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Artificial Neural Network Approach for Estimating Biochar Yield from Biomass Composition and Pyrolysis Temperature

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Abstract: *Biochar yield from biomass pyrolysis is influenced by complex interactions among feedstock properties and pyrolysis conditions. This study proposes the generation of an artificial neural network (ANN) model to predict biochar yield using input variables including volatile matter, fixed carbon, ash content, elemental composition (C, H, O, N), and temperature on pyrolysis process. A multilayer perceptron (MLP) network was trained using experimental data collected from various biomass sources. The model achieved high performance, with correlation coefficients (R2) of 0.98812 for training, 0.96529 for validation, and 0.94148 for testing. Mean squared error (MSE) analysis showed optimal validation performance at epoch 31, while the error histogram and regression plots confirmed strong predictive accuracy across all datasets. These results demonstrate that ANN is a powerful tool for modeling biochar production, offering a reliable and efficient alternative to labor-intensive experimental methods.*

Keywords: *Artificial Neural Network (ANN), Biochar, Biomass, Machine Learning, Pyrolysis*

1. Introduction

Biochar has attracted escalating emphasis in recent years due to its prospect applications in sustainable agriculture, environmental remediation, and carbon sequestration [1], [2]. As a carbon-rich solid product obtained from the biomass thermochemical processing, biochar plays a critical role in improving soil fertility, carbon-negative energy system, improved energy efficiency, reducing greenhouse gas emissions, and managing agricultural waste. These environmental and economic benefits have spurred extensive research into optimizing biochar production processes.

Among the different thermochemical conversion techniques, pyrolysis is evaluated the most efficient and widely used method for biochar production [3]. Pyrolysis requires the thermal decomposition of organic materials in the absence or limited presence of oxygen, resulting in the formation of three primary products: bio-oil (liquid), biochar (solid), and syngas (gas). The yield and quality of biochar are strongly affected by several factors, including the properties of the feedstock and the operating conditions, particularly the pyrolysis temperature [4].

Numerous theoretical models have been developed to project biochar yield under different pyrolysis conditions [5]. These models are often based on reaction kinetics, mass balance, or empirical correlations. However, the heterogeneous nature of biomass and the difficulty of thermal decomposition reactions limit the accuracy and generalizability of such models. As a result, there is a growing need for alternative predictive approaches that is able to handle complex, nonlinear relationships between process outputs and input variables.

In this context, machine learning (ML) techniques have developed as powerful tools for process modeling and prediction in bioenergy research. One of the most widely used models in this domain is the Artificial Neural Network (ANN), particularly the Multilayer Perceptron (MLP) architecture [6]. These networks are capable of capturing intricate patterns within large datasets and have demonstrated high predictive accuracy in various applications, including pyrolysis product prediction.

The aim of this study is to generate a prediction model using a Multilayer Perceptron neural network to estimate biochar yield derived from biomass properties and temperature process of pyrolysis. The input variables considered include proximate analysis data (fixed carbon, ash content, volatile matter), elemental composition (carbon, oxygen, hydrogen, nitrogen), and the operating temperature. This approach aims to provide a reliable, data-driven method for estimating biochar yield, contributing to the optimization and design of efficient pyrolysis processes.

2. Materials and Methods

2.1. Data Collection and Preprocessing

In order to facilitate the development of reliable and generalizable data-driven models, a comprehensive dataset comprising 301 individual records was systematically compiled from 17 peer-reviewed studies, as summarized in Table 1 [7], [8], [9], [10], [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22], [23]. This dataset represents a diverse selection of biomass feedstocks, including agricultural residues, bagasse, bamboo, cocopeat, coconut shell, coconut fibre, various pine derivatives (e.g., sawdust, wood), orange processing residues (pomace), cassava stem, rape stalk, and rhizome, palm kernel shell, cotton stalk, wood stem and barks.

The proximate composition—consisting of fixed carbon (FC), ash, and volatile matter (VM) —was uniformly expressed on a dry basis for the raw feedstocks. It is important to acknowledge that the limit of the current dataset is confined to biomass with composition of ash ranging from 0% to 15%, indicating the necessity for future dataset expansion to include feedstocks with higher inorganic content in order to broaden the relevance of the predictive models.

Furthermore, the ultimate (elemental) composition of the feedstocks was reported in terms of carbon (C), oxygen (O), hydrogen (H), and nitrogen (N). Due to the presence of data reported in both wet and dry bases across the source literature, all relevant values were standardized to a dry basis using a conventional conversion equation (Equation 1.) that incorporates the respective moisture content (MC), thereby ensuring consistency and comparability across the dataset [24].

$$\begin{aligned} FC_{dry} &= \frac{FC_{wet}}{1 - MC} \\ VM_{dry} &= \frac{VM_{wet}}{1 - MC} \\ ash_{dry} &= \frac{ash_{wet}}{1 - MC} \end{aligned} \qquad (1)$$

The dataset utilized for the development of the predictive model encompassed 7 input variables characterizing the physicochemical composition of feedstocks, in addition to one process parameter associated with the pyrolysis operation. These input features included fixed carbon (FC), ash content (Ash), volatile matter (VM), and elemental constituents—carbon (C), oxygen (O), hydrogen (H), and nitrogen (N)—alongside pyrolysis temperature (PT). The dependent variable, employed as the predictive target, was the biochar yield derived from the thermochemical conversion process.

To investigate the interdependence between any pair of variables—whether among input parameters or between output and input variables—the Pearson Correlation Coefficient (PCC), denoted (r), was utilized as a statistical metric to quantify the strength and direction of linear associations, as outlined in Equation (2) [25]. A PCC value of +1 or −1 denotes a perfect linear relationship (positive or negative), respectively, while a r value of 0 indicates the absence of a linear relationship. The absolute value of the r also serves as an indicator of the relative influence or predictive significance of each input variable on key output responses, including biochar yield, proximate properties (fixed carbon, ash, and volatile matter), and elemental composition (carbon, hydrogen, oxygen, and nitrogen). In this analysis, y and x represent the two variables under examination, and n denotes the total number of observations employed in the calculation.

$$r = \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \sum_{i=1}^{n} (y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^{n} (y_i - \bar{y})^2}} \qquad (2)$$

Table 1. Summary of the datasets and references

References	Biomass Feedstock	FC (%)	VM (%)	Ash (%)	C (%)	H (%)	O (%)	N (%)	T (°C)	BiocharYield (%)
Bhattacharjee & Biswas, 2019	Orange Bagasse	22.23	74.94	2.83	43.57	4.4	51.78	0.17	350–600	28.26–56.71
Biswas et al., 2017	Agricultural Residues	6.54–15.12	71.94–91.16	1.05–15.14	36.07–48.12	5.20–6.34	32.88–51.78	0.17–1.85	300–450	24.30–43.30
Chen et al., 2015	Bamboo	16.05	82.72	1.23	50.21	5.63	42.93	1.23	300–700	23.60–49.30
Crombie & Mašek, 2015	Straw Pellet	15.32	77.28	7.41	42	5.5	44.9	0.1	350–650	31.20–42.10
He et al., 2018	Agricultural Residues	7.49–17.96	75.66–86.09	4.38–13.07	36.71–43.95	5.47–7.77	33.24–45.51	0.49–2.08	300–700	17.68–74.49
Hong et al., 2020	Agricultural Residues	10.16–10.17	76.86–82.63	7.39–12.98	40.06–43.95	5.47–5.81	40.23–41.12	0.69–1.12	300–600	34.98–74.32
Lee et al., 2013	Agricultural Residues	11.73–23.18	70.24–87.83	0.44–8.05	51.71–64.23	4.37–6.89	27.61–45.51	0.23–1.40	500	22.30–38.70
Li, A., 2016	Pinewood Sawdust	61.78–86.37	10.11–35.04	1.63–4.13	-	-	-	-	400–700	21.74–31.09
Liu & Han, 2015	Agricultural Residues	11.10–13.15	80.85–85.45	1.40–8.05	47.75–48.15	5.61–6.70	43.60–45.51	0.90–1.35	200–330	50.21–91.00
Liu et al., 2014	Corncob	18.01	78.71	3.28	48.12	6.48	43.51	1.89	300–600	21.70–77.30
Patra et al., 2021	Agricultural Residues	4.33–7.22	84.56–87.05	5.73–9.96	40.80–45.70	4.10–5.50	40.50–45.70	0.20–3.90	300–600	23.10–52.30
Bian et al, 2016	Agricultural Residues	45.84–68.14	13.14–31.66	14.56–31.79	-	-	-	-	400	35–40
Rout et al., 2016	Coconut Shell	12.46	83.98	3.56	64.23	6.89	27.61	0.77	450–600	25.66–32.48
S. Matali, 2016	Oil Palm Frond	27.88–44.53	56.0–79.18	2.9–8.52	-	-	-	-	200–300	43.2–95
Shariff et al., 2016	Agricultural Residues	9.08–16.07	81.51–87.76	1.05–7.28	41.78–48.88	5.82–5.97	48.88–51.07	0.00–0.26	400–600	25.98–36.78
Tag et al., 2016	Agricultural Residues	23.50–27.80	68.20–70.90	4.00–9.61	35.70–48.07	5.27–6.36	40.98–48.07	1.03–9.61	250–600	27.60–72.10
Ucar & Ozkan, 2008	Rapeseed Oil Cake	17.67	75.28	7.05	45.92	6.21	40.09	6.9	400–500	33.23–38.40

2.2. Multi-layer Perceptron Neural Network

Multilayer Perceptrons (MLPs) are fully linked feedforward neural networks frequently applied in supervised regression tasks. They are trained using the Levenberg–Marquardt backpropagation algorithm, which efficiently minimizes error. During training, inputs are processed through the network using randomly initialized weights. The output is evaluated to target values, and weights are iteratively updated in the inversely related direction of the mean squared error gradient to reduce prediction error [26].

The architecture of a Multilayer Perceptron Neural Network (MLP-NN) typically comprises three fundamental layers: an input layer, one or more hidden layers, and an output layer [27]. Each layer is composed of numerous interconnected processing elements known as neurons. In the present study, the implemented MLP-NN structure includes eight input layer, one output layer, and one hidden layer. A schematic representation of this neural architecture is illustrated in Figure 1.

In this study, a Multilayer Perceptron Neural Network (MLP-NN) model was constructed to predict biochar yield based on biomass properties and the temperature on pyrolysis process. The dataset was partitioned into 70% for training, 15% for validation, and 15% for testing, confirming effective model learning while minimizing overfitting. The network architecture consisted of a single hidden layer comprising 10 neurons. The entire model development and training procedures were conducted using the MATLAB Neural Network Fitting, which provides an interactive environment for designing and analyzing neural network models.

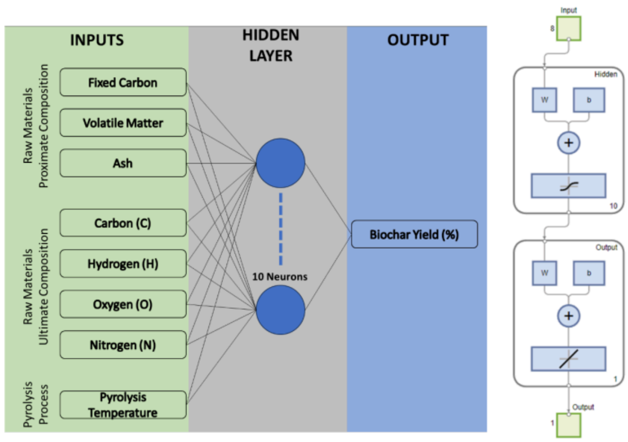

Figure 1. A Schematic illustration of the neural network architecture

3. Results and Discussions

3.1. Exploration of Dataset

	FC	VM	Ash	C	H	O	N	T (°C)	Yield
FC	1	-0.966	0.005	0.109	0.122	0.270	0.134	0.235	0.091
VM	-0.966	1	-0.237	0.317	-0.068	-0.008	-0.332	-0.244	-0.104
Ash	0.005	-0.237	1	-0.543	-0.080	-0.384	0.231	-0.012	0.157
C	0.109	0.317	-0.543	1	0.038	-0.242	-0.239	0.076	-0.127
H	0.122	-0.068	-0.080	0.038	1	-0.415	-0.101	0.007	0.063
O	0.270	-0.008	-0.384	-0.242	-0.415	1	-0.210	-0.058	-0.008
N	0.134	-0.332	0.231	-0.239	-0.101	-0.210	1	-0.047	0.032
T (°C)	0.235	-0.244	-0.012	0.076	0.007	-0.058	-0.047	1	-0.643
Yield	0.091	-0.104	0.157	-0.127	0.063	-0.008	0.032	-0.643	1

Figure 2. Pearson correlation coefficients (*r*) of inputs and output from several variables

The linear relationships among the input variables (fixed carbon [FC], ash content, volatile matter [VM], elemental composition [C, H, O, N], and temperature [T (°C)]) and the output variable (biochar yield) were quantified using Pearson correlation coefficients (r) and depicted in the form of a heatmap, as shown in Figure 2. The r values range from −1 to +1, where data points close to ±1 demonstrate strong linear correlations, and values near 0 indicate weak or no linear correlation. Strong negative correlations were observed between FC and VM (r = −0.966), C and ash (r = −0.543), and O and H (r = −0.415), indicating potential trade-offs between these biomass properties. In terms of the relationship between input and output, the temperature variable exhibited the strongest (and negative) correlation with biochar yield (PCC = −0.643), suggesting that higher pyrolysis temperatures are correlated with lower yield, a trend consistent with previous findings on biochar production. Other variables showed relatively weak correlations with biochar yield (|r| < 0.2), including ash (r = 0.157), FC (r = 0.091), and VM (r = −0.104), implying that while biomass composition influences yield, temperature is the dominant factor under the conditions studied [28].

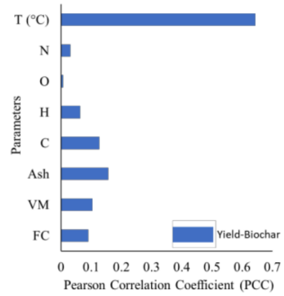

Figure 3. The degree of importance of input variables in predicting biochar yield using PCC

Similarly, Figure 3 shows the significance of input variables in predicting biochar yield using the Pearson correlation Coefficient. Temperature (T [°C]) is the most influential factor, indicating its dominant role in determining yield, the result is further compared to relevant works from Yize Li [31]. Other variables such as ash, nitrogen, and volatile matter (VM) also contribute, but to a lesser extent. In ontrast, carbon (C), hydrogen (H), and oxygen (O) show minimal impact, suggesting that biomass composition is less significant than process temperature in this prediction model.

3.2. Predictive Performance of Multi-layer Perceptron Neural Network

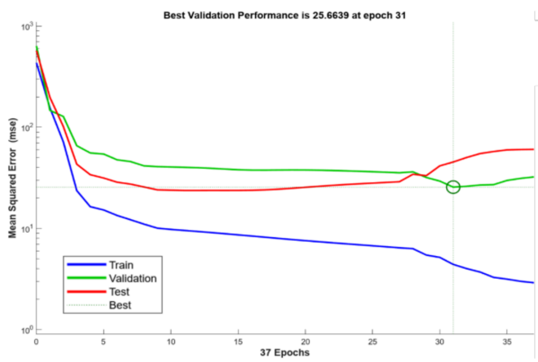

Figure 4. The training performance of the artificial neural network (ANN) model for predicting biochar yield

Figure 4 illustrates the training execution of the artificial neural network (ANN) model for estimating biochar yield, based on the mean squared error (MSE) over 37 epochs. The validation (green), training (blue), and test (red) error curves demonstrate the learning progression of the model. The best validation performance was achieved at epoch 31 with an MSE of 25.66, as showed by the green circle. After this point, the validation and test errors began to increase slightly, indicating the onset of overfitting [29]. This behavior highlights that the model achieved optimal generalization performance at epoch 31, which was selected as the final trained model.

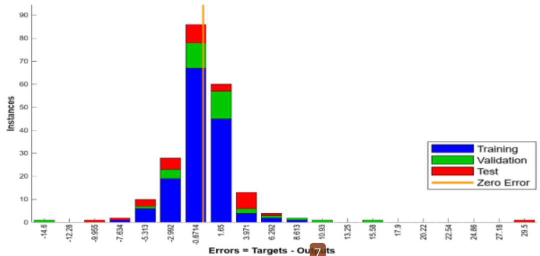

Figure 5. The error histogram of the artificial neural network (ANN) model

Figure 5 illustrates the error histogram of the ANN model, constructed with 20 bins to evaluate the distribution of prediction errors across the validation, training, and test datasets. The histogram reveals that the majority of errors are concentrated around zero, indicating that the model exhibits a low bias and is capable of generating accurate predictions for most instances. The distribution is relatively symmetric, with a high density of instances within a narrow error range (approximately −3 to 4), suggesting that the model generalizes well and maintains consistent performance across all data subsets. The presence of a few outliers with larger errors is minimal and does not significantly affect the overall predictive capability. The orange line depicts the zero-error reference, emphasizing that most predictions closely align with actual values.

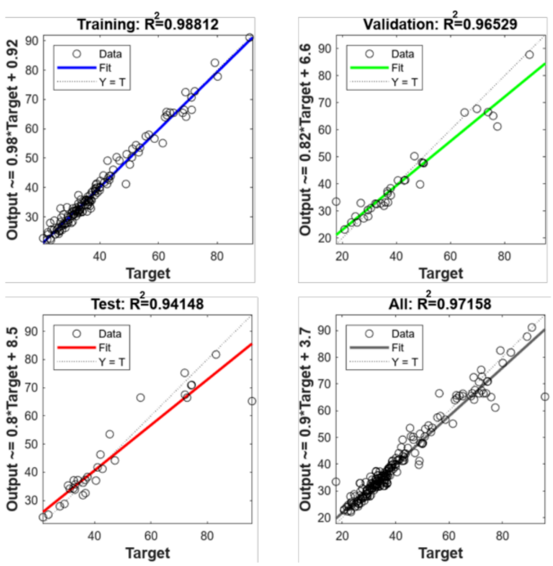

Figure 6. The regression visualizations for the artificial neural network (ANN) model

Figure 6 presents the regression plots for the ANN model, illustrating the correlation between predicted and existing values across the training, test datasets, and validation, as well as the overall performance. The R2 values indicate a strong linear relationship in all datasets: 0.98812 for training, 0.965 for validation, 0.941 for testing, and an overall R^2 of 0.971. These results propose that the model is capable of accurately predicting the target variable with minimal deviation across different data subsets. Comparing the test result, it is noteworthy that previous studies in the biochar yield prediction literature have reported relatively consistent coefficient of determination (R^2) values, such as Zhu ($R^2 = 0.855$) [25], Cao ($R^2 = 0.804$) [30], Pathy ($R^2 = 0.844$) [31], and Khan ($R^2 = 0.930$) [32]. The close alignment of the regression lines to the ideal reference line Y = T (where predicted output equals the target) further confirms the model's dependability and generalization ability. Minor deviations in the test data indicate slight overfitting, yet the overall high correlation validates the ANN model as a reliable predictive tool for estimating biochar yield based on biomass characteristics and pyrolysis conditions.

4. Conclusion

This study demonstrated the successful application of ANN model to predict biochar yield based on the physicochemical properties of biomass and temperature of pyrolysis process. The network achieved high accuracy, with R2-values of 0.98812 (training), 0.96529 (validation), and 0.94148 (testing), indicating strong predictive capability and good generalization. Error distribution analysis showed that most prediction errors were close to zero, reinforcing the model's robustness with no overfitting. These results point out the potential of ANN as an effective tool for modeling complex nonlinear relationships in biomass pyrolysis processes. The developed model can assist in optimizing biochar production by providing rapid and accurate yield estimations without requiring extensive experimental work. For future work, the model can be extended using more complex and diverse datasets that include a wider range of biomass types and pyrolysis conditions. Additionally, incorporating more input variables such as heating rate, particle size, residence time, and reactor type may further improve prediction accuracy and model generalizability.

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