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PREDICTIVE MODELING OF SYNGAS COMPOSITION AND GAS YIELD IN CATALYTIC BIOMASS REFORMING USING A MIMO-ANN FRAMEWORK

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Abstract
The catalytic reforming of biomass represents an efficient thermochemical pathway for converting solid feedstock's into combustible gaseous products such as CO, H_2, CO_2, and CH_4. Accurate prediction of these individual gas fractions is essential for optimizing process performance and designing advanced biomass-to-energy systems. In this study, a multiple-input multiple-output (MIMO) Artificial Neural Network (ANN) framework is developed to model and forecast gas yields generated under catalyst-assisted biomass conversion. A dataset of 300 plus experimentally characterized fuel samples, obtained from an operational gasification setup, forms the basis of the model training and evaluation. The ANN architecture incorporates 11 physicochemical and process-related input variables, including elemental composition (C, H, N, S, O), moisture content, ash, temperature, volatile matter, lower heating value, and equivalence ratio and predicts five key outputs: CO, CO_2, CH_4, H_2, and total gas yield. Network training is performed using the Levenberg-Marquardt (LM) and Bayesian Regularization (BR) algorithms to assess their comparative effectiveness. Model performance, evaluated through mean squared error metrics and regression analysis, demonstrates that the LM-trained ANN achieves superior predictive accuracy relative to BR. Overall, the developed ANN models exhibit strong agreement with experimental measurements, highlighting their potential as reliable predictive tools for catalytic biomass reforming processes.

INTRODUCTION

Biofuels have emerged as an intriguing alternative fuel source due to the depletion of hydrocarbon deposits and the harm they cause to the environment. [1]. As a result, the modernization of the world has been accompanied by measures to meet energy demand. Moreover, the utilization of fossil fuels causes numerous environmental problems, including global warming and greenhouse gas emissions, smog in cities, skin-deforming disease, and disruption of the weather cycle due to the melting of ice at the

North Pole. To sustain the growing energy demands in the world and enhance sustainable growth, the pulverized coal boiler has been developed and used for the combustion of biomass all over the world. [2]. Over the last 20 years, fantastic research has been carried out to seek new and alternative sources of energy regarding renewable resources. As a result of numerous benefits, including high availability and reduced CO_2 emissions, biomass has been regarded as the most appropriate energy source among all other sources of renewable energy. The International Energy Agency (IEA) estimates that in 2050, 27 percent of all transportation fuel in the world will have been substituted with biofuels. Since it captures carbon in the atmosphere when it is growing and emits the same when it is burned, biomass is also called a carbon-neutral fuel. The most common materials used for energy are plants, wood, and waste. [3]. Depending on the source and origin of the biomass, namely from plant and animal products, from a mixture of plant and animal products, or manufactured material, the chemical composition of biomass has been shown to consist of approximately 50% cellulose, 30% hemicellulose, and 20% lignin. Additionally, it contains various inorganic compounds and alkali metals such as phosphorus, magnesium, and calcium, along with chlorine in amounts ranging from 1% to 25%. Biomass also includes proteins and other organic substances like acids and salts [4].

Gasification is a process that produces carbon monoxide, hydrogen, and carbon dioxide at high temperatures (typically between 500–700 °C) without combustion, utilizing a controlled amount of steam or oxygen from organic or fossil-based carbonaceous waste [5]. This process involves the chemical transformation of solid or liquid waste into gas. Gasification begins with the thermo-chemical degradation of biomass into hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), and methane (CH_4), accompanied by by-products such as water and tar [6]. Among various thermochemical conversion methods, biomass gasification is considered the most effective for producing gaseous fuel [7]. During biomass gasification, the carbon-based material is subjected to elevated temperatures in a reactor known as a gasifier, where it interacts with gasification agents steam, oxygen, and air [8].

The efficiency of gasification is influenced by several factors, including the type of gasifier, the gasification agents used, the size of the particles, the types of catalysts employed, and the composition of the resulting gases. The use of catalysts in gasification offers several advantages, including increased output of the desired products and improved economic efficiency through lower gasification temperatures and the conversion of tar into gas [9].

Three main types of catalysts used in the gasification process include alkaline earth metals, transition metals such as nickel, and dolomite-based catalysts. Catalysts need to be not only cost-effective but also capable of enhancing the gasification process while addressing issues related to sintering and regeneration. Alkaline metals and calcium oxide (CaO) are particularly effective in this regard, as they have well-established and confirmed catalytic actions. [10]. The interest in creating prognostic models for time-consuming and expensive investigations is furthered by breakthroughs in computer science and soft computing. Researchers are encountering difficulties in collecting authentic data for the development of a new product due to elevated costs and delayed trials stemming from diverse operational conditions, requiring a series of experiments. [11]. A neural network or circuit of three layers is called a neural network. The first layer, the input layer, has a "neuron". Towards the Second layer, the hidden layer neurons are set to store what has been learned. Upon the Output Layer – for every output, one neuron. In the neural network, feedback is weighed separately, and a feature known as the activation or transfer mechanism passes the total. The output operation is commensurate with the weighted average output for linear units. The output is set at one of two levels for threshold units, depending on whether the total input is more than or less than a certain threshold value.

Artificial Neural Networks are a reliable method for predicting experimental results that eliminates these problems. It has the potential to learn and generalize in addition to using processing power from parallel structures. It is frequently employed to resolve non-linear issues. The network's training has an impact on prognostic performance and generalization. The generalization concerns how the ANN performs for inputs that were not included in the network's training. Artificial Neural Networks (ANN) have been extensively utilized in recent years, among other machine learning methodologies, owing to their accuracy, precision, speed, and cost-effectiveness in predicting non-linear system data. It is a non-linear modeling method that can be utilized to address various engineering issues even in the absence of sufficient experimental evidence. The human brain serves as the inspiration for the ANN. It makes use of parallel processing networks to manage the intricate interactions between the variables that make up the input and output. Some researchers have discussed the application of the ANN technique to biomass gasification.

The preliminary study was developed based on the documented facts on fixed-bed gasification, specifically concerning biomass gasification systems utilizing artificial neural networks (ANN)[13]. An artificial neural network model for biomass gasification using a fixed-bed down-draft gasifier was developed by employing input factors such as carbon, hydrogen, oxygen, ash, moisture content, and reduction zone temperature. This study aims to create an ANN model that forecasts the composition of gases and confirm it on the existing data. Data collected from experiments and literature review. Additionally, the impact of four variables, i.e., Steam/biomass ratio, temperature, CaO/biomass ratio, and weight percentage of coal bottom, was investigated. Using published kinetics data, it is expected that the process of gasification will take place in a single-pass fluidized bed gasifier together with CO_2 capture. Parametric studies are carried out to investigate the viability of the proposed system's suggested EFB-based enriched hydrogen product gas manufacturing process and are implemented in MATLAB to examine the impact of temperature and the ratio of steam to biomass on the hydrogen yield, efficiency, and concentration. The established model is meant to be utilized to work on heat integration and cost reduction to create an effective EFB hydrogen generation process. Energy production and environmental monitoring depend on the capacity to predict biomass gasification gases, but this is difficult because of the intricate linkages and variability. A potent technique for managing and optimizing these procedures is machine learning. To identify the best model for predicting the compositions of CO, CO_2, H_2, and CH_4 under various circumstances, this study uses Bayesian optimization to calibrate parameters for several machine learning algorithms, including Random Forest, Extreme Gradient Boosting, Light Gradient-Boosting Machine, Elastic Net, Adaptive Boosting, Gradient-Boosting Regressor, K-nearest Neighbours, and Decision Tree. The correlation coefficient (R), root mean squared error (RMSE), mean absolute percentage error (MAPE), relative absolute error (RAE), and execution time were used to evaluate performance, and a Taylor diagram was used to display visual comparisons. The significance of hyper-parameter optimization was examined using the t-test effect size, etc. With high R values under ideal conditions (0.951 for CO, 0.954 for CO_2, 0.981 for H_2, and 0.933 for CH_4) and great performance under sub-optimal conditions (0.889 for CO, 0.858 for CO_2, 0.941 for H_2, and 0.856 for CH_4), XG Boost beat other models. On the other hand, Elastic Net and K-nearest neighbours (KNN) showed the least stability and performance. This study highlights the importance of hyper-parameter tweaking in improving model performance and demonstrates the improved accuracy and robustness of XG Boost [14]. The co-gasification of pine wood, palm kernel shell (PKS), and bamboo using different proportions of polyethylene (PE) as a catalyst is analyzed to enhance syngas production and to determine the effects that the various experimental variables have.

Gasification is done using oxygen-rich carrier gases with an equivalent ratio (ER) of 0.3 and 750 o C. Gasification experiments are created utilizing the Taguchi technique with the Box-Behnken Design (BBD), highlighting four important experimental variables: biomass feedstock. PE ratio, oxygen concentration, and catalyst. In both the Taguchi technique and the BBD, the greatest cold gas efficiency (CGE) is 65.70%, while the highest carbon conversion (CC) value is 86.17%. The settings generating these findings employ the P1 catalyst, 29% oxygen content, pinewood feedstock, and 50% PE ratio. The major variable affecting CGE is the polyethylene (PE) ratio within the feed, whereas for CC, it is the catalyst type. The ANOVA-developed prediction model from the BBD now obtains an R^2 of 0.9191 for CGE and 0.9129 for CC. In comparison, the Taguchi-based ANN prediction model provides the R 2 values of 0.9644 and 0.9708 in the prediction of CC and CGE, respectively. Also, an ANN model involving BBD gives an R 2 value of 0.9471 in CC and 0.9734 in CGE. The models that have been developed can predict CGE and CC accurately. However, the BBD models are more accurate in predicting when compared to the Taguchi model. This shows the importance of the two methods in the prediction of the outcomes of gasification, the neural network model being more accurate when it comes to the prediction of the experimental outcomes. [15]. To promote H_2 and inhibit tar, machine learning techniques are used to optimize the biomass gasification process. Four machine learning prediction models are developed, and PSO-SVR is the most effective method, achieving $R^2 = 0.8701$ for the prediction of tar yield and $R^2 = 0.9105$ for the prediction of H_2 concentration. The optimal temperature for gasification is between 920 and 980°C, which will result in the highest predicted H2 concentration and significantly lower tar emission. Additionally, adding catalysts, using steam as a gasification agent, upgrading fluidized beds, and doping ores with catalytic effects in reactors all have positive impacts. [16]. A bench-scale fixed-bed gasifier was used to gasify a mixture of coal and biomass to produce H2-enriched syngas for power generation. The impact of two essential gasification factors, namely, catalyst and temperature, on gasification products (syngas and tar) and gasification systems' efficiency was explored. The co-gasification test was carried out using coal + pine sawdust (PSD) at temperatures of 700, 800, and 900 °C. Two operational process conditions, namely, With Catalyst (WICAT) and Without Catalyst (WOCAT), were studied. The catalysts employed are Pine Sawdust-Biochar (PSD-BC) and Nickel-Pine Sawdust-Biochar (Ni-PSD-BC). When Ni-PSD-BC and PSD-BC (WICAT) were utilized, the syngas production was greater than that of WOCAT by 11.33% and 5.82% respectively. Syngas output at 900 °C was greater than that of 700 °C by 14.07%. When the gasification temperature was increased from 700 to 900 °C, the H_2 and CO contents increased from 29.95 to 41.87% and 19.45 to 25.18%, respectively. The quantity of tar in the produced gas ranged from 8.01 to 12.96 g/Nm^3 at 700 to 900 °C temperature settings and 4.55 to 4.96 g/Nm^3 when the PSD-BC and Ni-PSD-BC catalysts were employed, respectively. The quality of gases generated at 700, 800, and 900 °C WOCAT is not acceptable for use in fuel cells and gas turbines, but those produced at 900 °C WICAT can be utilized in internal combustion engines and gas turbines [17]. Conserve environmental health; shift input data for the modeling of gasification materials, such as gases and solids, and limit reliance on fossil fuel providers. It embraced the construction of hybrid frameworks that connected an Extra Tree Regressor (ET) model with two optimization methods, namely Equilibrium Slime Mold Algorithm (ESMA) and Manta Ray Foraging Optimization (MRFO). The gasification process was simulated using the dataset from 312 experiments that were reported in the literature. With $R^2 = 0.99$ and RMSE = 0.0694 for gas yield and $R^2 = 0.986$ and RMSE = 6.943 for char yield during the training phase, respectively, the obtained result showed that the ETES hybrid model had a satisfactory fitness accuracy. These findings show that the hybrid models might significantly improve the prediction of char and syngas from gasification processes [18]. Artificial neural network models were developed based on mass loss data of sewage sludge and peanut shell during burning, gained by thermos-gravimetric analysis, to predict the experimental outcomes. The influences of mixture ratio and temperature on SS-PS combustion were discussed. Mixing ratio and experimental temperature are the input parameters of the ANN model, and sample mass is an output parameter. The best ANN models (ANN12 for combustion) were obtained, which are able to well predict the thermos-gravimetric curves of combustion with an R^2 of 0.99999. The projected results are in good accordance with experimental data of the ANN model, which confirms the dependability and accuracy of the application of ANN for the thermos-gravimetric studies [19]. A new poly-generation system incorporating biomass and waste plastic chemical looping co-gasification (BPCLG) for hydrogen production, power generation, and dimethyl ether synthesis is established and optimized by combining process simulation and machine learning for efficient utilization of organic solid waste. The artificial neural network is adopted to build surrogate models for predicting the molar fractions of key components in syngas and the system energy consumption. Then, the non-dominated sorting genetic algorithm-II is used to maximize the two objectives, including the highest molar percentage of hydrogen in syngas and the lowest energy consumption. This improved poly-generation system enhanced H_2 production by 4.36% and reduced energy consumption by 3.59%[20]. Coupling green hydrogen with the coal chemical sector is of importance for clean coal usage and low-carbon transformation. This work intends to estimate syngas composition effectively by using artificial intelligence-assisted machine learning models, notably the BP-MLPNN model, considering raw material variety and process uncertainty. The reliability and resilience of the BP-MLPNN model in predicting syngas components are as follows: MSE and RMSE values ranging between 0.002 to 11.61 and 0.05 to 3.41, respectively, while the R2 value ranges from 0.84 to 1.00. A basic interface input app was designed to achieve human-machine interaction. This model may alleviate uncertainties in assessing the integrated coal chemical industry and green hydrogen production system, giving technical guidance and references toward the estimation of its benefit and possibility in generating diverse chemical goods [21]. Machine learning (ML) and deep learning (DL) methodologies are applied during gasification and examined for their merits and downsides. AI algorithms have become very widespread in many fields and applications related to energy conversion systems. The usage of hybrid models has been quite common recently, especially due to their proven efficiency in modeling and optimization tasks. The main point is that the use of these algorithms significantly enhances the strength of the model to handle complex challenges, as deep learning methods have evolved to provide enhanced accuracy with reduced vulnerability to errors. The current study has made an effort to present a comprehensive review of machine learning and deep learning techniques and their applications, identifying gaps in current research knowledge [22]. The methodology makes use of sewage sludge, corn byproducts, sugarcane and orange harvest residues, coffee leftovers, eucalyptus leftovers, and urban waste. To develop the model, the three-layer feed-forward neural network technique is applied to simulate hydrogen conversion from each type of biomass using simulation data from Aspen Plus® software. The model demonstrated excellent performance with R2 values above 0.9941 and 0.9931 on the training and testing datasets, respectively. Sewage sludge showed the highest HHV of 18.1 MJ/kg, urban and orange waste exhibited the best cold gas efficiency, which was 82.2% and 80.6%, respectively, while the highest carbon conversion efficiency was obtained for sugarcane bagasse and orange residue, which is 92.8% and 91.2%, respectively. On the other hand, sewage sludge and corn waste showed the highest hydrogen mole fraction with 0.55 and 0.52, respectively. For sugarcane straw leftovers, the system may reach relative energy efficiencies of 24.4%, while for sugarcane bagasse, they can reach 42.6%. In all, the energy efficiency ranged from 23.7% for coffee waste to 39.0% for sugarcane bagasse.[23]. The fundamental driving force for the adoption of predictive models is the search for cost-effective and highly accurate solutions. This research will apply the model of the Multi-layer Perceptron, known for its prowess in identifying complicated linkages between input variables and gas production outputs. Additionally, the addition of the Reptile Search Algorithm Optimization (RSA) and the African Vultures Optimization (AVOA) significantly boosts the model's predictive power, boosting its precision. The investigation undertaken indicates the exceptional predictive capabilities of the MLRS model, positioned in the third layer, notably in anticipating hydrogen (H_2). This model obtained an amazing R^2 value of 0.994 during the validation phase. Conversely, for the nitrogen (N_2) prediction, the MLRS model in the second layer consistently outperformed all other models, having an exceptional R^2 of 0.997 during both the testing and validation stages [24]. A hybrid approach combining ML techniques with Aspen Plus to enhance gasification outcome prediction. In the paper, a base case gasification process flow-sheet simulation was done in Aspen Plus based on projected thermodynamic equilibrium conditions, which can result in inaccurate results. Experimental data were gathered using six machine learning techniques to address this problem, and their accuracy and efficiency were assessed. The importance of the features, improvement in accuracy, and the effect of using machine learning predictions within the gasification block on the rest of the flow-sheet were analysed[25]. We present an overview of several difficulties linked to feedstock biomass heterogeneity, multiple reaction pathway interactions, and technological defects. This research attempts to illustrate how different domains of AI and ML, such as predictive modeling and real-time optimization, promote gasification by reviewing current progress in the fields [25].

2. Methodology

There are many different sensors applied to the detection and measurement of accurate readings of solid particles in biomass gasification. The general outline of the experimental process study includes two qualitatively different segments. The preliminary intense step of the 'Gasification' procedure is gaining the proper datasets from the tentative method as has been explained in [26].

2.1. Experimental Data

In this study, the data set of the experimental design had 315 fuel sample properties. In ANN and ANFIS modeling the eleven input features have been compromised and the five output variables are compromised. The second part comprises the creation of the ANN and ANFIS model in MATLAB 2020a to estimate the fuel samples by using online computation methods. It has been divided into training data of %70, validation data of %15, and testing data of %15, where there are 221 training samples, 47 validation samples, and 47 testing samples.

2.2. ANN Model

Increment into the accuracy of the gas composition and thus that of the gas yield, a structure for an artificial neural network is formulated. Hidden layer neurons relay the signals coming after the input layer and then transmit them to the output layer neurons, it denotes that to produce the output signal, the network in the hidden layer must add its weighted inputs and employ the activation function. The activation function's way to function is given mathematically by (1).

$$y_j = F_{Activation}(\sum_{i=1} Wij\ Xij + b_j) \quad (1)$$

Where wij is the weight of the Ith input and jth neuron of the hidden layer or output layer, and bj is the Bias of the jth layer. An activation function of type Tansigmoid has been employed in the training of the model. The ANN model has one hidden layer which has 11 input features, 5 output features, and 50 neurons which are present in the hidden layer. The suggested ANN model deploys the Levenberg-Marquardt (LM) feed-forward-back propagation (BP) learning algorithm with the Tansigmoid function (2).

$$F_{Activation}(X) = \frac{1}{1-e^{-x}} \quad (2)$$

Regarding the feed forward-back propagation, the literature review shows that focuses on the specification of the architecture [27]. The architecture of the ANNs used in the current research is described in the following section with the help of Figure 2.

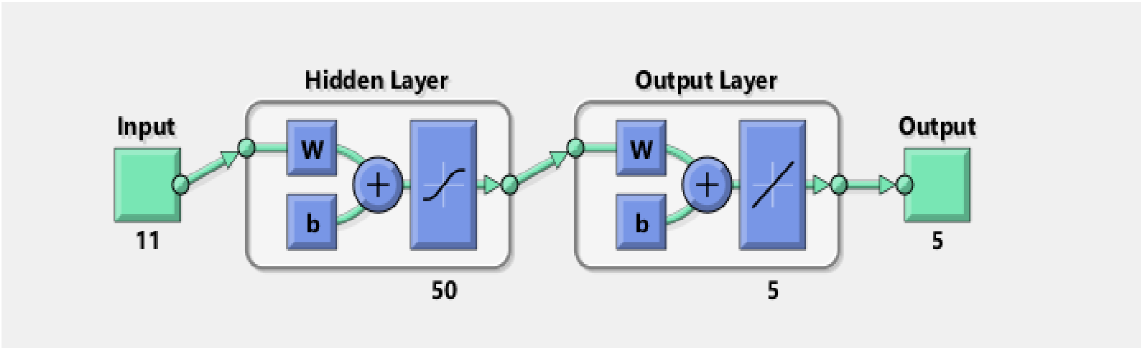

Figure 1. Architecture of ANN

- **Input layer:** The no. of input layer neurons is ordinarily based on the no. of input features that are determined in that procedure. Therefore, the input layer of the proposedstructure contains 11 neurons.
- **Hidden layers:** In this case, it is a simple multi-layer perceptron that consists of one hidden layer composed of 50 neurons. The no. of hidden layer neurons is chosen reasonably, also as selective as possible to minimize the error and possibly yield the best results.
- **Output layer:** The no. of output layer neurons is ordinarily based on the no. of output features that are determined in that procedure. Therefore, the output layer of the proposed structure contains five neurons.
-

2.3. Tuning of ANN Model

The above ANN model regulation process of analysis has entirely been accomplished via "NNTOOL". When tuning these parameters as input features, Carbon, Hydrogen, Sulphur, Nitrogen, Tg, Equivalence ratio (ER), LHV (Lower Heating Value), Oxygen, Volatile matter (VM), Moisture content (MC), and Ash value. As listed in the above CO_2, H_2, CH_4, CO, and gas yield are all output features with value. In this ANN model the no. of samples are 315 samples which are split into training data 70%, test data 15%, and validation data 15%. This split of data was done randomly by MATLAB. However, the distribution provided here can be modified for the required change if needed. The chosen parameters of the proposed model that were tuned optimally are presented in Table 1.

- Training operations are performed in batches with noises introduced in the model.
- Levenberg Marquardt (LM) with the 2^{nd}-order method, which is more accurate than the 1^{st}-order method as the time used up by the second order isa smaller amount while it includes noises during data collection.

The moment the ANN model regulation is over, it comes to a stop by itself and presents the shortest way which might be determined by the MSE measure of fuel samples. You can use the average of the squared error between the target and output to explain the mean square error (MSE) [28]. Figure 3 illustrates the suggested model's topology. In addition, the ANN algorithm's training flow sheet is shown in Figure 3. The trained parameters are optimally shown in Table 1. Figure 5 provides the ANN Regression analysis (R^2), and the findings are as follows:

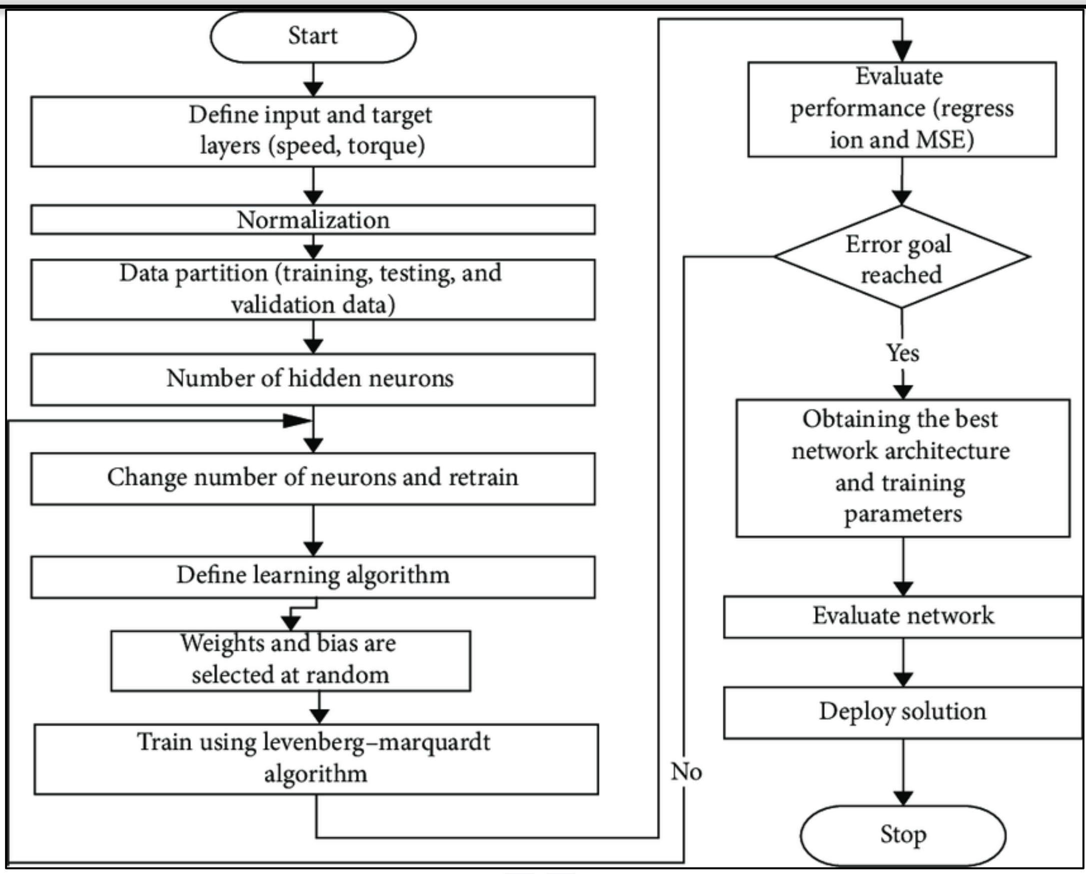

Figure 3: ANN training flow sheet

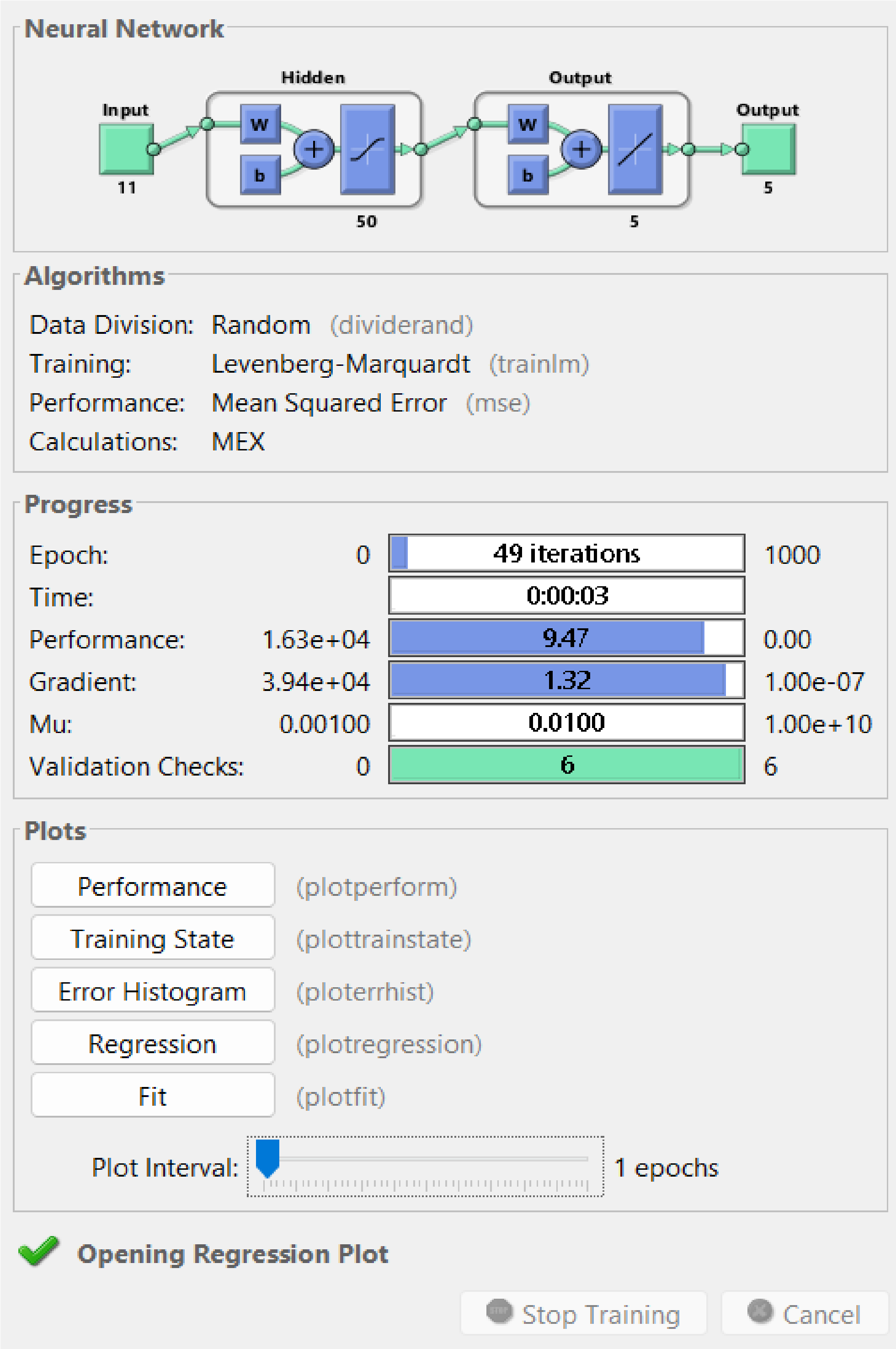

Figure 4: Training algorithm for ANN

Table 1: Optimal parameter selection for artificial neural network

Parameter	Selected Value	Details / Justification
Network Type	Feed-Forward Backpropagation	Matches the architecture shown in the network diagram.
Number of Inputs	4	Four input variables are connected to the ANN.

Parameter	Selected Value	Details / Justification
Number of Outputs	5	Outputs include CO, CO_2, H_2, CH_4, and Gas Yield.
Number of Hidden Layers	1	Single hidden layer as shown in the architecture image.
Hidden Layer Neurons	50	Exact neuron counts clearly displayed in the figure.
Hidden Layer Activation Function	Tansig	The figure and MATLAB default for this architecture confirm Tansig.
Output Layer Activation Function	Purelin	Used for continuous numerical prediction.
Training Algorithm	Levenberg–Marquardt (LM)	Most efficient for moderate-sized datasets and shown in training report.
Performance Metric	Mean Squared Error (MSE)	The performance plot in the image is labeled "Performance (MSE)".
Training Data Split	70% Train, 15% Validation, 15% Test	Follows standard ANN configuration and visible in the training window.
Epochs (Maximum Iterations)	1000	Default maximum iteration setting used for convergence.
Learning Rate	0.01	Stable learning rate for LM optimization.

2.4. Regression analysis for ANN

The regression analysis for training, testing, and validation is shown in Figure 5.

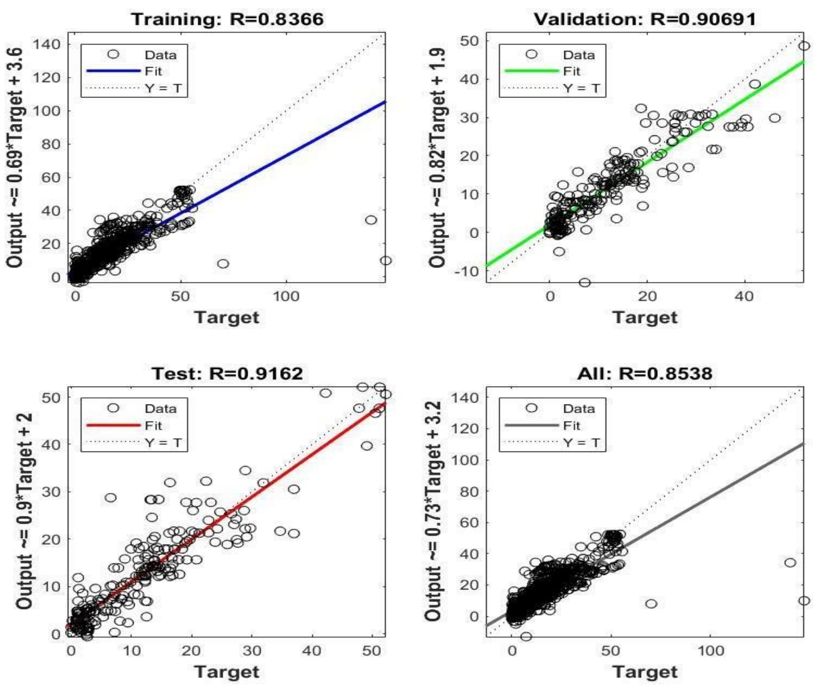

Figure 2. Regression Analysis of ANN

3. Results and Discussion

We obtained the final data after completing all experimental operations on the revised ANN model. We investigated and calculated values of ANN over many phases. The difference between the reported and testing findings is highlighted as follows, expressed in terms of the mean square error (MSE) calculated using the appropriate formula.

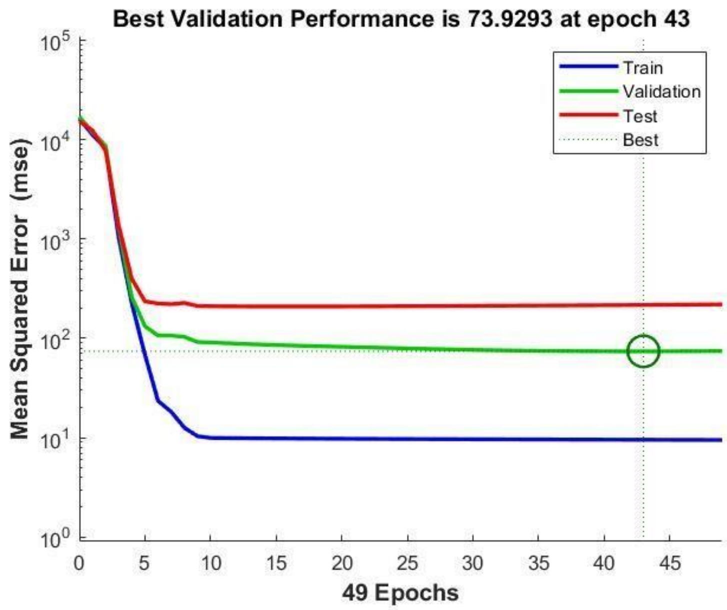

Figure 3. Convergence features of multiple input multiple output (MIMO) layer network: gas composition and gas yield using Levenberg Marquardt (LM)

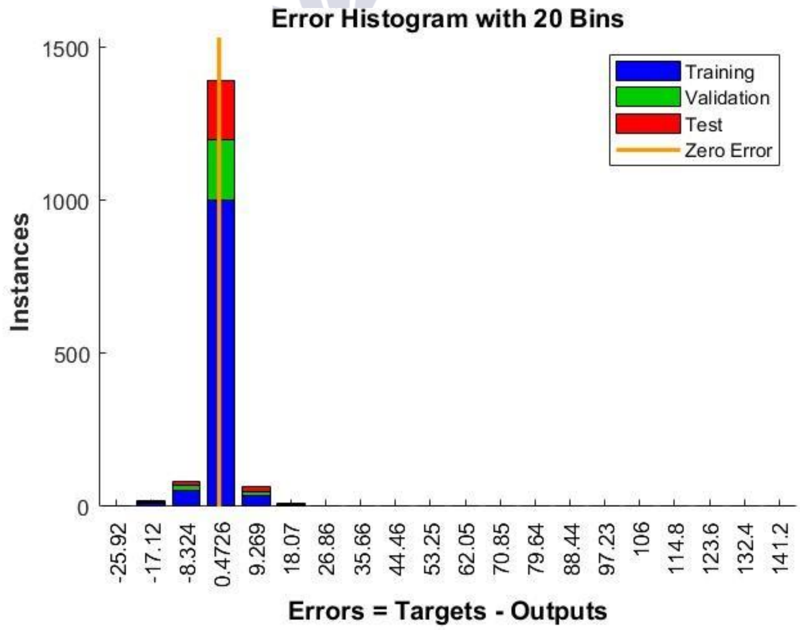

Figure 4. Error histogram: Multiple input multiple output (MIMO) network layer for gas composition and gas yieldusing Levenberg Marquardt (LM)

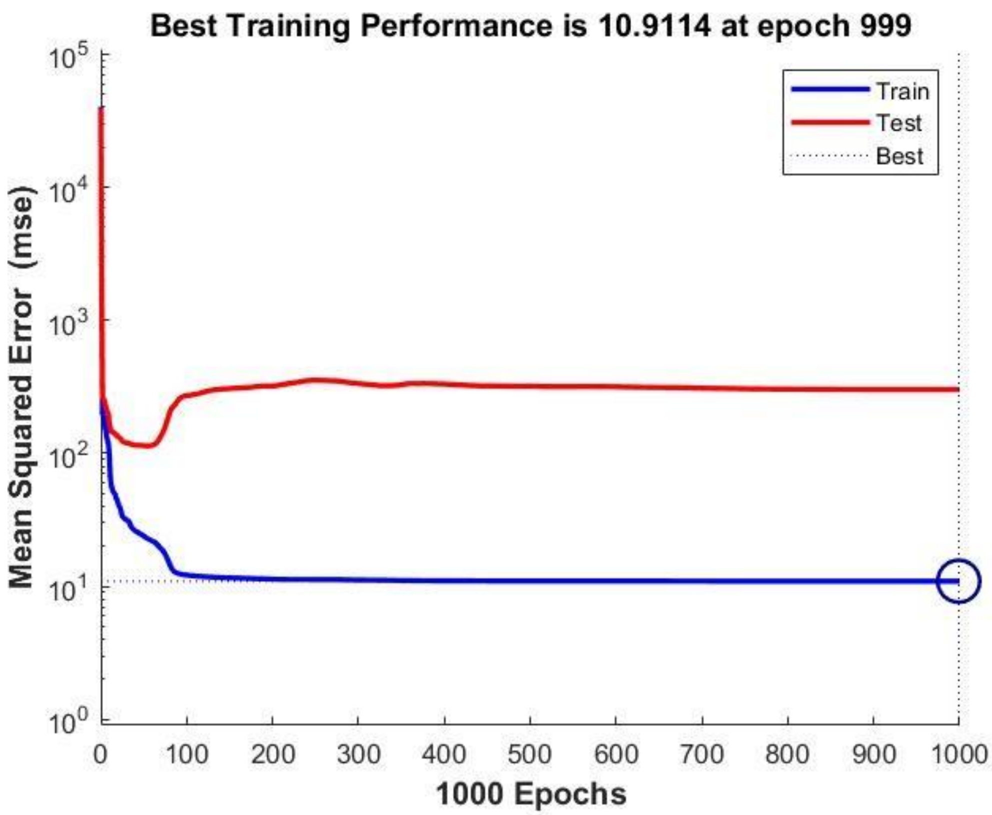

Figure 5. Convergence features of MIMO layer network: gas composition and gas yield using Bayesian Regularization (BR)

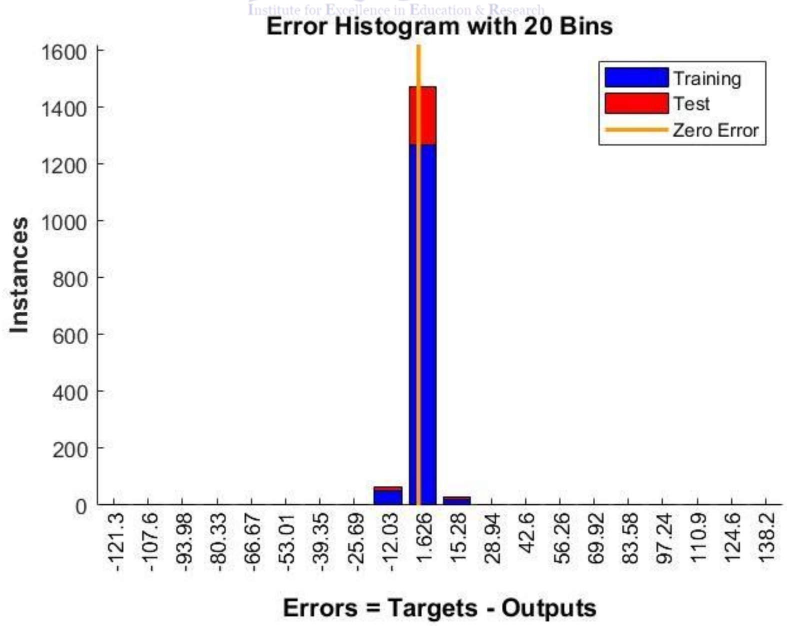

Figure 6. Error histogram: MIMO layer network of gas composition and gas layer using B

Figure 6 represents convergence features of the MIMO layer network: gas composition and gas yield and figure 7 represents the Error histogram: MIMO layer network of gas composition and gas yield using the Levenberg Marquardt (LM) respectively. And figure 8 represents the convergence features of the MIMO network layer: gas composition and gas yield using Bayesian Regularization (BR), and Figure 9 represents the Error histogram: MIMO network layer of gas composition and gas yield using Bayesian Regularization (BR) respectively. The results obtained showed that datasets trained by ANN using the LM algorithm are more significant and accurate than the datasets trained by ANN using the BR algorithm. Figure 6 shows the result of the network in terms of the convergence properties of the MIMO layer by using Levenberg Marquardt in the prediction of CO, H_2, CH_4, CO_2, and gas yield. LM was used while training the neural network where it had 49 iterations, and the best fitting was achieved at epoch 43. Therefore, stationary linearity in the purposes of convergence curve of training, testing, as well as validation, was observed inferring that the model was good fitting corresponding to the dataset investigated in the study. As seen from the convergence property of the responses in Figure 6, the CO, H_2, CH_4, CO_2, and gas yield, there was a significant reduction in the MSE while maintaining a stiff stability of the fitting curve.

LM algorithm MIMO network layer results

Table 2. LM algorithm MIMO network layer results

Input Variables	Algorithms	No. of Neurons	MSE	Epoch	Regression Coefficients Training	Validation	Testing	All	Output Variables
C, H, N, S, O, MC, Ash, T, VM, LHV, ER	LM	5	59.2	51	0.8	0.9	0.8	0.9	CO, H_2, CH_4, CO_2 Gas Yield
		10	25.5	50	0.8	0.82	0.9	0.8	
		15	54.6	15	0.9	0.6	0.8	0.9	
		20	21.8	25	0.9	0.9	0.8	0.9	
		25	54.1	10	0.9	0.7	0.9	0.9	
		30	32.4	13	0.93	0.7	0.91	0.92	
		35	33.5	13	0.9	0.8	0.8	0.9	
		40	17.3	17	0.92	0.91	0.9	0.93	
		45	12.5	13	0.9	0.6	0.4	0.9	
		50	0.47	49	0.836	0.906	0.92	0.853	

BR algorithm MIMO network Layer results

Table 3. BR algorithm MIMO network Layer results

Input Variables	Algorithms	No. of Neurons	MSE	Epoch	Regression Coefficients	Validation	Testing	All	Output Variables
					Training				
C, H, N, S, O, MC, Ash, T, VM, LHV, ER	BR	5	49.01	182	0.8	-	0.9	0.9	CO, H_2, CH_4, CO_2, Gas Yield
		10	34.94	355	0.9	-	0.7	0.8	
		15	33.17	277	0.95	-	0.8	0.91	
		20	23.73	1000	0.9	-	0.9	0.9	
		25	31	1000	0.9	-	0.82	0.9	
		30	28.65	1000	0.9	-	0.9	0.9	
		35	23.97	1000	0.9	-	0.8	0.8	
		40	18.59	583	0.93	-	0.7	0.9	
		45	32.2	1000	0.9	-	0.93	0.9	
		50	1.6	1000	0.9	-	0.8	0.9	

The summary of the results is shown in Table 2 as obtained from the LM algorithm using the hidden layer neurons of 5-50. Regarding this, predictive modeling was performed to assess the effectiveness of the MIMO layer network in improving the model outcomes. When there were 50 neurons in the hidden layer, the R^2 (regression) ranged from 85 to 94%, respectively. The LM algorithm produces a significantly better result than the BR algorithm. The coefficient of determination (R^2) of the number sequence obtained from Levenberg Marquardt (LM), MIMO, and Bayesian Regularization (BR), multiple input multiple output (MIMO) network layer for the gas composition and yield is provided in Tables 2 and 3. The findings in these tables were derived after applying all the input variables examined in this study.

The convergence characteristics of the MIMO (multiple input multiple output) layer network utilized for CO, CO_2, CH_4, H_2, and gas production exhibited stability, meaning that the design offered a superior fit for the analyzed variables in the given dataset. In this case, the results for the fitting, i.e. training, validation, and testing of the employed network are presented in Tables 2 and 3. The error identified from the output of Figure 1-4 could be influenced depending on the input and output variables under consideration; nevertheless, the application of two different types of algorithms which are in addition incorporate different numbers of neurons in an ascending sequence from 5-50 may substantially lessen the error. Below we have provided details about the MIMO layer network for the Bayesian Regularization algorithm. Both the tables are as follows Table 2 and Table 3 by Levenberg Marquardt for the C, H, N, S, O, MC, Ash, T, VM, LHV, and ER as the independent variables used in the prediction of the dependent variables which are the gas composition (CO, CO_2, CH_4 and H_2) as well as the gas yield. For Figure 7, the MSE reported is much lesser as compared with the values reported for Figure 9, whereas the coefficient of determination of the fitting curves of training, validation, and testing given in Table 2 is relatively higher than the values in Table 3.

From Table 2, it is possible to conclude that there is a substantial improvement in the results when the model was trained by Levenberg Marquardt and the prediction of the composition of the gases (CO, CO_2, CH_4, H_2) and the yield of the gases is concerned. The performed comparison of the models used the C, H, N, S, O, MC, Ash, T, VM, LHV, and ER input variables to predict gas composition and gas yield using the BR and LM algorithms. Indeed, the BR algorithm results were compared to those of LM with 50 hidden neurons, where it was found that the later was better. When the case of R^2 and mean square error is being looked at, the relative implication derived from this study is that the LM algorithm is relatively superior to the BR for predicting the composition of tgas and the yield of the process. In this research, to check the learning performance of ANN models, three parameters were managed under observation i.e. MSE (mean square error), iterations, and R^2 (regression value). All are shown in Tables 2 and 3. If the value of MSE is equal to close to zero, this indicates the difference between experimental outputs and predicted the outputs which is then considered nearer to zero. While, if the values are equal to zero then it would represent absolutely no difference and no error in the experimental output and predicted outputs. Meanwhile, regression (R) depicts the correlation level between the experimental and predicted results. There is a possibility that the value of regression could be equal to one. In that case, there would be a minimum or no difference between experimental and predicted values. The R and MSE values for training, validation, and testing of data using ANN are represented in Table 2 and 3.

Statistical values for the proposed ANN model

Table 4. Statistical values for the proposed ANN model

Type of Data	MSE	Regression (R^2)
Training	0.04726	0.836
Testing	0.0337	0.906
Validation	0.0422	0.916

Moreover, if the mean squared error (MSE) value approaches zero, it indicates that the tuning of the suggested model is effective for all datasets. Furthermore, the observed and predicted outcomes are almost identical results. For assessment of the performance, a comparison of network outputs with intended output is made and the value of MSE achieved is very low and hence can be considered as almost negligible. They are near to satisfying and quite reasonable R^2 (regression) and MSE (mean square error) values.

4. Conclusion and Future work

The global energy crisis necessitates continued exploration of efficient, sustainable, and technologically advanced pathways for energy production. In this study, a comprehensive dataset comprising **315 experimental records** from biomass, coal, and blended feedstock gasification was employed to develop and evaluate a **Multiple-Input Multiple-Output (MIMO) Artificial Neural Network (ANN)** model. The model incorporated key physicochemical parameters, including elemental composition (C, H, N, S, O), proximate analysis (MC, Ash, VM), operational conditions (T, ER, LHV), and gas composition (CO, CO_2, CH_4, H_2), with overall gas yield as the output variable. The ANN was trained using both the **Levenberg–Marquardt (LM)** and **Bayesian Regularization (BR)** algorithms. Performance analysis revealed that networks with **5–50 neurons in the hidden layer** exhibited stable convergence behavior. Among these, the LM algorithm demonstrated **superior predictive accuracy**, characterized by lower Mean Square Error (MSE) and higher coefficients of determination (R^2) compared to BR. The strong agreement between experimental and predicted results confirms that the ANN framework efficiently captures the nonlinear relationships governing catalytic gasification. These findings highlight the potential of ANN-based models to significantly reduce the labor, cost, and time associated with experimental trials in thermochemical conversion research. Model validation was conducted using multiple statistical performance indicators, including **MSE, RMSE, MAE, MAPE,** and **Regression (R)**. The near-zero MSE values affirm minimal deviation between experimental and predicted outputs, confirming high model reliability and generalization capability.

Future advancements will focus on integrating the current ANN framework with more sophisticated deep-learning architectures such as **Recurrent Neural Networks (RNNs),** particularly **Long Short-Term Memory (LSTM)** units, and **Convolutional Neural Networks (CNNs)**. Additionally, evolutionary and swarm-based optimization methods may be employed to enhance hyper-parameter tuning and improve predictive robustness. Expanding the model to include larger datasets and more diverse operating conditions will further strengthen its applicability for real-time process control, optimization, and industrial-scale gasification systems.

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