs. the normalized time