Journal of Petroleum Research and Studies

journal homepage: https://jprs.gov.iq/index.php/jprs/

Print ISSN 2220-5381, Online ISSN 2710-1096

AI-Driven Modeling of Catalytic Pyrolysis for Sustainable Fuel Production: A Neural Network Approach

Idres M. Khder[1], Saba A. Gheni[1*], Zainab F. Hassan[2], Marwan I. Hamd[3], Nalan Turkoz Karakullukcu[4], Ataallah K. Tahah[5]

[1]Chemical Engineering Department, College of Engineering, Tikrit University, Iraq.
[2]Petroleum Research and Development Center, Ministry of Oil, Baghdad, Iraq.
[3]North Oil Company, Ministry of Oil, Iraq
[4]Advanced Technology Research and Application Center, Ondokuz Mayis University, Samson, Turkey
[5]North Refineries Company (NRC), Baiji, Salahuldeen, Ministry of Oil, Iraq.
[*]Corresponding Author E-mail: ghenis@tu.edu.iq

Article Info

Received 06/03/2025
Revised 07/05/2025
Accepted 13/05/2025
Published 21/12/2025

DOI:
http://doi.org/10.52716/jprs.v15i4.1090

Abstract

The growing demand for solutions to plastic waste and sustainable fuel options around the world has inspired research into catalytic pyrolysis as a potential method to convert waste plastic into profitable biofuels. The intensity of pyrolysis processes affected by many process factors makes traditional modeling methods difficult. This research uses artificial nervous network (ANNS) to create a prediction model aimed at increasing biofuel conversion in catalyst pyrolysis. The range of variables considered in the study, including temperature, residence time, catalyst type, conversion, density, particular gravity, API, viscosity, and higher heating value were used to train the ANN model, giving accurate predictions of biofuels production under various conditions. The Levenberg-Marquard method was employed for network training, guaranteed better accuracy and low error. The comparative comparison of traditional modeling functioning and AI-operated approaches reflect the advantage of the artificial nervous network (ANN) model in real-time managing non-linear interactions and optimizing processes. Conclusions suggest that the AI-operated approaches clearly promote process efficiency, reduce waste, and improve decision making in industrial contexts.in this study a perfect match was achieved between the predicted data and experimental data, with R2 value of 1, indicating a perfect alignment between the predictions and experimental results. This research highlights the ability of artificial intelligence to increase permanent chemical engineering functioning and improve biofuel production from waste plastic.

Keywords: Catalytic pyrolysis, Waste Plastics, artificial intelligence, Green fuel.

النمذجة المعتمدة على الذكاء الاصطناعي للتحلل الحراري التحفيزي لإنتاج وقود مستدام: منهجية الشبكات العصبية

الخلاصة:

ألهم الطلب على معضلة النفايات البلاستيكية وخيارات الوقود الدائم في جميع أنحاء العالم البحث في التحلل الحراري التحفيزي كطريقة محتملة لتحويل النفايات البلاستيكية إلى وقود حيوي مربح. إن شدة عمليات التحلل الحراري المتأثرة بالعديد من عوامل العملية تجعل طرق النمذجة التقليدية صعبة. يستخدم هذا البحث الشبكة العصبية الاصطناعية (ANNS) لإنشاء نموذج تنبؤ يهدف إلى زيادة تحويل الوقود الحيوي في التحلل الحراري للمحفز. تم استخدام مجموعة بيانات تحتوي على درجة الحرارة ومدة الإقامة ونوع المحفز لتدريب نموذج الشبكة العصبية الاصطناعية (ANNS)، مما يعطي تنبؤات دقيقة لإنتاج الوقود الحيوي في ظل ظروف مختلفة. تم استخدام طريقة Levenberg-Marquard لتدريب الشبكة، مما يضمن دقة أفضل وخطأ منخفض. تعكس المقارنة المقارنة بين أداء النمذجة التقليدية والأساليب التي تعمل بالذكاء الاصطناعي ميزة نموذج الشبكة العصبية الاصطناعية (ANN) في إدارة التفاعلات غير الخطية في الوقت الفعلي وتحسين العمليات. تشير الاستنتاجات إلى أن الأساليب التي تعمل بالذكاء الاصطناعي تعزز بوضوح كفاءة العملية وتقلل من النفايات وتحسن عملية اتخاذ القرار في السياقات الصناعية. يسلط هذا البحث الضوء على قدرة الذكاء الاصطناعي على زيادة الأداء الدائم للهندسة الكيميائية وتحسين إنتاج الوقود الحيوي من نفايات البلاستيك إلى نفايات البلاستيك.

1. Introduction

Artificial Neural Networks (ANNs) are computational models inspired by the human brain's structure. They consist of layers of synthetic neurons that analyze complex datasets for tasks like categorization and pattern recognition. ANNs adjust neuron weights via backpropagation, optimizing predictions by reducing discrepancies between expected and actual values. ANNs have revolutionized industries by enabling automation, predictive analytics, and optimization particularly in healthcare, finance, and engineering, where they improve efficiency, accuracy, and problem-solving skills[1] .

AI has grown to be a crucial tool in the advancement of contemporary era, revolutionizing industries by means of permitting wise automation, predictive analytics, and optimization. AI-pushed methodologies have revolutionized fields including healthcare finance and engineering. In engineering AI-powered gear enhance efficiency, accuracy and problem-fixing abilities[2].

These include structural and civil engineering where AI is primarily used to assess structural health monitoring Mechanical engineering has benefited from AI-based predictive maintenance strategies that detect faults in machinery and electrical systems before failures occur, reducing downtime and maintenance costs[3]. In aerospace and automotive engineering AI improves aerodynamic design optimization, enhances fuel efficiency and ensures safety in autonomous vehicles[4]. In biomedical engineering deep learning models can support medical diagnostics drug discovery and personalized healthcare solutions[5].

The role of synthetic neural networks in chemical engineering has been transformative in modeling and optimizing complicated procedures enhancing performance and lowering expenses. ANNs were extensively used to model nonlinear and complex chemical processes in which traditional mathematical modeling processes battle[6]. Their utilization has been hired to decorate the efficacy of catalysts and optimize distillation columns. Research has illustrated the effectiveness of artificial neural networks within the development of response kinetic fashions. Engineers can forecast conversion prices and efficiency with a high diploma of accuracy by means of employing sophisticated strategies. AI-primarily based controllers in method manipulate have exhibited superior overall performance in evaluation to conventional Proportional-Integral-Derivative (PID) controllers. Particularly, in dynamic structures together with multiphase drift reactors and heat exchangers[7, 8]. In the face of fluctuating operating situations, AI-driven control structures autonomously regulate procedure parameters in real time to make certain balance and efficiency.

Advanced artificial intelligence has greatly contributed to predictive renovation techniques in chemical flora via the usage of sensor statistics styles to locate anomalies in pumps, compressors, and heat exchanger cars. AI can predict future apparatus malfunctions previous to their prevalence with the aid of analyzing ancient statistics, thereby decreasing unnecessary delay and improving safety. The layout of catalysts and the prediction in their efficacy are essential packages of AI in the field of chemical engineering. The pastime and stability of catalysts in heterogeneous catalysis approaches, along with hydrocracking and catalytic pyrolysis, were predicted the usage of AI-driven fashions. The identity of imaginative catalyst compositions that enhance the efficiency of biodiesel manufacturing and plastic waste conversion has been extended with the aid of AI-incorporated methodologies that appoint Density Functional Theory (DFT) simulations[9].

By optimizing water remedy strategies, forecasting pollutants dispersion, and improving carbon dioxide seize systems, artificial intelligence has considerably advanced sustainable chemical engineering. The oxidative desulfurization strategies for diesel gasoline have been progressed by using AI-driven models, which has brought about a big discount in Sulphur emissions[10]. By predicting flammability thresholds, explosive risks, and noxious gasoline dispersion styles in industrial settings, synthetic intelligence has more advantageous the safety protocols and chance assessment of chemical centers. These AI-driven methodologies make sure compliance with protection regulations and enhance emergency preparedness[11].

The application of artificial neural networks (ANNs) and AI-driven techniques has significantly advanced process optimization in chemical engineering, improving efficiency, sustainability, and control automation. AI technologies are enabling chemical engineers to create more efficient and environmentally sustainable processes, improving safety in industrial practices. Compared to traditional methods, AI and machine learning models offer distinct advantages in simulating complex processes like the pyrolysis of mixed plastic waste. This research plays a crucial role in real-world applications by optimizing biofuel production from plastic waste and providing a scalable approach for industrial implementation. The primary reasons for this are as follows:

1. The process of converting plastic into diesel using a hydrothermal reactor improves energy efficiency by dynamically adjusting variables such as time and temperature, which reduces energy consumption and increases yield. In contrast, traditional conversion processes operate under fixed conditions, leading to higher energy consumption and lower efficiency. Therefore, optimizing the conversion process with a hydrothermal reactor by controlling temperature and time provides greater energy efficiency and cost savings compared to conventional methods.
2. Without the necessity of detailed reaction mechanisms, AI can assess not linear relations between variables including feedstock structure, heat, residency time frame, catalysis kind, as well as distribution of the product.
3. Polyethylene (PE), polypropylene (PP), polystyrene (PS), PET, PVC, and numerous other polymers exhibit distinct breakdown routes, rendering mixed plastic garbage intrinsically heterogeneous.
4. Traditional models are less adaptable to real-world fluctuations due to the necessity of making numerous assumptions about feed composition and response rates.
5. The predictions of AI-pushed fashions can be more dependable as they're educated on experimental information and autonomously adjust to varying feed compositions.
6. In order to resolve mass and energy balances, conventional modelling relies on straightforward assumptions and correlations, which occasionally fail to account for minor yet significant components.
7. The accuracy and adaptability of forecasts can be improved by the simultaneous optimization of various parameters and the management of high-dimensional information by Artificial Intelligence.
8. In particular, this is advantageous for predicting the conversions of pyrolysis products (solid,

liquid, and gas), reaction efficiency, and energy requirements.

9. Comprehensive kinetic models and extensive experimental calibration are required in traditional modelling to determine rate constants, activation energies, and heat transfer coefficients.
10. AI algorithms, especially neural networks, may learn directly from experimental data and discern concealed patterns in intricate datasets. This facilitates swifter and more precise predictions without the necessity of deriving complex differential equations.
11. AI models can forecast system behavior in real-time, allowing dynamic process optimization to enhance efficiency, product conversion, and energy conservation.
12. Conventional material and energy balancing methodologies need repetitive hand recalculations, rendering them computationally intensive and time-consuming.
13. AI-driven control systems may autonomously modify response conditions according to real-time sensor data, therefore reducing energy waste and enhancing product quality.
14. In actual pyrolysis operations, sensor readings and experimental data exhibit intrinsic noise resulting from measurement inaccuracies, ambient fluctuations, and feedstock variability. AI models exhibit resilience to noisy and partial data, but traditional models falter with absent or inaccurate inputs. This enhances the reliability of AI for practical applications in industrial environments.
15. AI models may be trained on laboratory-scale experimental data and subsequently scaled to pilot and industrial levels with great precision.
16. Significant parameter modifications and recalibrations can be essential whilst transitioning from laboratory to commercial scale for conventional models.

Through the mixing of AI with pyrolysis modelling, this research objective to enhance method efficiency, refine biofuel manufacturing forecasts, and offer a scalable methodology for business programs. These further studies should adopt more advanced AI options, such as deep learning and reinforcement learning, to maximize the optimization of the process for AI chemical engineering the drive for renewable energy sources Advanced renewable energy sources further drive.

2. Methodology

2.1. Data Preprocessing

Preprocessing, an important segment in statistics analysis, facts mining, and system mastering,

involved the conversion of raw information into a format that become suitable for computational duties. The motive of this technique was to cope with inappropriate or disorganized records, remove redundancies, and rectify inconsistencies. It worried multiple tiers. Data acquisition discrepancies, such as inaccuracies from digital sensors or manual recording mistakes, are often the source of such mistakes. These mistakes may also lead to erroneous conclusions and unreliable outcomes all through the evaluation if improperly addressed. As a result, good sized attempt changed into dedicated to the improvement of preprocessing strategies if you want to improve the reliability and accuracy of subsequent computational models[12].

Temperature, time, and catalyst kind had been the 3 primary classifications into which the dataset changed into meticulously organized. Each of these additives performs an essential function within the conversion of biofuels. There were 4 columns inside the dataset: Temperature, Time, Catalyst Type, and Biofuel Conversion. One of the primary goals of the Artificial Neural Networks (ANN) model became to predict the conversion of biofuels the usage of the initial three parameters. The unprocessed facts become structured into a. **Xlsx** report throughout the initial phase of dataset education, which become vital for enter into the ANN model. The green management of good-sized datasets and the seamless interplay with device mastering algorithms have been facilitated by the effective framework provided by way of MATLAB for preparatory sports[12].

For education and evaluation functions, the dataset, which contains 32 rows, was divided into two companies. 30% of the records was allotted for evaluation and testing, whilst 70% changed into distinct for training [13]. Through this division, the model was confident to come upon a numerous array of occasions, thereby enhancing its generalization abilities. The unbiased variables within the enter. **Xlsx** document have been the columns for Catalyst Type, Time, and Temperature. An equitable distribution of facts among the schooling and trying out businesses turned into ensured by using the sturdy statistics manipulation abilities of MATLAB, which facilitated this division.

Biofuel conversion changed into the objective variable, as anticipated with the aid of the ANN version in MATLAB. The number one input records become retained within the data_prediction. Csv file. Later, this document changed into utilized to expect the conversion of biofuels in the MATLAB ANN framework[14]. An overall of seven facts factors are excluded from the schooling dataset for you to compare the model's accuracy and resilience. The actual experimental findings are explicitly contrasted to the model's anticipated outputs the usage of these absent values as

benchmarks. This validation level ensures the ANN model's dependability and applicability in real-international scenarios.

In this study, an ANN model was used with MATLAB to predict and optimize the catalytic pyrolysis process of plastic waste. Compared to previous studies that used dataset ranging from 16 to 40 data points, this study utilized an dataset containing 32*7 experimental data points, enhancing the model's accuracy and its ability to adapt to various variables[15, 16]. The main innovation in the methodology lies in optimizing operational parameters such as temperature and residence time using AI-driven modeling techniques. These parameters are dynamically adjusted using AI, rather than using fixed values as in many previous studies, contributing to improved prediction accuracy and increased production efficiency.

2.2. Data entering

By enabling instant get admission to to the facts contained inside the Excel sheets for each catalyst, the readtable feature facilitated the importation of records from Excel files into MATLAB. As a end result of this system, the variables have been without difficulty handy and manipulable, as the Excel facts turned into converted to MATLAB tables[17]. Each column of the facts changed into dependent to make certain its integrity for destiny processing, with every column representing specific bodily and chemical parameters, such as temperature, time, conversion, density, particular gravity, API, viscosity, and higher heating price.

The readable function made it possible to effectively convert Excel information into MATLAB tables, ensuring that each column turned into without a doubt labelled to reflect the specific characteristics of the catalyst. The catalyst name became replicated within the very last column of every desk to assure that each records point became as it should be connected to its corresponding catalyst kind, thereby making sure information integrity.

The code in the Figure (1) shows how to load an Excel file into MATLAB. The file path is specified using the variable file1, then the data is read from the file using the readtable function and stored in the variable data.

```
% Entering Data
file1 = ('C:\Program Files\Polyscape\R2019a\bin\book4.xlsx');
data = readtable(file1);
```

Fig. (1): Data entering.

2.6. Split the dataset

The facts are organized in MATLAB in a way that classifies all columns that constitute both chemical and physical attributes (e.g., temperature, time, density, specific gravity, API, viscosity, and higher heating fee) as input variables. The conversion is diagnosed as the output variable[18]. To reap this separation, the relevant columns for inputs and outputs are removed from the table imported from the Excel report. This strategy is vital for making certain that the information is meticulously prepared for predictive fashions, with a wonderful and systematic delineation between input and output statistics. This improves the efficacy and precision of the analytical and modelling techniques.

The code in the Figure (2) filters numeric columns from the dataset, then separates the data into inputs and outputs. The inputs exclude the 'Conversion' column, which is used as the output.

```
numeric_columns = varfun(@isnumeric, all_data, 'OutputFormat', 'uniform');
numeric_data = all_data(:, numeric_columns);

% separate the data to (Inputs) and (Outputs)
inputs = numeric_data(:, setdiff(numeric_data.Properties.VariableNames, {'Conversion'}));
outputs = numeric_data.Concersion;
```

Fig. (2): Split up the target column.

2.4. Z score standardization

The Z-Score Standardization procedure in MATLAB entailed computing the mean and standard deviation of both the input and output data. This formula was applied to each element in the input and output data[19]. This guaranteed that the data was standardized with a mean of zero and a standard deviation of one. The data was prepared for use in the model's training process following the calculation, which effectively mitigated the effects of differences in scale between the various features.

```
% Z-Score for input
mean_inputs = mean(inputs, 1, 'omitnan');
std_inputs = std(inputs, 0, 1, 'omitnan');
z_scores_inputs = (inputs - mean_inputs) ./ std_inputs;
z_scores_table_inputs = array2table(z_scores_inputs, 'VariableNames', inputs.Properties.VariableNames);
z_scores_table_inputs.Catalyst = all_data.Catalyst;

% Z-Score for output
mean_outputs = mean(outputs, 'omitnan');
std_outputs = std(outputs, 0, 'omitnan');
z_scores_outputs = (outputs - mean_outputs) ./ std_outputs;
z_scores_table_outputs = table(z_scores_outputs, 'VariableNames', {'Conversion_ZScore'});

disp('Z-Scores for Inputs with Catalyst:');
disp(z_scores_table_inputs);

disp('Z-Scores for Outputs (Conversion):');
disp(z_scores_table_outputs);
```

Fig. (3): z score standardization for data.

2.5. Building of ANN Model

Prior to constructing the Artificial Neural Network (ANN) model in MATLAB, the data undergoes a thorough preparation and preprocessing phase. The preprocessed data is then structured into matrices, where the target variable, such as biofuel conversion, is clearly represented as output values. Input variables, including features like temperature, residence time, and catalyst type, are also organized into matrices to be fed into the model. This organized approach ensures that the ANN model can learn the relationships between inputs and out puts effectively.

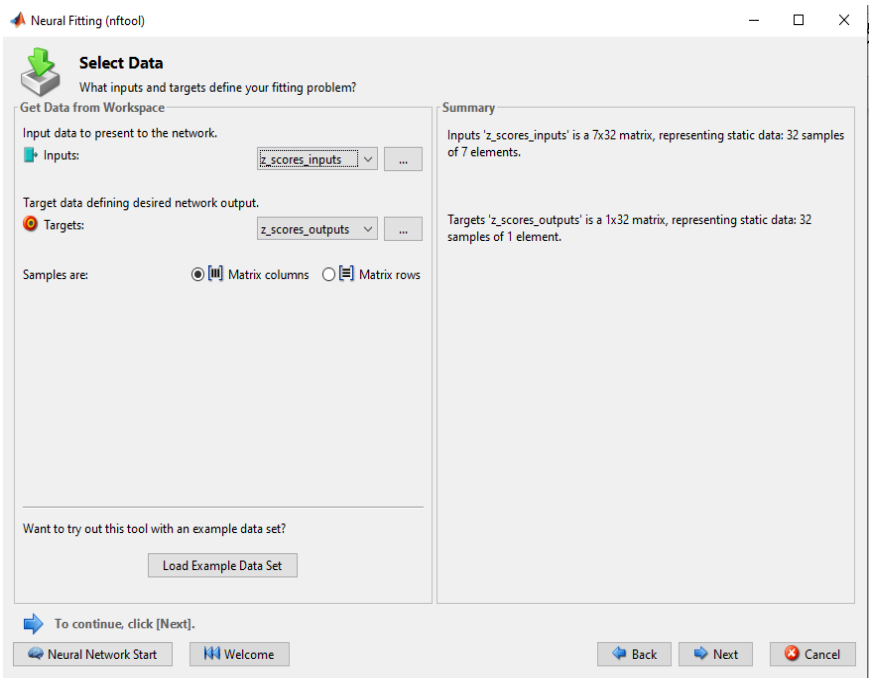

Fig. (4): Entering data from Workspace.

Once the data was imported into MATLAB, it was divided into three sets: **training, validation, and testing**. The **training set** was used to expose the neural network to the data, allowing it to learn underlying patterns and adjust its internal weights. The network iteratively minimizes errors calculated during training process, leading to continuous performance improvements. The validation set was employed to monitor the network's generalization capability, ensuring it doesn't overfit to the training dada.

It turned into supposed to assess the version's overall performance independently, without influencing the education process, using the check set. Novel facts were integrated into the take a look at set to make certain a specific evaluation of the version's anticipated overall performance. This technique facilitated the development of a version that become each specific and resilient, capable of generating dependable predictions using novel facts.

In the following figure, the data is split into three set during the training of the neural network using the Neural Fitting tool in MATLAB. 70% of the data is allocated for training, where the network's weights are adjusted based on the error of the network with this data. Then, 15% of the data is allocated for validation, which is used to measure the model's ability to generalize and stop training when generalization no longer improves. Finally, another 15% is allocated for testing, which doesn't affect training but provides an independent measure of the model's performance during and after training.

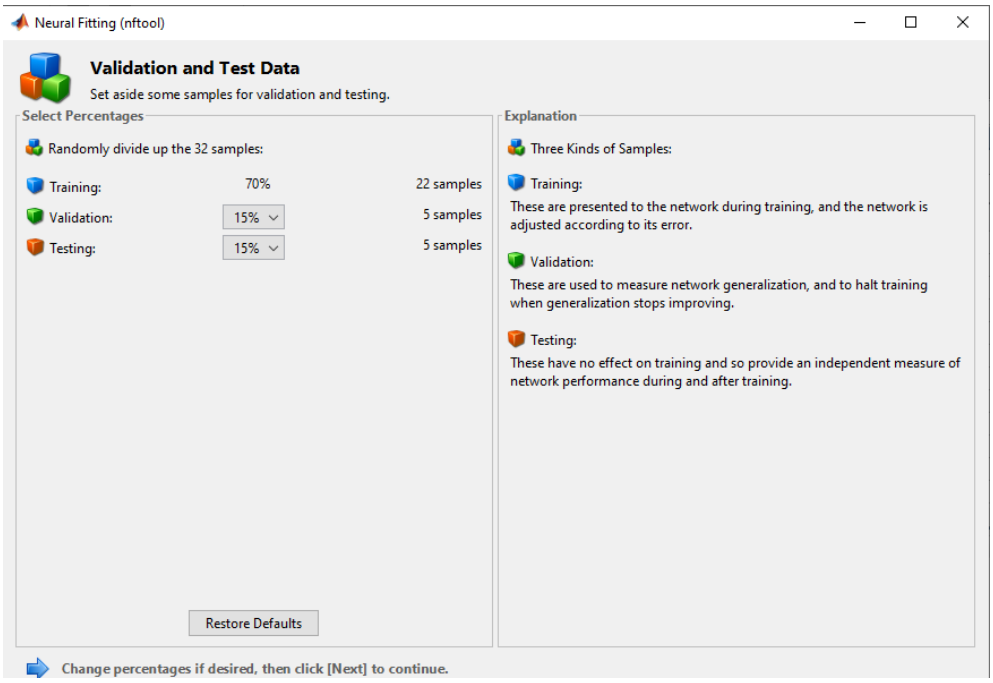

Fig. (5): Set the Validation and testing data.

Following the delineation of the **training, validation, and testing models** in MATLAB, the subsequent Phase worried the establishment of the hidden layer in the neural network. A vital element in the improvement of a powerful neural network version is the determination of the number of nodes (neurones) in the hidden layer, which become done for the duration of this phase. The capability of the model to pick out complicated patterns inside the facts turned into at once inspired by way of the wide variety of nodes.

In this research, the hidden layer contained 20 nodes, which suggests that the community utilised 20 neurones to analyse the input information and extract the critical homes for output prediction. In the occasion that the network's accuracy fails to satisfy the objective after schooling, this level may be revisited to contain modifications in the number of nodes to decorate performance.

A photograph illustration of the exhaustive network architecture became offered in the decrease phase of the MATLAB interface. The Hidden Layer, which consists of 20 neurones, was linked to the Input Layer, which incorporates 7 enter traits. Subsequently, the Output Layer, which represents the network's goal variable, was connected to the Hidden Layer.

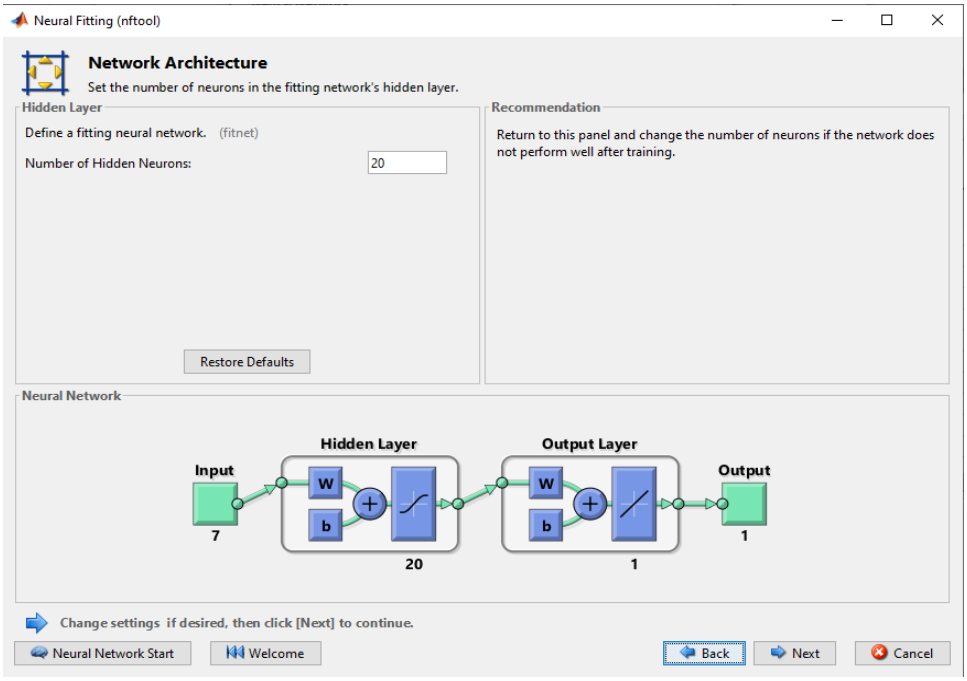

Fig. (6): Set the number of Hidden Neurons.

2.6. Training Network

After the **number of nodes** in the hidden layer of the neural network was determined, the final step was taken before the **training procedure** in MATLAB could commence. In this phase, the appropriate training algorithm was selected. For neural networks in MATLAB, the **Levenberg-Marquardt (train) algorithm** was chosen as the default and most frequently employed algorithm.

The Levenberg-Marquardt method has proven to be highly efficacy in training neural networks, particularly in situations where **precise models** are required. It has demonstrated strong performance with datasets of **small to medium sized datasets,** offering quick convergence and reduced errors. This approach works by adjusting the networks weights iteratively to minimize the discrepancy between the predicted and actual values, thereby improving the model's accuracy and reliability[16].

In order to **mitigate overfitting**, the network was configured to autonomously **terminate training** when the validation set's performance was no longer improved. The model was designed to generalize well to unseen data, ensuring that it didn't just memorize the training dataset. By evaluating its performance on the validation and tests, the model's ability to make accurate predictions on new, previously unseen data was assessed, confirming its robustness and reliability.

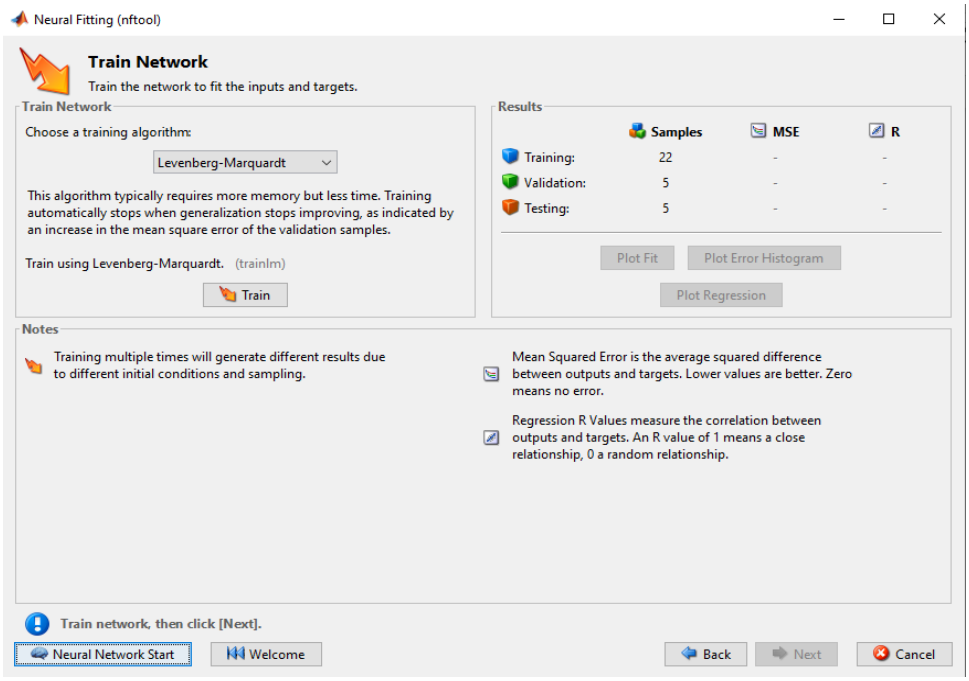

Fig. (7): Set the Training Network.

2.8. Prediction

Outcomes of the training procedure were preserved upon successful completion of data training in MATLAB. The values forecasted by the neural network derived from the training model were recorded in a MATLAB matrix designated as y_pred, which includes the anticipated conversion outputs. Optimization methods were employed to ascertain the optimal conditions for maximizing conversion, utilising the saved y_pred values. By utilizing these predictions, the model improved performance and facilitated data-driven decision-making, ensuring that the system operated under the optimal conditions identified by the trained neural network.

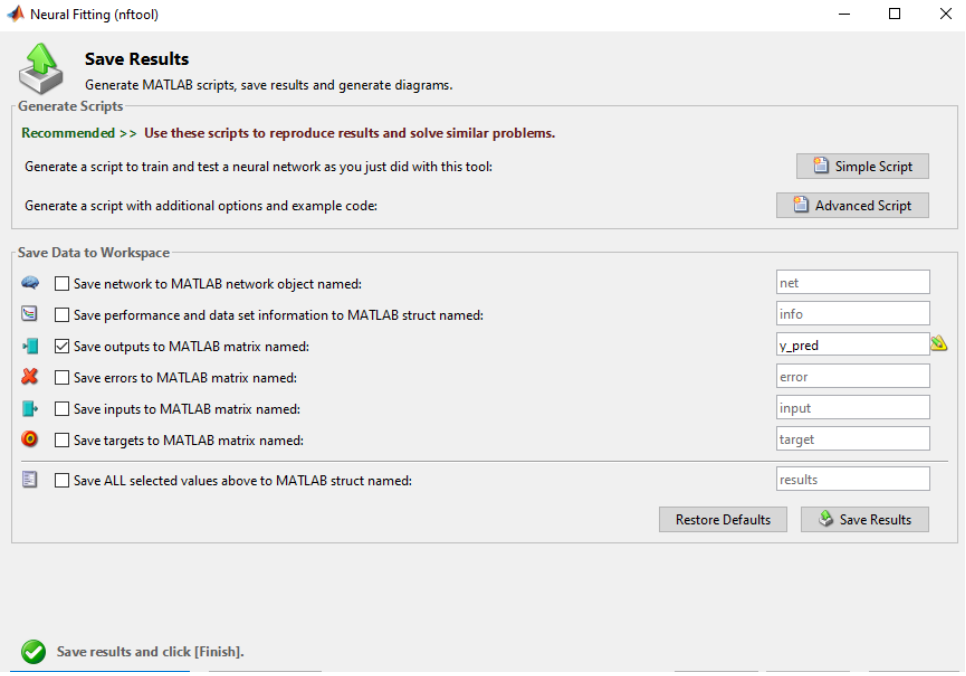

Fig. (8): Saving output data.

2.8. Optimization

In MATLAB, the **neural network** was fed input data from the **anticipated conversion (y_pred)** at this point. The outcomes generated by the previously trained model were represented in a matrix of data. The **objective function** was subsequently established utilizing characteristics including **temperature, time, and cofactor type**, which were structured into a **target matrix (output2)** including these variables. The **input (y_pred)** denoted the **conversion value** the network intended to assess, whilst the **output (output2)** indicated the ideal circumstances the network attempted to identify for optimizing conversion. This organized dataset delineated the correlation between **inputs and outputs**, allowing the neural network to **improve its forecast precision and ascertain the ideal circumstances for temperature, time, and cofactor to attain maximum performance**.

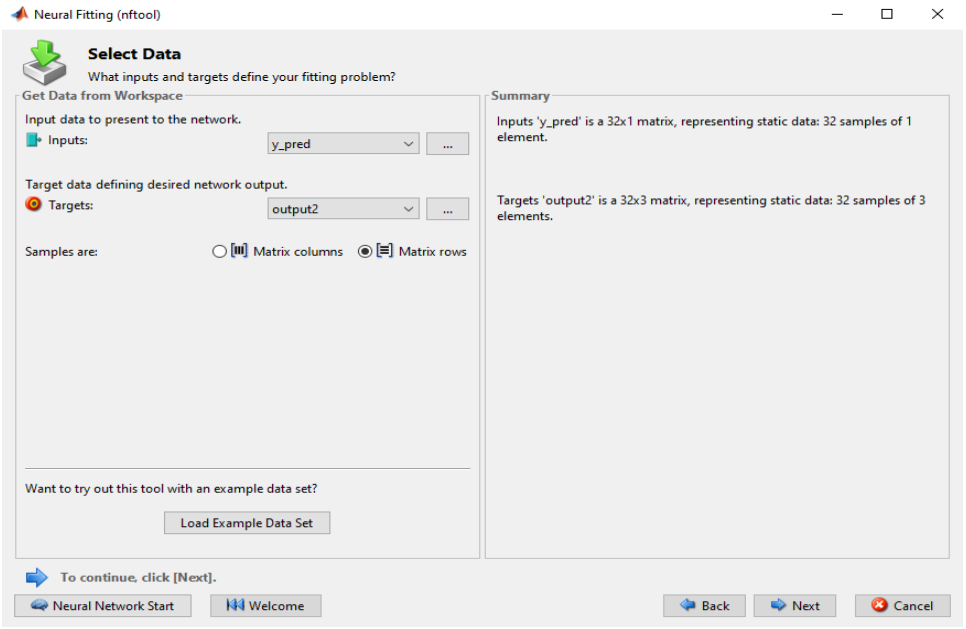

Fig. (9): Selected data to Neural Network.

Subsequent to the data entry procedure, the data is partitioned into training, validation, and test sets. 70% of the data is allocated for training, where the network's weights are adjusted based on the error of the network with this data. Then, 15% of the data is allocated for validation, which is used to measure the model's ability to generalize and stop training when generalization no longer improves. Finally, another 15% is allocated for testing, which doesn't affect training but provides an independent measure of the model's performance during and after training.

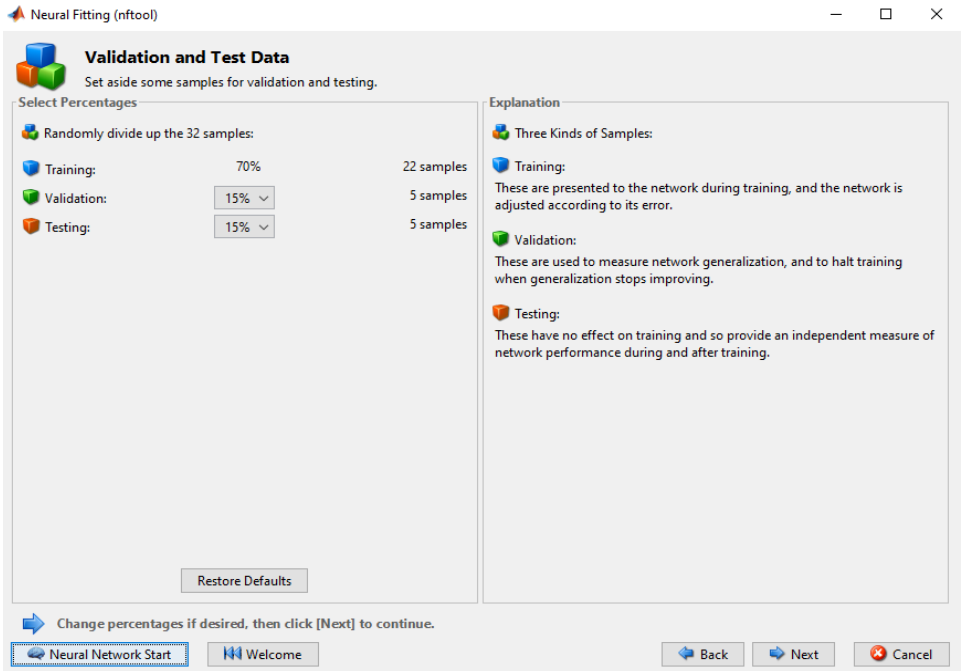

Fig. (10): Selected data to Neural Network.

Next, the number of neurons in the hidden layer is determined. In this example, 21 nodes were chosen in the hidden layer, a number that aims to balance the complexity of the model with its ability to generalize. The overall structure of the network is designed to consist of an input layer that handles one element (predicted Conversion), a hidden layer containing 21 nodes to process patterns, and an output layer containing 3 nodes representing the optimal factors: temperature, time, and type of catalyst.

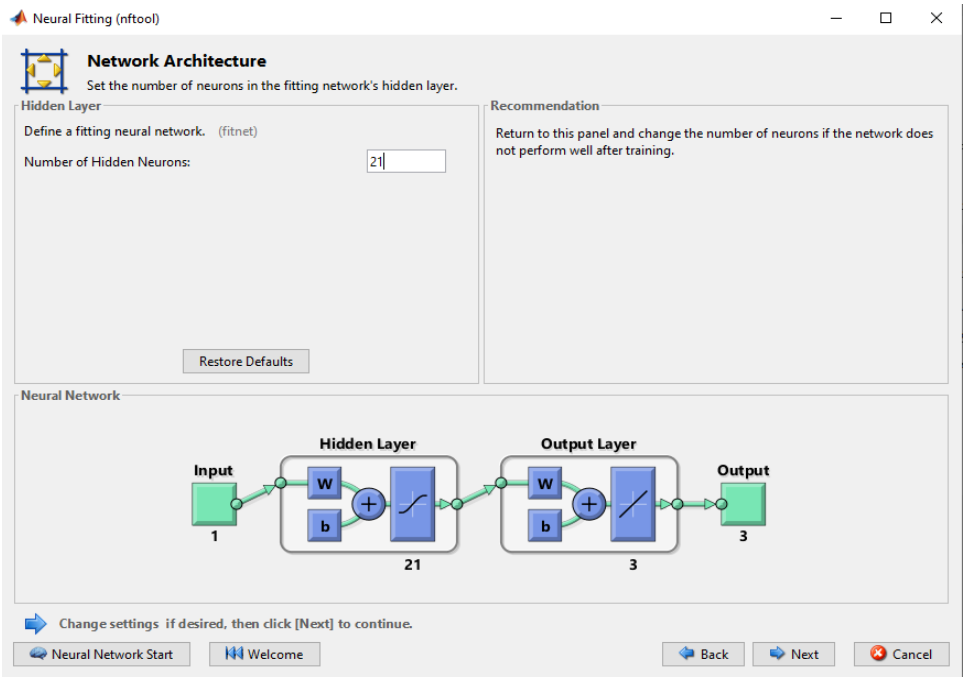

Fig. (11): Set up the number of hidden neurons.

Upon ascertaining the quantity of neurons in the neural network's hidden layer, the process advances to the selection of the training algorithm. This step employs the Levenberg-Marquardt algorithm, recognized as one of the most effective and rapid methods for training neural networks. This algorithm modifies the weights in the network to reduce the discrepancy between the predicted values and the goal values.

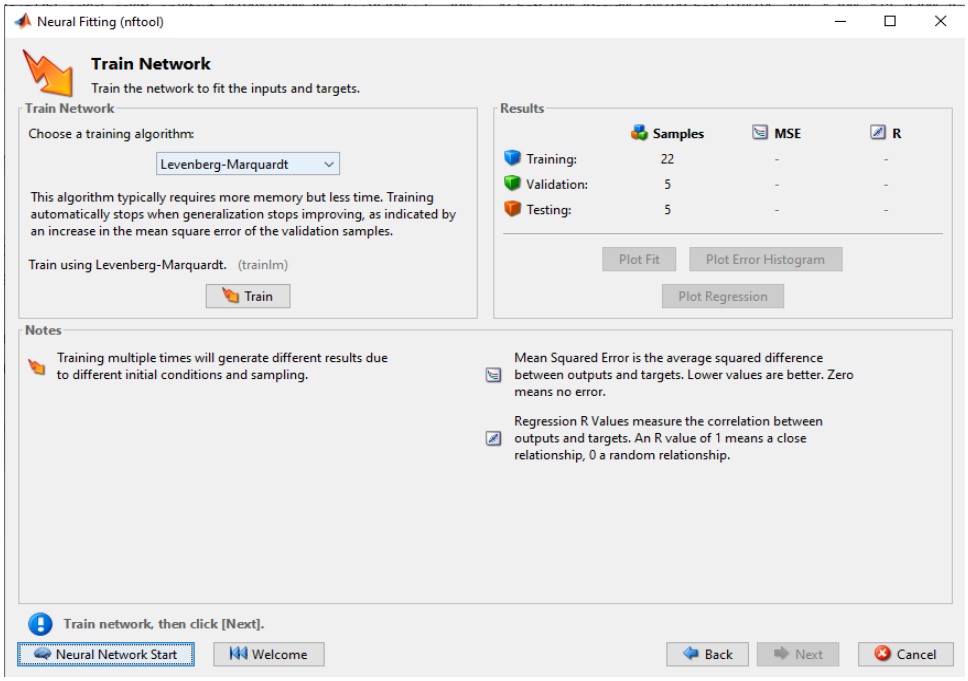

Fig. (12): Set up the training algorithm.

Upon concluding the neural community education method, the code changed into employed to check the excellent circumstances for maximizing expected conversion. The finest anticipated conversion (max_conversion) turned into diagnosed, and the related instances, which includes temperature, time, and catalyst kind, have been extracted from the authentic dataset. The imply rectangular errors (mse_optimized) was calculated to assess the accuracy and dependability of the trained model. The findings, encompassing the correct conversion and applicable instances, have been ultimately provided, supplying essential insights into the great configurations required to enhance gadget performance and maximize performance[20]. The code in the figure 13 finds the optimal conditions (temperature, time, catalyst) for maximum plastic-to-diesel conversion and calculates the Mean Squared Error (MSE).

```
%optimal conditions
[max_Conversion, max_index] = max(y_pred);
optimal_temperature = all_data.Temperature(max_index);
optimal_time = all_data.Time(max_index);
optimal_catalog = all_data.Catalyst{max_index};

% Mean Squared Error
mse_optimized = mean((y_test - y_pred).^2);

% Result
fprintf('Optimal Conditions:\n');
fprintf('Maximum Predicted Conversion: %.2f\n', max_Conversion);
fprintf('Temperature: %.2f°C\n', optimal_temperature);
fprintf('Time: %.2f minutes\n', optimal_time);
fprintf('Catalyst: %s\n', optimal_catalog);
fprintf('Optimized Mean Squared Error: %.4f\n', mse_optimized);
```

Fig. (13): Calculation of the optimal conditions for predicted conversion.

3. Simulation and optimization of the experimental results

3.1. Simulation results and discussion

Table (1) affords an in-depth comparison of experimental biofuel yields from the catalytic pyrolysis of polypropylene making use of the Fe-Ce/AC-activated Sepiolite catalyst, with and without the inclusion of algae. The correlation between the empirical findings and the predicted biofuel output is clarified via this comparison. The nonlinear regression technique became hired to meticulously educate the information, setting up a dating among the inputs and the projected outputs. This technique markedly stronger the model's accuracy, achieving results that were in perfect agreement with experimental data. When calculated based on unseen data, the error rate was R^2 = 1 and MSE =1.21, indicating a perfect match between the predictions and the experimental results. This outcome is attributed to the use of ANN techniques, which enable dynamic adaption to the data. In another study used CatBoost Regressor (CatB) Extreme Gradient Boosting (XGB) models for co-pyrolysis prediction, achieving R^2 values of 0.92-0.98. their multi-objective optimization indicated that higher plastic waste in the feedstock increased liquid yield, while more biomass favored biochar production[15].

Figure (14) illustrates the data training procedure and the degree of concordance between the projected yields and the experimental results. The results validate the efficacy of the implemented data training process in accurately predicting biofuel yields, significantly bolstering the credibility of this approach.

Table (1): Observed and predicted yield for Fe-Ce/AC-activated Sepiolite with and without algae.

Fe-Ce/AC-activated Sepiolite					
Run	**Temperature (℃)**	**Time (min)**	**Observed yield (%)**	**Predicted yield (%)**	**Error (%)**
1	225	30	32.42	32.42	0
2	225	60	40.6	40.6	0
3	225	90	43.2	43.2	0
4	225	120	48.37	48.37	0
5	250	30	44.7	44.7	0
6	250	60	53.4	53.4	0
7	250	90	70.2	70.2	0
8	250	120	78.31	78.31	0
9	275	30	68.56	68.56	0
10	275	60	76.4	76.4	0
11	275	90	81.6	81.6	0
12	275	120	88.24	488.2	0
13	300	30	80.023	80.023	0
14	300	60	86.4	86.4	0
15	300	90	89.65	89.65	0
16	300	120	93.52	93.52	0
17	325	30	87.22	87.22	0
18	325	60	92.87	92.87	0
19	325	90	94.1	94.1	0
20	325	120	96.21	96.21	0
Fe-Ce/AC-activated Sepiolite with algae					
21	225	30	35.42	35.42	0
22	225	60	48.22	48.22	0
23	225	90	50.81	50.81	0
24	225	120	53.98	53.98	0
25	250	30	50.15	50.15	0
26	250	60	55.41	155.4	0
27	250	90	74.4	74.4	0
28	250	120	81.63	81.63	0
29	275	30	74.2	74.2	0
30	275	60	80.189	80.189	0
31	275	90	83.46	83.46	0
32	275	120	91.85	91.85	0
33	300	30	85.11	85.11	0
34	300	60	91.84	91.84	0
35	300	90	93.14	93.14	0
36	300	120	95.05	95.05	0
37	325	30	91.21	91.21	0
38	325	60	95.54	95.54	0
39	325	90	96.2	96.2	0
40	325	120	97.42	97.42	0

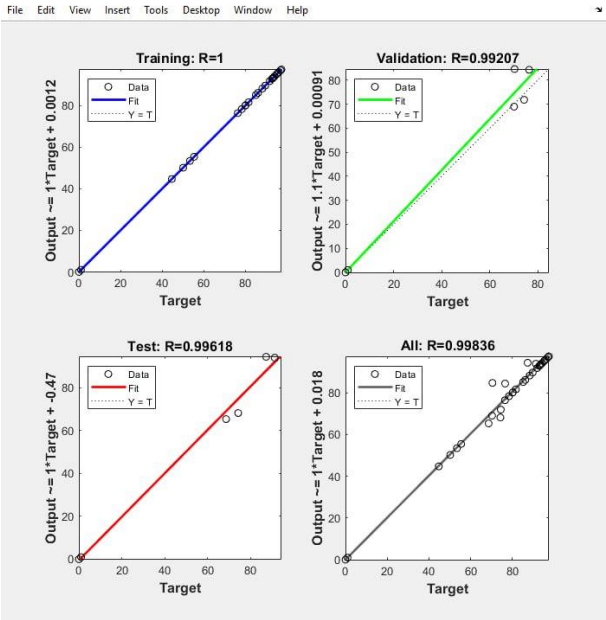

Fig. (14): Training, Validation, and Test process for Fe-Ce/AC-activated Sepiolite with and without algae.

3.2. Optimized output prediction

One way to determine the best operating conditions to achieve the highest biofuel yield is to use an artificial neural network (ANN) model in MATLAB. By training and running the model using MATLAB's optimization tools, a target can be set to increase the yield to values close to 100%. Based on the data shown in Table (2), optimal operating conditions and yields were forecasted utilizing MATLAB's computational capabilities.

Table (2): The best operating conditions and optimal yields.

Temperature (℃)	Time (min)	Type of Catalyst	Yield (%)
225	120	Fe-Ce/AC-activated Sepiolite	48.37
225	120	Fe-Ce/AC-activated Sepiolite with algae	53.98
250	120	Fe-Ce/AC-activated Sepiolite	78.31
250	120	Fe-Ce/AC-activated Sepiolite with algae	81.63
275	120	Fe-Ce/AC-activated Sepiolite	88.24
275	120	Fe-Ce/AC-activated Sepiolite with algae	91.85
300	120	Fe-Ce/AC-activated Sepiolite	93.52
300	120	Fe-Ce/AC-activated Sepiolite with algae	95
325	120	Fe-Ce/AC-activated Sepiolite	96.21
325	120	Fe-Ce/AC-activated Sepiolite with algae	97.42

The coefficient of determination (R^2) was established at 1, signifying exceptional predictive accuracy. This study utilizes the artificial neural network (ANN) model in MATLAB to get a maximum biofuel output of 97.42%. This is accomplished by the catalytic thermal degradation of mixed plastics into biofuel, further processed in a hydrothermal autoclave reactor. The optimal

working parameters to attain this yield were: temperature = 325 °C, duration = 120 minutes, and catalyst type = Fe-Ce/AC-activated Sepiolite with algae.

4. Conclusions

A significant improvement has been achieved in the catalytic pyrolysis process of sustainable biofuel generation. Real-time processes, fuel production, and overall process efficiency are continuously optimized through the use of AI-driven modeling in the study to develop a reliable prediction system.When comparing conventional modeling techniques with the the application of artificial neural networks (ANNs) in this study, it's evident that AL-driven modeling offers greater benefits. The ANN model used to predict nonlinear dependencies among the factors considered (temperature, residence time, and catalyst type) without an a priori specified response function, based on the experimental results, proves to be highly accurate.

The findings provide key insights into the optimal configurations needed to improve system performance and maximize efficiency. By using AI-based modeling techniques, the system can adapt to varying conditions and continuously optimize process parameters, leading to better biofuel conversion rates and reduced energy consumption. This approach helps enhance the reliability and scalability of the process.

The study therefore underlines the drive behind selecting favorable process conditions since the highest anticipated conversion efficiency of 97.42% is achieved using Fe-Ce/AC-activated Sepiolite with algae, residence period120minutes, and temperature325°C. These results confirm the effectiveness of using AI to enhance industrial performance and achieve high efficiency in biofuel production.

This study highlights that AI-driven approaches greatly enhance waste-to-fuel technology, enabling scalable biofuel production from plastic waste. Further research should focus on improving the catalytic process using deep learning and reinforcement learning techniques to enhance prediction accuracy and process efficiency. Additionally, exploring alternative feedstocks and developing new catalysts is essential to increase sustainability and biofuel production efficiency.

Author Contribution Statement: Idres M. Khder contributed to conception and data Analysis. Saba A. Gheni contributed to research design and data processing. Zainab Falah contributed to literature review. Marwan I. Hamd contributed to literature review. Nalan Turkoz Karakullukcu

contributed to data processing. Ataallah K. Tahah contributed to data analysis and interpretation. All authors have read and approved the final version of the manuscript.

References

[1] M. F. da Costa, R. d. S. Araújo, A. R. Silva, L. Pereira, and G. M. Silva, "Predictive artificial neural networks as applied tools in the remediation of dyes by adsorption—A review", *Applied Sciences*, vol. 15, no. 5, p. 2310, 2025. https://doi.org/10.3390/app15052310.

[2] Z. Sun, S. Jayasinghe, A. Sidiq, F. Shahrivar, M. Mahmoodian, and S. Setunge, "Approach Towards the Development of Digital Twin for Structural Health Monitoring of Civil Infrastructure: A Comprehensive Review", *Sensors*, vol. 25, no. 1, p. 59, 2024. https://doi.org/10.3390/s25010059.

[3] A. AGGARWAL, "A Critical Analysis of Methodologies for Detection and Classification of Power Quality Events in Smart Grid", *IEEE Access*, vol. 9, pp. 83507-83534, 2021. https://doi.org/10.1109/ACCESS.2021.3087016.

[4] H. Karali, G. Inalhan, and A. Tsourdos, "Advanced UAV Design Optimization Through Deep Learning-Based Surrogate Models", *Aerospace*, vol. 11, no. 8, p. 669, 2024. https://doi.org/10.3390/aerospace11080669.

[5] A. Esteva, B. Kuprel, R. A. Novoa, J. Ko, S. M. Swetter, H. M. Blau, and S. Thrun, "Dermatologist-level classification of skin cancer with deep neural networks", *Nature*, vol. 542, pp. 115-118, 2017. https://doi.org/10.1038/nature21056.

[6] E.G. Kirilova, "Artificial neural networks: Applications in chemical engineering", Modeling and Simulation in Chemical Engineering: Project Reports on Process Simulation, *Heat and Mass Transfer*, *Springer*, 127-146, 2022. https://doi.org/10.1007/978-3-030-87660-9_6.

[7] K. Srinivasan, A. Puliyanda, D. Thosar, A. Bhakte, K. Singh, P. Addo, R. Srinivasan, and V. Prasad, "Artificial intelligence and machine learning at various stages and scales of process systems engineering", *The Canadian Journal of Chemical Engineering*, vol. 103, no. 3, pp. 1004-1035, 2025. https://doi.org/10.1002/cjce.25525.

[8] M. Das, M. Catalkaya, O. E. Akay, and E. K. Akpinar, "Impacts of use PID control and artificial intelligence methods for solar air heater energy performance", *Journal of Building Engineering*, vol. 65, p. 105809, 2023. https://doi.org/10.1016/j.jobe.2022.105809

[9] H. Zhang, S. Kang, J. Li, Z. Li, J. Chang, Y. Xu, G.M. Lu, and C. Sun, "Near zero-waste biofuel production from bioderived polyhydroxybutyrate", *Fuel*, vol. 286, part 2, p. 119405, 2021. https://doi.org/10.1016/j.fuel.2020.119405.

[10] K. Ahmed, B. Khan, and M. Shahbaz, "Pathways to China's carbon neutrality and clean energy transition: Evidence from the three decades long stricter environmental regulations", *Sustainable Futures*, vol. 8, p. 100296, 2024. https://doi.org/10.1016/j.sftr.2024.100296.

[11] J. Park, and D. Kang, "Artificial Intelligence and Smart Technologies in Safety Management: A Comprehensive Analysis Across Multiple Industries", *Applied Sciences*, vol. 14, no. 24, p. 11934, 2024. https://doi.org/10.3390/app142411934.

[12] S. Albahra, T. Gorbett, S. Robertson, G. D'Aleo, S. V. S. Kumar, S. Ockunzzi, D. Lallo, B. Hu, and H. H. Rashidi, "Artificial intelligence and machine learning overview in pathology & laboratory medicine: A general review of data preprocessing and basic supervised concepts", *Seminars in Diagnostic Pathology*, vol. 40, no. 2, pp. 71-87, 2023. https://doi.org/10.1053/j.semdp.2023.02.002.

[13] D. Ardila, A. P. Kiraly, S. Bharadwaj, B. Choi, J. J. Reicher, L. Peng, D. Tse, M. Etemadi, W. Ye, G. Corrado, D. P. Naidich, and S. Shetty, "End-to-end lung cancer screening with three-

dimensional deep learning on low-dose chest computed tomography", *Nature medicine*, vol. 25, no. 6, pp. 954-961, 2019. https://doi.org/10.1038/s41591-019-0447-x.

[14] Y. Chen, and L. Huang, "Inputs and Outputs, MATLAB Roadmap to Applications: Volume I Fundamental", *Springer Nature Singapore*, pp. 219-240, 2025. https://doi.org/10.1007/978-981-97-8788-3.

[15] Y. Ayub, and J. Ren, "Co-Pyrolysis of biomass and plastic waste: Process prediction and optimization based on Artificial Intelligence and response optimizer surrogate model", *Process Safety and Environmental Protection*, vol. 186, pp. 612-624, 2024. https://doi.org/10.1016/j.psep.2024.04.049.

[16] F. Abnisa, S. D. Anuar Sharuddin, M. F. bin Zanil, W. M. A. Wan Daud, and T. M. Indra Mahlia, "The yield prediction of synthetic fuel production from pyrolysis of plastic waste by levenberg–Marquardt approach in feedforward neural networks model", *Polymers*, vol. 11, no. 11, p. 1853, 2019. https://doi.org/10.3390/polym11111853.

[17] MathWorks, https://www.mathworks.com/help/matlab/import_export/read-spreadsheet-data-into-table.html.

[18] MathWorks, https://www.mathworks.com/help/matlab/import_export/read-spreadsheet-data-into-table.html.

[19] MathWorks, https://www.mathworks.com/help/stats/zscore.html.

[20] MathWorks, https://in.mathworks.com/help/optim/ug/fit-ode-problem-based-least-squares.html.