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Efficiency Prediction for Emission Reduction in Highly Sour Diesel via Oxidative Desulfurization: A Python Neural Network Approach

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Abstract

Machine learning algorithms have gained popularity recently as a method for predicting the efficiency of industrial processes. The fluctuation of desulfurization process operation conditions, especially sulfur content in diesel fuel, has an impact on the efficiency of the process. This study presents the development of an artificial neural network (ANN) model using Python to predict the efficiency of the oxidative desulfurization (ODS) process in highly sour diesel fuel. Experimental data from a trickle bed reactor were used to train and validate the model. The dataset included variables such as ODS temperature, pressure, liquid hourly space velocity (LHSV), and sulfur content in the feed. The ANN model demonstrated a high prediction accuracy with sulfur conversion results matching the experimental data with approximately 98% accuracy and a regression coefficient (R^2) of 0.99. The model effectively captured the influence of the operating conditions, showing that higher temperatures and pressures significantly enhanced the desulfurization efficiency. Additionally, the optimization of LHSV contributed to achieving optimal sulfur removal. This work highlights the potential of machine learning techniques in enhancing the predictive capabilities and efficiency of industrial desulfurization processes.

Keywords: *Oxidative desulfurization; Python; Trickle bed reactor; Diesel fuel; Sulfur conversion.*

1. Introduction

The oxidative desulfurization (ODS) of diesel fuel is an essential process for reducing sulfur emissions, which are a major environmental concern due to their contribution to acid rain and air pollution. Traditional hydrodesulfurization (HDS) methods are often inadequate for removing sulfur compounds from highly sour diesel. As such, there is a growing interest in ODS as an alternative or complementary technology, given its potential to achieve higher desulfurization efficiencies under milder operating conditions. The combustion of diesel fuel releases sulfur oxides (SOx) into the atmosphere, leading to severe environmental and health issues. Sulfur oxides contribute to the formation of fine particulate matter (PM2.5), which can penetrate deep into the lungs and bloodstream, causing respiratory and cardiovascular diseases. Additionally, SOx emissions result in acid rain, which adversely affects soil, water bodies, and vegetation. Therefore, reducing the sulfur content in diesel fuel is critical to mitigating these environmental and health impacts. Predicting the optimum operating conditions for the ODS process is crucial for maximizing sulfur removal efficiency and minimizing emissions. Accurate prediction models can help in identifying the best combination of temperature, pressure, liquid hourly space velocity (LHSV), and sulfur content in the feedstock to achieve the desired desulfurization levels. This not only enhances the efficiency of the ODS process but also ensures compliance with stringent environmental regulations. Artificial neural networks (ANNs) are empirical modeling methods that mimic the functioning of organic brain structures, capable of revealing underlying complex correlations from input-output data alone. These potent tools

have seen extensive research and application in various fields, including chemical engineering for process modeling. Despite the challenges in modeling and validating trickle bed reactors (TBR) due to their heterogeneous nature and the complexity of transport and reaction phenomena, ANNs provide a promising approach to improve predictive capabilities. Artificial neural networks (ANNs) [4], and in particular feed-forward FANNs [4], have been the subject of much research to develop process models during the past ten years, and the industry has been using them more and more frequently [5]. These networks are now being used for number prediction in applications such as exhaust gas emission modeling [6], design of eco-friendly materials [7], computation of efficiency of wastewater treatment units [8-13], heavy metals in groundwater leaching modeling [7], and chemical [14] and microbial [15] coal desulfurization modeling [16-20]. Some studies have developed homogeneous and heterogeneous models for the TBR models [21]. These models are very useful in calculating parameters, but they do not provide more information about the reaction rate kinetics. Understanding these phenomena' effects on TBR performance in terms of conversion, selectivity, and temperature profile is very significant [21]. Many program software have been presented in literature used for modeling, simulating, and optimization of the three-phase models of TBR including gPROMS [22-25], Matlab [26-28], Aspen HYSYS [29-31], Fluent [32-34], Comsol [35-36], Fortan [22,37-39], and Python [40-42]. Choosing of favorable software technique represents a significant issue because selecting solution software can be considered one of the difficult tasks in a solution of three-phase reactors. Nawaf *et al.* [43] used gPROMS programming language to predict the efficiency of ODS of light gas oil using a manganese oxide catalyst. They also used it to obtain a highly accurate kinetic model of the ODS reactions in a trickle-bed reactor. The optimal kinetic model parameters are found using an optimization method based on the reduction of the sum of squared errors between the experimental and predicted composition of the oxidation process. For a broad variety of operating circumstances, the projected product conversion demonstrated extremely excellent agreement with the actual results, with absolute average errors of less than 5%. Ramírez-Castelán [44] used Matlab programming language to simulate the behavior of an industrial hydrotreating unit under various conditions and assumptions, such as those of the linear gas velocity, the model is solved using the method of lines with a finite difference scheme for discretization in the axial direction. To find out how the system behaves as the feed's content of sulfur compounds changes, a study of dynamics is conducted. A sensitivity analysis of the most important model parameters was also carried out and high precision results were achieved. Lindfors [45] computed the demetallization (HDM) and desulphurization (HDS) conversions of heavy oils on catalysts under hydrogen pressure for a variety of temperature, pressure, and liquid hourly space velocity (LHSV) combinations using the simulation tool that is described. The code was fed with HDM, HDS, T, p, and LHSV data from at least one (test) run for the simulation pattern to work. This test data set serves as a "fingerprint" of the catalyst, oil, hydrogen, and reactor system that was employed. A procedure for estimating the catalyst's lifespan up to the point of maximal metal absorption is included in the software. Using the information on the density, volumetric flow rate, and metal content of the oil, as well as the mass of the catalyst in the reactor and the maximum amount of metal that the catalyst can absorb this computation is carried out at the simulated demetallation level. Because the software is interactive, in a question-and-answer format, the user provides the information that the computer requests. The software may be used in the following ranges: 5–15 MPa, 320–420 °C, and LHSV 0.5–3.0 h^{-1}. HDS and HDM test results should fall between 10 and 100%. Yang *et al.* [46] used Python programming language to code response surface methodology (RSM) and backpropagation artificial neural network (BP-ANN) to optimize the four critical process parameters of pressure, temperature, time, and the mass ratio of input oxygen to wastewater COD to obtain the best possible performance. The model findings and experimental data correlation coefficients show that BP-ANN outperforms RSM in both simulation and prediction. All of the parameters are significant for the resulting quadratic model, according to the analysis of variance in RSM, but their interactions are not significant. Temperature is the most important parameter, with a relative relevance of 35.61%, followed by pressure (29.74%) and time (19.53%). The connection weights technique is used to evaluate

the relative importance of these factors for process efficiency. This study aims to develop an ANN model using Python to predict the efficiency of the ODS process for highly sour diesel fuel. By leveraging experimental data from a continuous ODS process in a TBR, this work seeks to demonstrate the model's predictive accuracy and its potential to optimize desulfurization conditions. The focus will be on key operating parameters such as temperature, pressure, LHSV, and sulfur content in the feedstock, aiming to enhance the overall efficiency of the desulfurization process.

2. Experimental work

The experimental results that were used in the present study to develop the ANN models were obtained via ODS of diesel fuel with molecular oxygen over an activated carbon-based homemade catalyst. The details of the experimental work were published elsewhere [49]. The operation variables are shown in Table 1.

Table 1. Experimental variables studied in the ODS process.

Variables	Level	Value
Temperature, ℃	5	80, 90, 100, 110, 120
Pressure, bar	5	1, 3, 5, 7, 9
Liquid hourly space velocity, h^{-1}	5	1, 2, 3, 4, 5
Wt. % of sulfur content	7	0.1

In this study, Iraqi sour diesel fuel was used as a feedstock. The diesel fuel is supplied by North Refineries Company (NRC), Baiji, Iraq. The main specifications and physical properties of diesel fuel are shown in Table 2.

Table 2: The diesel fuel feedstock specifications

Specifications	Value
Density @ 15.0℃	828
Flashpoint, ℃	70
Pour point, ℃	-15
Viscosity @400 ℃/cSt	2.2
API	39.4
Physical form	Liquid
Color	0.5
Doctor test	-ve
Sulfur concentration, wt%	0.7361
Salt content, mg/L	10

3. Methodology of prediction of ODS efficiency

3.1 Data preprocessing

The dataset contains three categories of data based on the effects of Temperature, Pressure, and LHSV and there are five columns such as LSHV, P, T, S %wt, and sulfur conversion. The sulfur conversion is the target column that is going to be predicted from the ANN Model. First of all, all of the data have to be compiled from the raw dataset and make a CSV file to feed into the ANN Model. All the raw data was preprocessed and placed in the 'TBR_Combined.csv' file, which is attached as a supporting file S1. All the data in TBR_Combined.csv were used to train and evaluate the ANN Model performance. There were 368 rows in the dataset, 80% of them were used for training and 20% were used for evaluation tasks. More clearly, all the LSHV, P, T, and S %wt data were placed in the CSV file to feed into the model

and they predicted the sulfur conversion percentage. Then, another CSV file was used to predict the sulfur conversion percentage from the raw data. The file was 'raw_data_for_prediction.csv' where all the raw data were stored. To check how accurately the model can perform, 7 values were separated from the original dataset to feed into the model and later matched with the experimental results.

3.2. Import necessary modules

The necessary modules were imported from some Python Libraries; Numpy and Pandas facilitate analysis and manipulation of the data, and Matplotlib and Seaborn for data visualization to find any anomaly in the dataset. Additionally, some other Python Libraries were needed to build the present ANN model, in that case, Tensorflow, Keras, and Scikit-Learn were utilized.

3.3. Read the dataset

The complete dataset was read and loaded with Python. A CSV format file was used to make Pandas read and load the dataset. Five columns and 368 rows were created. The ANN model was trained with these data and after that, the trained model predicted the sulfur conversion percentage.

3.4. Split the dataset into train and test sections

The dataset was split for processing. The sulfur conversion column was kept in the 'Y' variable and the rest of the data in the 'X' variable. This is because the sulfur conversion column is the target column that the present ANN Model is going to predict. Scikit-Learn was used to split again our dataset into the Train and Test section. We have 368 rows and will take 20 % that is 368 * 0.2 = 73 Rows for our Testing purpose. More clearly, 80% of the total data was used to train the present ANN model, and the remaining 20% of the data will be used to evaluate the model's performance.

3.5. Normalization

The train and twist data were trained, for this MinMaxScaler function was used from Scikit-Learn. Fit and Transform functions were used to scale the train.

3.6. Building of ANN model

Up to this stage, the dataset has been preprocessed to feed into the ANN Model. Now Tensorflow and Keras were used to build the ANN model. Here, 5 layers with 5 Neurons along with Activation, Optimizer, and Loss functions were created to facilitate the evaluation of the ANN model performance. Figure 1 shows the ANN model layers and neurons.

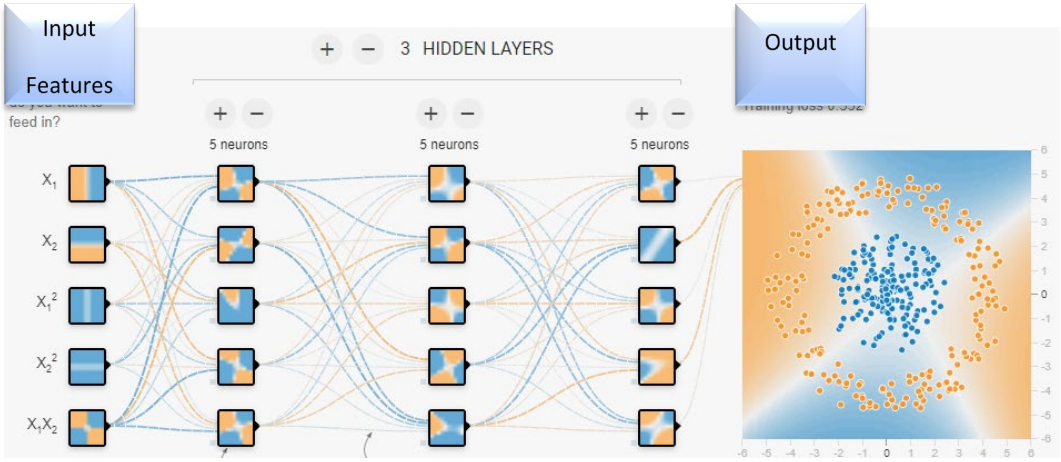

Figure 1. The ANN model layers and neurons.

In machine learning and deep learning analysis, the most used activations are step function, sigmoid function, hyperbolic tangent, and Rectified Linear Unit (ReLU). The activation function is chosen based on the problem. In the present work that is based on a regression process, ReLU was used as it provides better performance compared to others. ReLU works on the principle of:

$$f(x) = \max(0,z) \quad (1)$$

It means if the output is negative, it is considered as 0, if the output is greater than zero then go ahead and process the output. Also, it was used as an activation function popular because it's simple and fast, and its ability to introduce non-linearity into neural networks enables them to learn complex patterns and relationships in data, making it an essential tool in various applications [47]. The Rectified Linear Unit is the most commonly used activation function in deep learning models [48]. The function returns 0 if it receives any negative input, but for any positive value x, it returns that value.

Surprisingly, such a simple function (and one composed of two linear pieces) can allow a model to account for non-linearities and interactions so well. However, the ReLU function works great in most applications, and as a result, it is very widely used in diverse engineering applications [49]. Activation functions serve two primary purposes;

1) Help a model account for interaction effects: The interactive effect is when one variable such as A affects a prediction differently depending on the value of another variable such as B. For example, if my model wanted to know whether a certain body weight indicated an increased risk of diabetes, it would have to know an individual's height. Some body weight indicates elevated risks for short people while indicating good health for tall people. So, the effect of body weight on diabetes risk depends on height, and we would say that weight and height have an interaction effect.

2) Help a model account for non-linear effects: This just means that if I graph a variable on the horizontal axis, and my predictions on the vertical axis, it isn't a straight line. Or said another way, the effect of increasing the predictor by one is different at different values of that predictor.

The ReLU captures interactions and non-linearities via the following mechanism; for a single node in a neural network model. For simplicity, assume it has two inputs, called A and B. The weights from A and B into our node are 2 and 3 respectively. So the node output is f(2A + 3B). We'll use the ReLU function for our f. So, if 2A + 3B is positive, the output value of our node is also 2A + 3B. If 2A + 3B is negative, the output value of our node is 0. For concreteness, consider a case where A=1 and B=1. The output is 2A + 3B, and if A increases, then the output increases too. On the other hand, if B=-100 then the output is 0, and if A increases moderately, the output remains 0. So, A might increase our output, or it might not. It just depends on what the value of B is. This is a simple case where the node captured an interaction. If more nodes and more layers were added, the potential complexity of interactions only increases. However, it is required to see how the activation function helped capture an interaction. For non-linearities; a function is non-linear if the slope isn't constant. So, the ReLU function is non-linear around 0, but the slope is always either 0 (for negative values) or 1 (for positive values). That's a very limited type of non-linearity. However, two facts about deep learning models allow us to create many different types of non-linearities from how we combine ReLU nodes. First, most models include a bias term for each node. The bias term is just a constant number that is determined during model training. For simplicity, consider a node with a single input called A, and a bias. If the bias term takes a value of 7, then the node output is f(7+A). In this case, if A is less than -7, the output is 0 and the slope is 0. If A is greater than -7, then the node's output is 7+A, and the slope is 1. So the bias term allows us to move where the slope changes. So far, it still appears we can have only two different slopes. However, real models have many nodes. Each node (even within a single layer) can have a different value for its bias, so each node can change the slope at different values for our input. When we add the resulting functions back up, we get a combined function that

changes slopes in many places. These models have the flexibility to produce non-linear functions and account for interactions well (if that will give better predictions). As more nodes in each layer (or more convolutions if we are using a convolutional model) were added, the model gets even greater ability to represent these interactions and non-linearities.

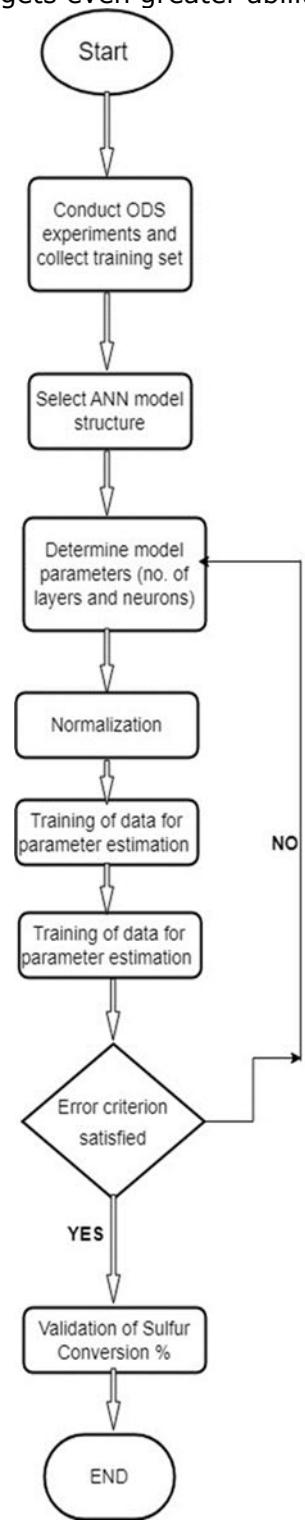

Figure 2. Algorithm of developing and validation of the ANN model by Python.

3.7. Training of the model

The crucial part here is to set batch size and number of epochs. Batch size means how much data we allow the model to train at a time. The performance of the present ANN model can be checked by changing the parameters. Of course, it is required to make sure to use the Graphics Processing Unit (GPU) to make faster training.

3.8. Loss function

Below plot the true loss and validation loss. The good thing is it doesn't fluctuate much. If the deviation is more then we should rebuild the model until the result is good.

3.9. Prediction

For the prediction of sulfur conversion percentage and optimization of the operations conditions to drive the conversion to a higher value, 20% of the dataset that was left untrained was used to predict the sulfur conversion percentage from the developed and well-trained ANN model. Also, the accuracy of the model can be predicted in terms of regression coefficient (R^2). Also, another metric used to evaluate the model performance is Mean Absolute Error (MAE). Figure 2 shows the algorithm of the model developing, running, and validation.

For reusing the Python ANN model, all new data ('LSHV', 'P', 'T', and 'Wt') in the CSV file S3 can be added and the Google Colab with GPU can be run to obtain the predicted sulfur conversion percentage.

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4. Results and discussion

Statistical insights of the dataset present a brief but informative overview of the data using mean, standard deviation, minimum, maximum, and percentile as shown in Table 3.

Table 3. Statistical insights of the dataset.

	LHSV, h^{-1}	Pressure, atm	Temperature, °C	Wt.% sulfur	Sulfur conversion, %
Mean	2.991	4.3	99.7	0.2958	59.8
STD	1.415	2.6	14.1	0.0966	13.1
min	1.0	1.0	80.0	0.0737	40.0
25%	2.0	2.0	90.0	0.213	48.0
50%	3.0	4.0	100.0	0.294	60.0
75%	4.0	7.0	110.0	0.382	71.0
Max	5.0	9.0	120.0	0.441	90.0

Successfully identifying outliers, correlation, grouping, and clustering the data always play a pivotal role. If data points belong to different groups or clusters, scatterplots can reveal these groupings. Different colors or shapes can be used to distinguish between groups, making it easy to identify patterns within each subgroup. Figure 3 shows the clustering and grouping of the data.

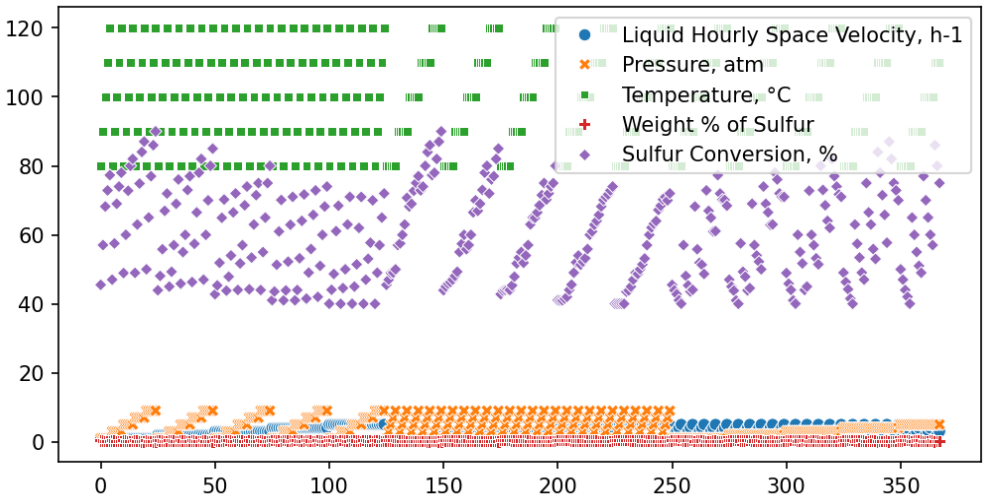

Figure 3. Clustering and grouping the data.

A clear and defined correlation among temperature, pressure, weight of sulfur, liquid hourly space velocity(LHSV), and sulfur conversion paves a greater path to the next level of analysis. Figures range between (4 to 7) draw the actual picture indicating the effect of each operation variable on the sulfur conversion rate.

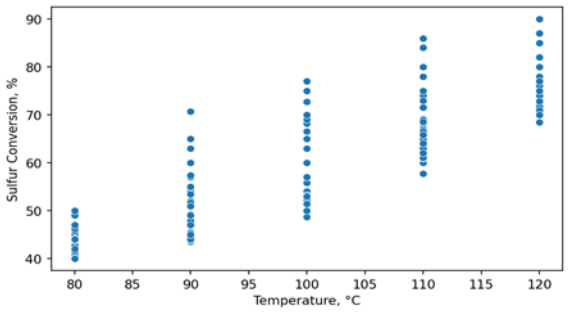

Figure 4. Effects of temperature on sulfur conversion.

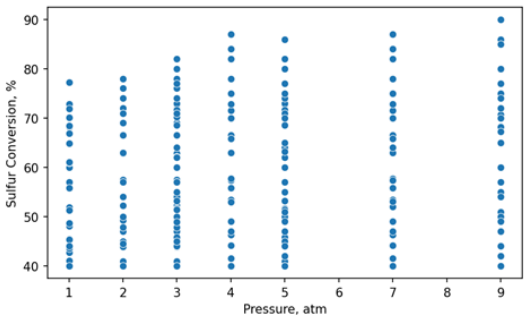

Figure 5. Effects of pressure on sulfur conversion.

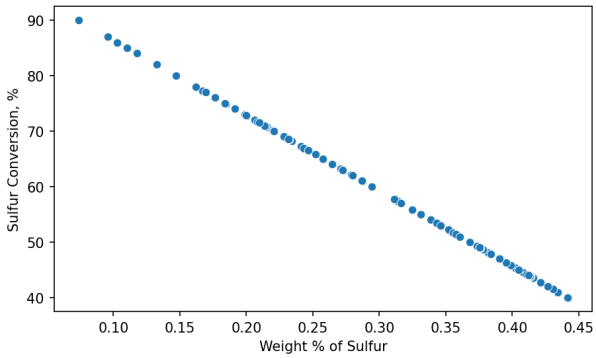

Figure 6. Effects of the weight of sulfur content in diesel fuel on sulfur conversion.

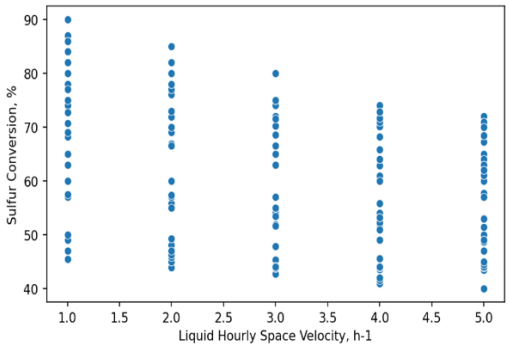

Figure 7. Effects of liquid hourly space velocity on sulfur conversion.

The heatmap is extremely useful for visually assessing the strength and direction of the relationship between two variables (Figure 8). A positive correlation implies that as one variable increases, the other also tends to increase, while a negative correlation suggests an inverse relationship.

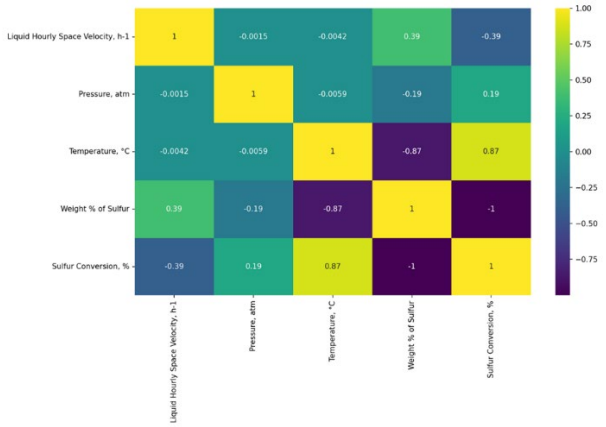

Figure 8. Heatmap provides the correlation score using color combination.

The bar chart shown in Figure 9 provides a visual representation of how temperature, pressure, weight of sulfur and Liquid hourly space velocity(LHSV) positively and negatively affect the sulfur conversion rate and this result is in line with previously published works [50,51].

A distribution plot is frequently used to visualize the distribution of a single variable as shown in Figure 10. It can show the frequency or probability distribution of values, providing insights into the central tendency and spread of the data. It can be used to visually assess normality or test distributional assumptions. This is particularly useful in statistical analyses where assumptions about the underlying distribution are important. It also allows users to overlay multiple distributions in a single plot, making it easy to compare distributions across different groups or conditions.

Grouping data helps visualize how well data is separated based on the values of two or more continuous features. This aids in understanding the discriminative power of the chosen variables. When analyzing the importance of features in a machine learning model, a scatterplot with hue can illustrate how the importance of two features varies across different categories. It helps visualize trends or patterns in the relationship between two variables within different subgroups, providing insights into potential interactions. Figure 11 shows this trend. Figure 12. Line plots of the training and validation loss of the dataset for 400 epochs.

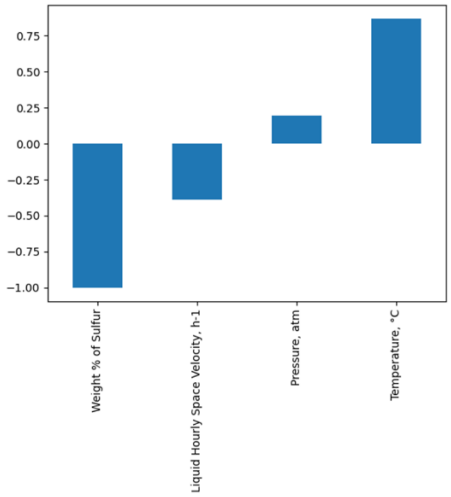

Figure 9. Correlation of the ODS reaction parameters.

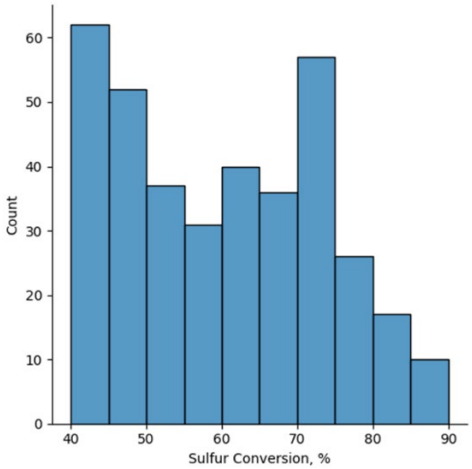

Figure 10. Distribution of sulfur conversion processing in the ANN model.

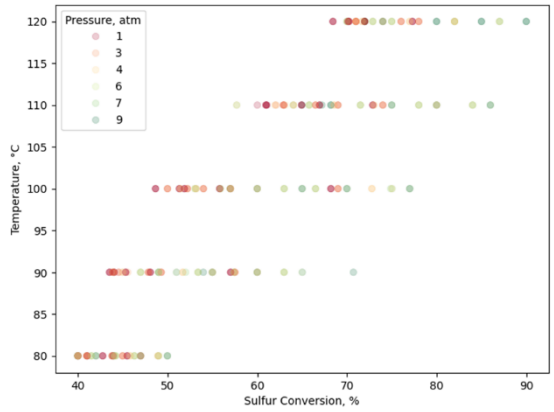

Figure 11. Visualizing trends of temperature vs. sulfur conversion across subgroups of ODS pressure.

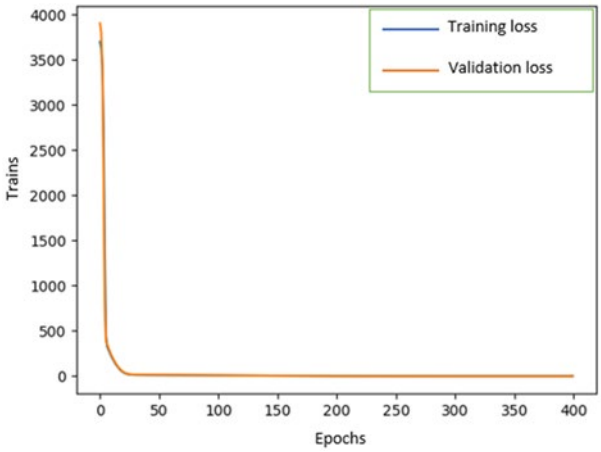

Figure 12 shows the training and validation of the loss function of the ANN model.

Here red line represents the predicted results from our ANN model and the blue dots represent the experimental results and they were trained for 400 epochs. It can be seen that both data results are pretty close. That means the model developed predicts nearly experimental results. Figure 13 shows the parity chart between experimental and ANN-predicted data obtained in the present work. Thus, it can be considered that the Python ANN model can predict sulfur conversion with around 98% accuracy and it can be seen that the outstanding matching between the trained and validated regression coefficient (R^2) is 0.999.

The optimum operating conditions for the highest possible sulfur conversion percentage can be obtained by running the ANN model on the Google Colab website with GPU with a target objective function of sulfur conversion percentage approaches 100%. The predicted optimum operating conditions and the sulfur conversion percentage are shown in Table 4.

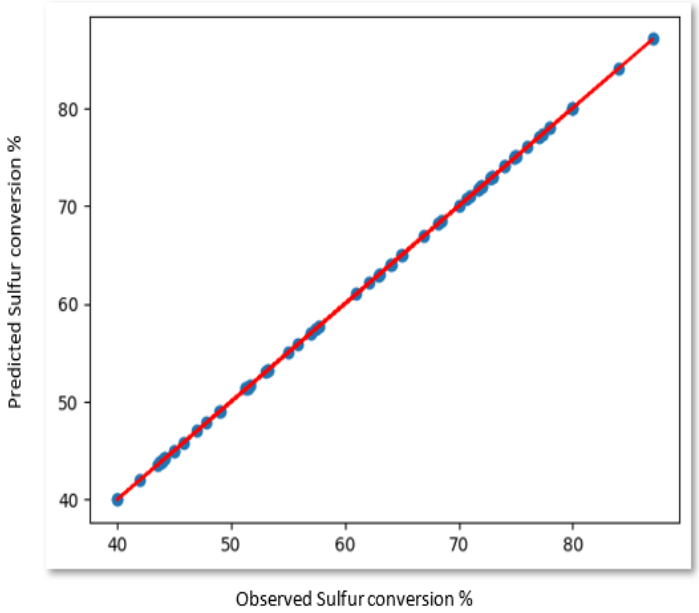

Figure 13. Prediction vs experimental sulfur conversion in trickle bed reactor.

Table 4. Results of experimental ODS of sour diesel fuel by AC-based catalyst in TBR at different operation conditions.

LSHV, h^{-1}	Pressure, atm	Temperature, °C	Sulfur compounds, %wt.	Sulfur conversion, %
4	5	110	0.234	68.210
5	5	110	0.257	65.000
1	5	120	0.076	97.851
2	5	120	0.1103	85.022
3	5	120	0.147	80.037
4	5	120	0.191	74.017
5	5	120	0.206	72.006

Here, it can be found that the MSE is 1.5 % which is an outstanding precision of prediction. The highest sulfur conversion percentage obtained in the present study using the Python ANN model was 97.851 in the ODS process of the highly sour diesel fuel processed in the trickle bed reactor. The optimum operating conditions to achieve that conversion were; liquid hourly space velocity= 1 h^{-1}, temperature=120°C, pressure= 5 atm, and sulfur content Wt.%= 0.076.

5. Conclusions

The application of Python programming language in developing an artificial neural network (ANN) model for predicting sulfur conversion in the oxidative desulfurization (ODS) process demonstrated significant potential. The model, developed with ReLU function and trained using experimental data, effectively simulated the optimization process. During testing, the ANN model estimated sulfur conversion with a high degree of accuracy, achieving a correlation coefficient (R^2) of 0.99 and a mean square error of 1.5%. This study highlights the novel use of ANN in the ODS of sour diesel fuel, providing a robust tool to assess the relationships between process parameters and predict sulfur removal. The model and related data can be confidently employed as an expert system in ODS trickle bed reactors, minimizing the need for complex and time-consuming laboratory tests.

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