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Artificial Neural Network Model for Predicting the Desulfurization Efficiency of AL-Ahdab Crude Oil

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Abstract. In this paper, an artificial neural network (ANN) model was used to model and predict the desulfurization efficiency of AL-Ahdab crude oil (AHD). This study implements the artificial neural network (ANN) in modeling and predicting sulfur removal from AL-Ahdab crude oil for a better understanding and optimizing of the process operation. This study was based on data sets collected from previous work on AHD sour crude oil (3.9 wt% sulfur content). The developed model's accuracy was assessed by the mean squared error and goodness of fit (R^2). In this study, fifteen neural network models for the desulfurization process were designed and validated. Results show that the developed model (9) is in excellent agreement with experimental data. Model (9) is the best model with the lowest mean square error (0.001), two hidden layers and 20 neurons and the value of the correlation coefficient (R^2) is 0.999.

INTRODUCTION

Due to economic development, as an energy source, the requirement for crude oil is rising steadily. The crude oil is classified as sweet (less than 0.5% sulfur content) or as sour (greater than 0.5% sulfur content). The sulfur content in crude oil depends on the geographical location of the crude oil reservoir. In addition to its adverse effects on the environment, the high content of sulfur in crude oil has a negative impact on the refining process, such as corrosion issues in pipelines and refining equipment [1]. The majority of low sulfur crude oil has led companies to improve desulfurization techniques for improving crude oil quality [2-5]. The important features of heavy crude oil include high density, high acidity, high viscosity and high sulfur [1]. Thiols (RSH), sulfides (RSR9), polysulfides (RSSR9), thiophene and alkyl-substituted thiophene compounds are found in crude oil [6]. In the next decade, the future of the industry will also not be the same, (1) The decline in conventional reserves and (2) the increase in demand for oil and gas products worldwide are the most significant explanations for this technological and methodical transition in the industry [7]. Several techniques, such as hydrodesulfurization (HDS) [8], biodesulfurization [9] (BDS), adsorption [1, 10] and oxidative desulfurization (ODS) [11, 12], have used to remove sulfur contain from crude oil [13]. To understand and optimize the operation of the process, modeling and simulation can be used. It offers an excellent theoretical framework for investigation, scaling-up, and automated control implementation [14, 15]. Several studies have reported modeling the desulfurization process using Artificial neural networks (ANN) models [14, 16-23]. Lv et

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al. in 2020 used ANN, back-propagation (BP) logarithm, to predict the desulfurization rate of flue gas by controlling the flue gas parameters [16]. Noora in 2015 investigated the desulfurization of diesel oil on activated carbon using ANN, back-propagation BP logarithm. Comparing the output of ANN modeling and the experimental data (target) showed satisfactory agreement [24]. Salari et al. in 2008 investigated the desulfurization of fuel using an artificial neural network, back-propagation (BP). Comparing the output of ANN modeling and the experimental data reveals an excellent agreement [25].

To the best of our knowledge, no study has investigated modeling and predicting crude oil desulfurization efficiency using ANN Model. Due to this lack of research, we present insight into modelling and predicting AL-Ahdab crude oil desulfurization efficiency using a back-propagation BP logarithm.

ARTIFICIAL NEURAL NETWORKS TECHNOLOGY

The neural network is described as a massively parallel distributed system composed of computational units that have a natural tendency to store and make available experiential information for usage [26]. For several chemical engineering applications, ANN has been used [27, 28]. A significant benefit of this modeling approach is that a system high accuracy mathematical model can be constructed within a reasonable period without detailed knowledge of the system's phenomena [14]. The neural nets learn to recognize the patterns of the data sets during the learning process. The data set patterns that allow the expert to do more relevant, flexible work in a changing setting are learned by neural networks themselves. While a sudden major shift will take some time for the neural network can learn, it is excellent to adapt the information to evolve continuously. The programmed systems, however, are limited by the designed scenario. Informative models are generated by neural networks, although more traditional models struggle to do so. The neural network performance is at least as high as conventional statistical modeling and much better in most cases [29]. Figure 1 illustrates a single ANN processing unit.

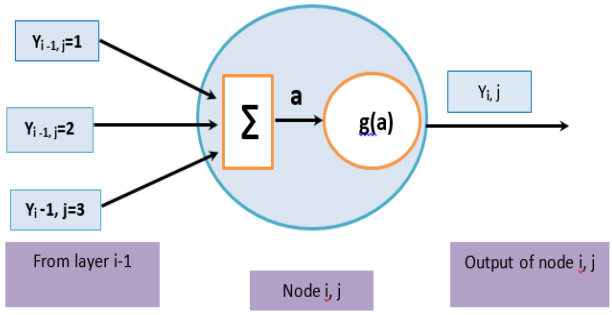

FIGURE 1. The Single Processing Node Structure with Sequence of Information Processing [30]

One or more yi data inputs may be accessed by a node from many other network nodes or from another place, such as additional data input. Each input's value is modified to wi,j (not shown in Fig.1), which is referred to as the weight coefficient and is generally referred to as the ANN coefficient. Conceptually, these weights are analogous to the synaptic force in the human brain between two connected neurons. The signal of the weighted nodes are measured, and the received data (a), called the activation, is being sent to a transfer function, (g), which can be any mathematical function, like the sigmoid function, which is usually regarded as a simple differentiable bound function [31], as present in Eq. 1 [32], if plotted in a graph, that would be as can be seen in Fig. 2:

$$f(x) = \frac{1}{1 + e^{-x}} \quad (1)$$

f : Sigmoid function (S-shaped curve) is one of the most commonly used transfer functions, x: refers to inputs.

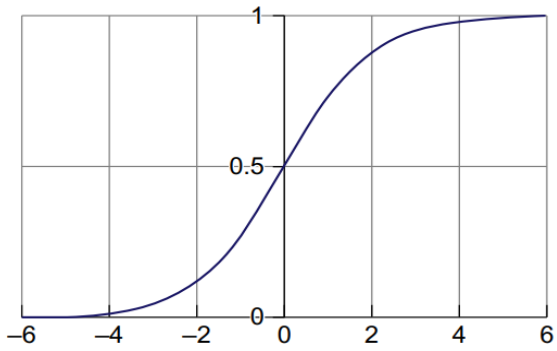

FIGURE 2. Graph of the standard logistic sigmoid function[32]

Feed-Forward Neural Network

Feed-Forward Neural Network training is mainly undertaken using the back-propagation (BP)-based learning algorithms. Feed-forward neural networks use the association between independent variables serving as network inputs and dependent variables designated as network outputs [33]. A node in the network named the input layer accepts a signal from a certain outside entity in the feed-forward form of ANNs. Hidden nodes are the network's remaining nodes due to not receiving the signal or sending information to an external entity. The hidden nodes are grouped into one or more layers. Each arc has a weight associated with it (the lines between the circles in Fig.3) [31].

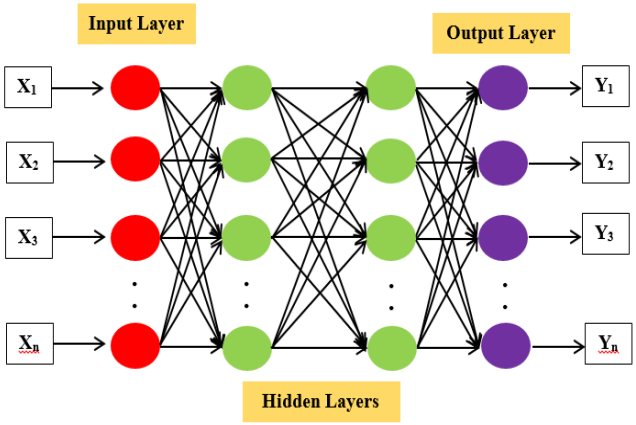

FIGURE 3. Schematic Representation of Perceptron's Two Hidden Layers [31]

ANN training

Learning or training is the process of computing the weight values and building the structure of the network, as well as an algorithm were doing this is named a “learning algorithm”. It is more than just any kind of optimization algorithm. A few simple calculations can answer once a network is trained, which is one of the advantages of using an ANN [31]. The ANN training method is explained elsewhere [30].

ARTIFICIAL NEURAL NETWORK DESIGN

The neural network design used in the present work is shown in Fig. 4; It is a three-layer neural network of data processing units consisting of feed-forward-back-propagation (nodes or neurons). The optimum number of hidden layers and the number of neurons in each hidden layer were determined by trial and error, based on the mean square error value. Hidden neurons allow the network to learn complicated tasks by gradually extracting more meaningful

characteristics from the input patterns. In the input layer of this network, four neurons are representing four process variables (mixing velocity, temperature, sorbent dose (AC) and contact time), adjustable neuron numbers (20) in a single hidden layer, and one neuron representing the residual sulfur in the output layer.

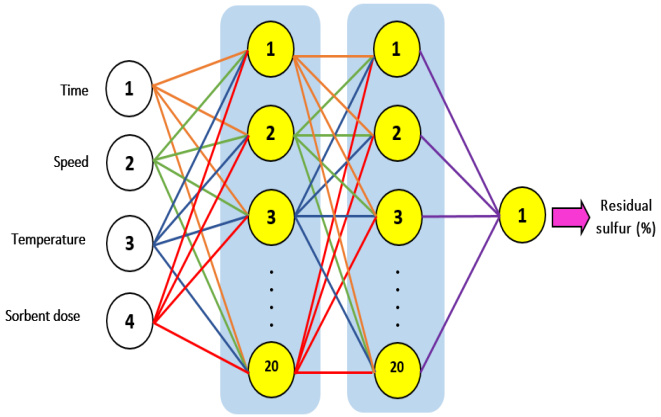

FIGURE 4. The Input and Output Layers of Operation Conditions[30].

Several transfer functions were tested with supervised training algorithms and the method of feed-forward back-propagation. Sixty per cent of input patterns were dedicated to training data sets. For the analyses, the remainder of the data was used. The learning rate is 0.75, and 0.1 momentum were adapted to the tested network, and for 1000 epochs, the network can be trained to gain the necessary output errors. Based on the highest R^2 and the lowest mean square error values, optimum topologies were specified. For the neural network training in the current study, a data set consisting of random selection data points covering the full set of the (15) experimental tests mentioned in Table 1 could be used. Some other data set containing data points that were not present in the training set is being used as a testing sample to check the network's predictive capabilities.

TABLE 1. Predicted (Output) versus ANN Structure Target Values [30]

No.	AC dose(g)	Temp. (C)	Time(min)	Speed (rpm)	%R	Training Data	
						Target	Output
1	1	60	60	500	42.56	2.24	2.2382
2	1	60	60	500	33.84	2.58	2.5714
3	0.7	60	60	400	28.71	2.78	2.7674
4	0.7	50	60	500	25.64	2.9	2.885
5	0.7	60	60	200	22.82	3.01	2.9928
6	0.7	60	60	100	19.23	3.15	3.13
7	0.7	40	60	500	18.717	3.17	3.1496
8	0.7	60	30	100	11.28	3.4	3.375
No.	**AC dose(g)**	**Temp. (C)**	**Time (min)**	**Speed (rpm)**	**%R**	**Testing Data**	
						Target	**Output**
9	0.7	60	60	300	23.84	2.97	2.9815
10	0.7	60	60	500	32.76	2.622	2.6509
11	0	60	60	500	31.53	2.67	2.6965
12	0.5	60	60	500	19.20	3.151	3.152
13	0.7	30	60	500	16.41	3.26	3.257
14	0.7	60	45	500	15.64	3.29	3.2855
15	0.7	60	15	500	6.92	3.62	3.599

DISCUSSION OF THE PERFORMANCE OF THE ANN MODEL

Table 2 compares numerous eligible neural network models for the choice of the appropriate design in this study. Model (9) is the model with the lowest mean square error (0.001), two hidden layers and 20 hidden layer neurons, according to the results in Table 2.

TABLE 2.: Various trained models for neural networks **[30]**

Parameters	Model No.								
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
No. of hidden layers	1	1	1	1	1	1	1	2	**2**
No. of neurons	5	10	12	13	25	26	36	20	**20**
R^2 (Training)	1	1	0.999	1	1	0.944	0.937	0.943	**0.999**
R^2 (Test)	0.859	0.850	0.443	0.926	0.317	0.958	0.959	0.959	**0.999**
Number of trial and error	10	100	1200	1200	1200	1200	5000	1000	**1000**
Training function	trainlm	trainlm	trainlm	trainlm	trainlm	trainrp	trainrp	trainrp	**trainrp**
Transfer Functions	tansing	hardlim	purelin	tansing	tansing	Purelin	logsig	logsig	**Logsig**
Mean Squared error	5.3	2.2	1.23	0.97	0.88	0.73	0.50	0.09	**0.001**

Figures (5, 6 and 7) [30] allow easy visual comparison between the predicted residual sulfur (S) values estimated by the ANN model and the experimental values for the treated crude oil samples. The production well tracks the goals, and the value of the R^2 is over 0.999. Consequently, the network response is sufficient in this situation.

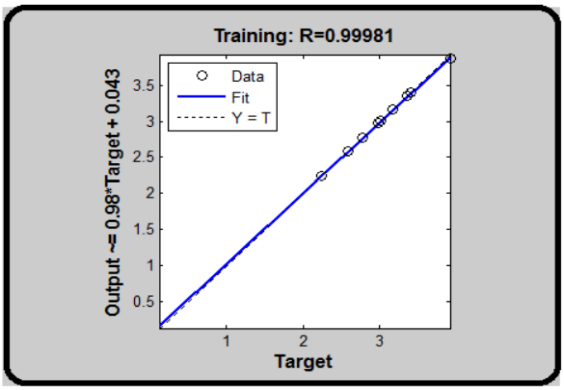

FIGURE 5. Regression Plot of Prediction Collection of Training

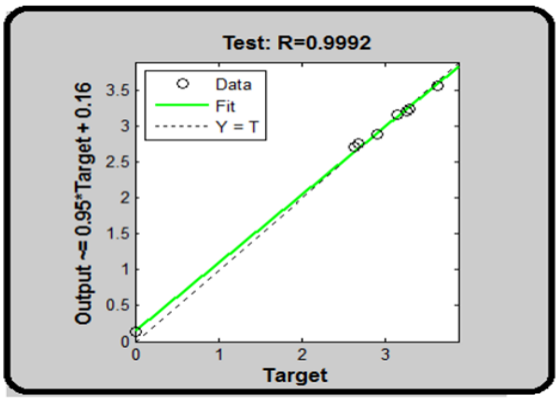

FIGURE 6. The Test Prediction Set

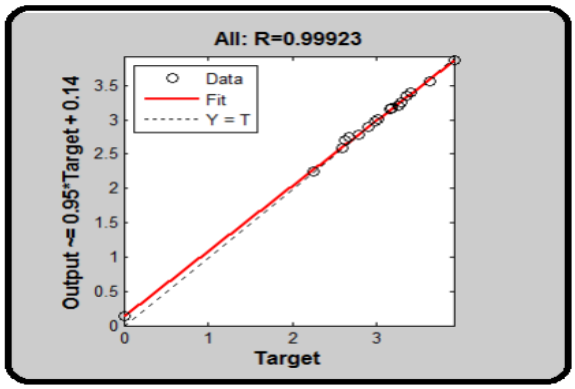

FIGURE 7. The All Prediction Set

The optimal combination of the neurons for the first and second layers that minimize the error is determined using the feed-forward back-propagation neural network, as seen in Fig.8. In Figure 8, training and test errors are presented. The outcome is rational in this design since the final mean-square error is 0.001, and it is possible to achieve lower values by including more experimental data points.

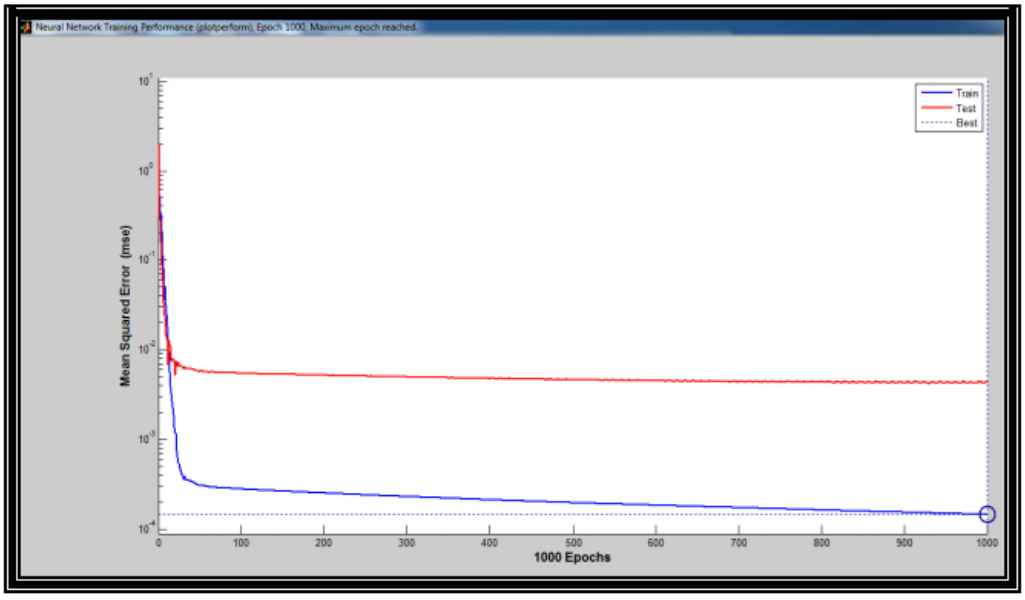

FIGURE 8. Evolution of training and test errors during ANN training as a result of the number of learning epochs[30]

COMPARATIVE STUDY

The comparison between the results obtained from this study with other studies of using an artificial neural network to model the desulfurization efficiency is shown in Table 3.

TABLE 3. Comparative study for Different Desulfurization Technique

No.	Learning algorithm	Feed type	Desulfurization technique	Input layers	Hidden layers	Output layer	R^2	Ref.
1	BP-ANN	diesel oil	Adsorptive desulfurization	5	15	1	0.9998 & 0.99658	**[24]**
2	BP-ANN	fuel oil	Oxidative desulfurization	5	8	1	0.946	**[25]**
3	BP-ANN	crude oil	Adsorption-Assisted Oxidative desulfurization	4	20	1	0.999	**This study**

* A back-propagation neural network

CONCLUSIONS

The artificial neural networks technique was used as a tool to predict the sulfur removal from AL-Ahdab crude oil. The multilayer feed forward type of ANN has been designed and validated. Three neuron layers, the input, the hidden and the output layer, were included. It was found that the predictions are in good agreement with the measured results. The mean square error and the correlation coefficient defined the trained neural networks' data predictions' validity and reliability. This shows that neural networks offer a valuable alternative to classical modeling using first principles. The predictions of desulfurization efficiency effectively model the experimental data using ANN (consisting of two hidden layers and twenty neurons in each layer). The output monitors the goals very well; Model (9) is the best model with the lowest mean square error (0.001), a back-propagation neural network (BP-ANN) with two hidden layers and 20 hidden layer neurons and the value of the correlation coefficient R^2 - is 0.999.

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