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Energy Optimization of Sugarcane Bagasse by Oxidative Torrefaction: A Multiple Linear Regression Method

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Abstract. Biomass is widely recognized as a promising substitute for fossil fuels due to zero CO_2 emissions, global availability, storage capacity, and immediate response to demand. Therefore, this research aimed to develop and apply a multiple linear regression model to predict the calorific value in oxidative torrefied sugarcane bagasse. An innovative method was used to enhance the efficiency of torrefaction process, focusing on predicting the calorific value through temperature and oxygen concentration. Detailed analyses of collected data were carried out in the RStudio software environment, which showed the capacity of the model to explain calorific value of sugarcane bagasse, achieving a coefficient of determination R2 of 88.29%. The results showed that the model enhanced the understanding of biomass torrefaction processes and provided valuable tools for optimization, promoting more efficient and sustainable practices in energy generation from agricultural residues such as sugarcane bagasse. The novelty of this research was in presenting a specific and rigorous method to address a significant challenge in the field of renewable energy, offering tangible results that could have a significant impact on the industry.

Keywords: Biomass; Multiple linear regression model; RStudio; Sugarcane bagasse; Torrefaction

1. Introduction

The persistent expansion of energy consumption in recent decades is contributing to the depletion of fossil fuel resources, high environmental pollution, and increased climate change (Hu *et al.*, 2018). To replace fossil fuel, renewable energy sources offer a significant solution for a sustainable future (Germán *et al.*, 2023). Therefore, research has been conducted to develop renewable energy sources and other efficient technologies to prevent potential global energy and environmental crises (Kartal and Özveren, 2022). In this context, biomass offers several advantages as a suitable alternative to fossil fuels (German *et al.*, 2023; Lamandasa *et al.*, 2021; Prihantini *et al.*, 2021). These include zero CO_2 emissions, global availability according to demand, and storage capacity (Kalak, 2023).

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Biomass is an incredibly adaptable material that can be converted into biofuels and biochemical products through various thermochemical conversion technologies, such as pyrolysis (Cen *et al*., 2021; Huang *et al*., 2020), gasification (Fan *et al*., 2020) and combustion (Tu *et al*., 2018). However, thermochemical use of biomass is constrained by high moisture content, low calorific value, volumetric energy density, and significant hygroscopicity (Xu *et al*., 2021). These challenges lead to reduced conversion efficiency, alongside high costs associated with the collection, storage, and transportation of biomass (Chen, Peng, and Bi, 2015).

Among the available biomass options, lignocellulosic has been proven effective as the most preferred due to both technical and social factors (Fandiño *et al*., 202). This preference is based on several factors, including lack of competition with food resources, higher energy density, lower requirements for fertilizers, water, pesticides, and rapid growth (Verdugo *et al*., 2022). Consequently, it is essential to explore new methods for efficiently using biomass from sectors such as agro-industry and the paper industry, as well as improving the inherent characteristics (Gutiérrez *et al*., 2022).

Several preprocessing methods such as torrefaction have shown potential to address some of the limitations associated with the use of raw biomass in pyrolysis, gasification, or combustion processes (Parkhurst, Saffron, and Miller 2016; van der Stelt *et al*., 2011). Torrefaction or mild pyrolysis, is a thermochemical process occurring in the range of 200 to 300°C at atmospheric pressure, with limited or no oxygen presence (Thengane *et al*., 2020). This process is conducted in a non-oxidizing environment at temperatures ranging from 200 to 300°C (Chen *et al*., 2021). Torrefaction can also be carried out with a limited amount of oxygen in the gas phase (oxidative torrefaction) (Devaraja *et al*., 2022), thereby potentially reducing costs due to the exothermic oxidation reactions of biomass leading to widespread application in the industry (Leontiev *et al*., 2018). Although research has examined the applications of torrefaction and enhanced biomass, information on system integration and practical applications in the industry remains insufficient (Kusrini *et al*., 2018). There has been a significant increase in commercial advancement and adoption of biomass torrefaction technology recently, as shown by a significant increase in the number of operational demonstration plants (Hazra *et al*., 2023; Wilén *et al*., 2014; Koppejan *et al*., 2012).

The widespread adoption has shown the need to develop a model that predicts the properties of torrefied biomass or improves torrefaction conditions (Adeleke *et al*., 2020). This will facilitate the design of large-scale torrefaction equipment and optimize the process overall (Liu *et al*., 2023). Torrefaction technology requires development to create predictive models that can be used for assessing the viability of the process. For example, (Watts *et al*., 2023) used a regression model to determine the optimal torrefaction temperature using thermogravimetric data. This shows the need for idea identification of variations among the parameters influencing oxidative torrefaction.

Various regression methods that are available vary based on the type of variables and the assumed functional relationship. Among these methods, linear regression is the most fundamental and powerful in terms of information (Mahbobi and Tiemann, 2015). Linear regression assumes that the relationship between two variables is linear or can be linearized through some transformation. In this context, the observed data show a potential linear relationship among variables. However, multiple linear regression is considered the fit model since the Higher Heating Value (HHV) is the dependent variable, while temperature and oxygen concentration serve as independent variables. This model assumes that more than one independent variable influences or correlates with the value of the dependent variable (Granados, 2016).

Angelique (Conag *et al*., 2019), proposed a new predictive model for the HHV based on components of Sugarcane Residue (SCR), which were both raw and torrefied due to the inadequacy of existing models. Although moisture correlated negatively with the HHV of fuels, it is often excluded in conventional models. Despite the negative contribution of moisture because of combustion, its removal was observed to require additional energy which affected HHV. The model was established through multivariate linear regression with experimental and bibliographic data, achieving a minimum R2 of 0.90, with a mean absolute error of less than 6% and a mean bias of less than 1%. This model aimed to anticipate the potential use of SCR as a renewable energy source (Conag *et al*., 2019).

Wei-Hsin Chen et al. investigated the production of biocarbon and the yield of sugarcane bagasse torrefaction. The experiment was carried out using bilinear interpolation (BLI), inverse distance weighting interpolation (IDW), and regression analysis for predictions. The results showed that torrefied biomass at 275°C for 60 minutes or at 300°C for 30 minutes or more was suitable for biocarbon generation, as a low-carbon impact alternative to coal with low energy efficiency at 300°C. All three methods were suitable for predicting yield, with IDW showing an error below 5%. Therefore, second-order regression analysis was recommended for more accurate predictions (Chen *et al*., 2017).

(Oladosu *et al*., 2024) conducted an experiment using a tubular furnace for torrefaction, exploring the effects of temperature, retention time, moisture content, and particle size on HHV as well as energy yield (EY) of Bambara groundnut shell (BBGS). The results showed an optimal HHV of 21.78 MJ/kg with 1 mm particles, a temperature of 260°C, 23 minutes retention, and 10% moisture. The model obtained was applied to validate the input-output relationships using Response Surface Methodology (RSM) and Bayesian Information Criterion (BIC) stepwise regression, developing a regression model with a balance between interpretability and solid predictive performance.

Ighalo *et al.* (2020) explored an innovative method to predict HHV of biomass using a linear regression algorithm (LRA) and stochastic gradient descent (SGD) in a machine learning environment. The experiment was based on a dataset comprising 78 proximate and ultimate analyses. The results showed that LRA model had higher accuracy compared to SGD. The evaluation was also carried out using stratified cross-validation, stratified random splits, and holdout testing, obtaining a coefficient of determination R2>0.999 in all cases. The research suggested that LRA and SGD were highly accurate artificial intelligence models for predicting biomass HHV (Ighalo *et al*., 2020).

Qian *et al.* (2018) developed regression models based on proximity to anticipate the HHV of poultry waste (PW). The data of PW was obtained from literature to build the models, which were validated with additional samples and compared with previous models. The most accurate model integrated linear terms (all proximate components), polynomial terms (quadratic and cubic terms of volatile matter), and interaction effects (fixed carbon and ash). The results showed a higher R2 (91.62%) and lower estimation errors compared to previous models, serving as a potential tool for predicting PW HHV without the need for expensive equipment (Qian *et al*., 2018).

Based on the description, this research represents a significant contribution to the existing knowledge on oxidative torrefaction of sugarcane bagasse and the prediction of calorific value by developing and applying a multiple linear regression model. By addressing the influence of temperature and oxygen concentration, the analysis aims to explore biomass conversion mechanisms. This offers a precise tool to optimize the processes, promote more efficient, and sustainable practices in energy production from agricultural waste. Therefore, the hypothesis states that both temperature and oxygen concentration during oxidative torrefaction have a significant impact on the calorific value of sugarcane bagasse. Therefore, this research aimed to develop a predictive model for the calorific value of sugarcane bagasse following torrefaction process using temperature and oxygen concentration as input parameters.

This research presents a novel method by developing a predictive tool to estimate the calorific value of sugarcane bagasse torrefied under controlled conditions of temperature and oxygen concentration. Compared to previous reports, this research integrates a detailed analysis of the correlation between specific variables such as oxygen concentration and temperature, providing greater precision in the estimation of energy value of the biofuel. Furthermore, the use of mathematical models to represent the experimental data contributes significantly to improving the understanding of torrefaction process which serves as fundamental for future optimizations in the production of fuels from biomass.

2. Methods

Experimental research was conducted using sugarcane bagasse as biomass, subjected to an oxidative torrefaction process. Initially, particle size was controlled within a range of 500 µm to 850 µm (Abdulyekeen, Daud, and Patah, 2024) and 1 kg was used. The sample was dried at 105°C for 24 hours according to the procedures of (Liborio et al., 2023). This control of particle size and standardized drying process ensured homogeneous initial conditions for biomass before torrefaction process, thereby contributing to the consistency and reproducibility of experimental results (He *et al.*, 2023).

2.1. Experimental Setup

The reactor consisted of a sealed chamber designed for torrefaction, supplied with inert gases such as nitrogen and oxygen to create a controlled environment. The role of nitrogen (N2) in the oxidative torrefaction process was essential to creating a controlled environment within the reactor. Nitrogen acted as an inert gas that prevented the undesired oxidation of biomass during the process. By introducing nitrogen into the sealed chamber, an oxygen-free environment was created, preventing spontaneous combustion and other undesired effects associated with the presence of oxygen. This enables torrefaction to be conducted in a more controlled and predictable manner, ensuring the quality and consistency of the final products obtained from the process. Within this chamber, temperature and oxygen concentration are monitored and regulated to ensure optimal conditions throughout the process. Exhaust gases were also maintained, allowing thorough monitoring of the products from torrefaction, as shown in Figure 1.

The oxidative torrefaction process included controlling the flow of nitrogen, acting as an inert gas, and oxygen (1). To regulate this flow, Pure nitrogen, and synthetic air were used as a mixture of oxygen and nitrogen. Both gases passed through a mixer before entering the reactor (2), where temperature was monitored (3). The resulting gases were filtered to capture particulate matter.

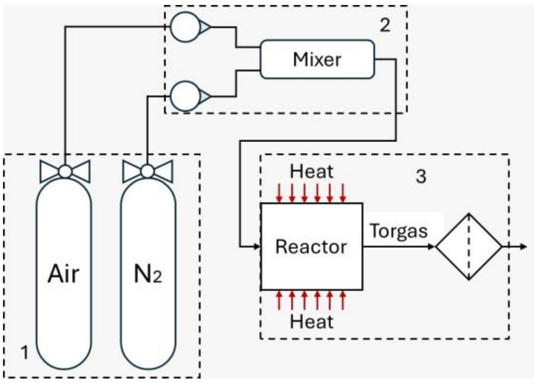

Figure 1 Schematic diagram of the experimental setup

2.2. Parameters

To conduct torrefaction, temperatures ranging from 200 to 300°C were applied, alongside oxygen concentrations of 0%, 10%, and 20%, each for 30 minutes, as shown in Table 1. The 0% oxygen setting showed pure nitrogen input, while 20% represented the atmospheric oxygen level, and 10% denoted an intermediate mixture between these extremes. The variation in these parameters facilitated subsequent biomass analysis using a calorimetric bomb to obtain diverse HHV.

The 30 minutes time period was selected in the experimental protocol for torrefaction of sugarcane bagasse to allow adequate assessment of how torrefaction conditions vary during the period. This specific period, along with variations in temperatures and oxygen concentrations, included a significant range of torrefaction conditions. Furthermore, the duration was considered sufficient to induce significant changes in the properties of sugarcane bagasse, including HHV, while maintaining a practical and manageable duration for the experiments.

Table 1 Temperatures and Concentrations

Temperature °C	Oxygen concentration (%)		
200	0	10	20
220	0	10	20
240	0	10	20
260	0	10	20
280	0	10	20
300	0	10	20

2.3. Model

A multiple linear regression model was used for this analysis, where the dependent variable was HHV, while the independent variables consisted of temperature and oxygen concentration per volume. Using the RStudio software environment, comprehensive assessments were conducted, including the analysis of collinearity among variables, inspection of regression residuals, determination of the coefficient of determination (R2), coefficients associated with the linear equation, as well as F-tests and other relevant statistical diagnostics. This method allowed for a comprehensive and rigorous evaluation of the relationship between predictor variables and the response variable within the context of multiple linear regression model. In the context of the multiple linear regression model, it was presumed that events follow a functional structure defined by equation 1:

$$y_j = b_0 + b_1 x_{1j} + b_2 x_{2j} + \cdots + b_k x_{kj} + u_j \quad (1)$$

where:

- y_j represents the dependent variable, in this case, the calorific value of the torrefied sugarcane bagasse for sample j.
- b_0 is the independent term or intercept, which shows the expected value of y_j when all independent variables x_{ij} are equal to zero.
- b_1, b_2,..., b_k are the regression coefficients showing the expected change in y_j for each unit change in the independent variables x_{1j}, x_{2j},..., x_{kj} respectively.
- x_{1j}, x_{2j},..., x_{kj} represent the independent variables, in this case, the experimental conditions such as oxygen concentration and temperature for sample j.

- u_j is the error or random disturbance term, which captures the influence of factors not included in the model.

This formulation aims to capture the linear relationship between predictor variables and the response variable, thereby enabling a quantitative interpretation of the influence of temperature and concentration on HHV.

3. Results and Discussion

The results obtained through the calorimetric bomb are presented in Table 2, where values of HHV are recorded based on temperature and concentration. The independent and dependent variables were initially assessed for collinearity, as shown in Table 2. This was carried out to determine the existence of linear relationship, an essential condition for the application of the regression model. The analysis was based on a correlation matrix, the content of which was visualized in Figure 2.

Table 2 Data obtained from the calorimetric bomb

Temperature °C	Concentration %	HHV (kJ/kg)
200	0	18934
220	0	19493
240	0	20241
260	0	21328
280	0	21658
300	0	23827
200	10	18950
220	10	20381
240	10	21130
260	10	21493
280	10	24860
300	10	25841
200	20	19683
220	20	20716
240	20	21027
260	20	21602
280	20	24718
300	20	26988

Oxidative torrefaction could be more favorable because the presence of oxygen during the process was able to reduce energy loss, improve efficiency and profitability, modify biomass properties. This phenomenon contributed to high handling and energy density, offering an enhanced final product quality with lower formation of undesired compounds. According to Table 2, there was an increasing trend in HHV as torrefaction temperature rose. This suggested that higher temperatures led to greater biomass densification and decomposition, causing elevated fixed carbon content and calorific value. Additionally, HHV values were higher for lower oxygen concentrations (0% and 10%), compared to an oxygen concentration of 20%. This showed that the presence of oxygen during torrefaction contributed to partial oxidation of the biomass, which could reduce carbon content and calorific value. The analysis was based on a correlation matrix, as shown in Figure 2.

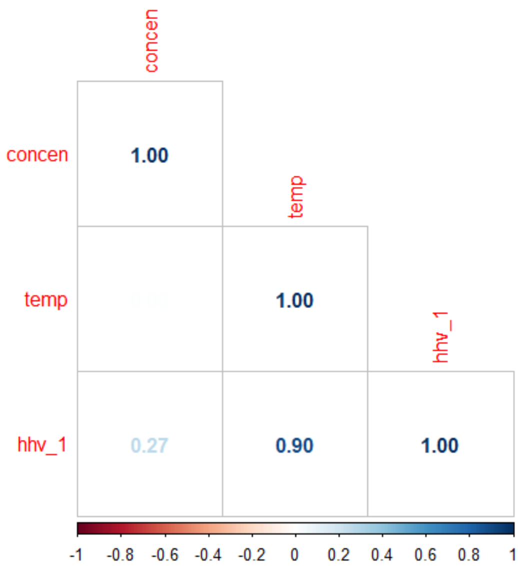

Figure 2 Correlation matrix among the variables

Figure 2 shows a correlation matrix between the variables used in the research: oxygen concentration (concen), temperature (temp), and Higher Heating Value (HHV_1). Each component of the matrix is described below:

- Correlation between concentration (concen) and temperature (temp): The correlation coefficient was 0.0, showing that there was no significant linear relationship between these two variables. This suggested that oxygen concentration did not vary proportionally with temperature in the roasting process.
- Correlation between temperature (temp) and Heating Value (HHV_1): The coefficient of 0.90 suggested a strong positive correlation, showing a corresponding increase in temperature alongside heating value. This showed the importance of temperature as a significant factor in optimizing torrefaction process to improve energy content of bagasse.
- Correlation between concentration (concen) and Heating Value (HHV_1): The coefficient of 0.27 showed a weak positive correlation, suggesting that oxygen concentration has a minor influence on heating value compared to temperature.

The matrix included a color code on the lower scale, ranging from -1 (perfect negative correlation) to 1 (perfect positive correlation). The colors showed the magnitude and direction of the correlations, where darker shades show a stronger relationship and lighter represent weak or no correlations. Following this confirmation, RStudio software was used, setting HHV as a function of temperature and concentration, with the result shown in Table 3.

3.1. Residual Value

The initial exploration of the summary of linear regression showed the assessment of residuals. Based on Table 3 and Figure 3, the residuals showed a uniform distribution, which tended to be symmetric. This suggested that the mean value was close to zero, while the maximum and minimum values including 0.25 and 0.75 percentiles showed similarities with opposite signs. The observation suggested that the model was appropriate as the residuals did not show significant systematic patterns, thereby supporting the validity of the applied linear regression.

Table 3 Distribution and evaluation of linear regression model residuals

Residues:	Min	1Q	Median	3Q	Max
	-1611.42	-334.73	67.22	374.35	1309.66

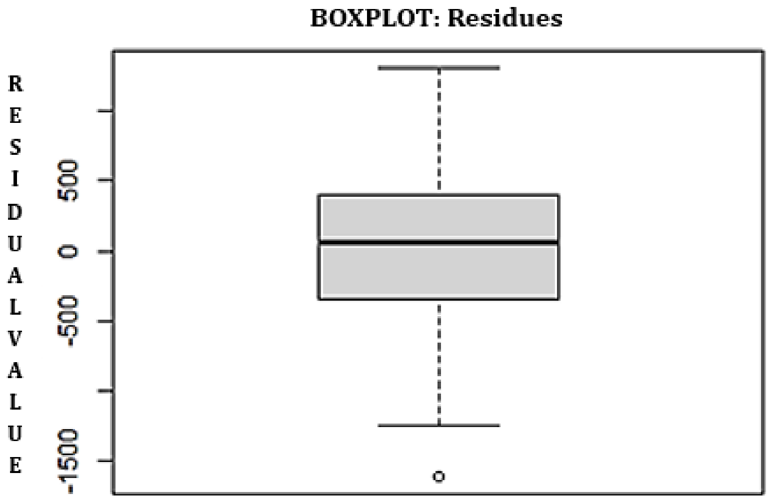

Figure 3 Boxplot of the distribution of residual values

Figure 3 shows a boxplot of the residuals obtained from the predictive model used in the research. This plot provided valuable information for analyzing the distribution of the residuals, identifying possible outlier, as well as evaluating the symmetry and dispersion of the errors.

- Median: The central line within the box represented the median of the residuals, which was close to 0. This showed that the model errors were balanced between overpredictions and underpredictions, suggesting a good model fit.
- Box (IQR - Interquartile Range): The box enclosed the interquartile range (IQR), which represented 50% of the data. In this case, the residuals were mainly concentrated between values of approximately -500 and 500. The concentration was around the median showing that most of the model errors were within a reasonable range.
- Whiskers: The whiskers in the plot extended to the minimum and maximum values, excluding outliers. In this case, the whiskers showed a dispersion that extended from approximately -1500 to 1000, showing some limited variability in the residuals.
- Outliers: A point outside the range of the whiskers was observed, which corresponded to an outlier. This showed a specific data point where the model had a considerably larger error, suggesting the need for a detailed review to determine a special case or an error in the data. This boxplot showed that the model residuals were properly distributed, with acceptable symmetry and a limited presence of outliers. Most of the errors were concentrated near 0, which supported the accuracy and stability of the proposed predictive model.

3.2. Coefficients

After analyzing the residuals and confirming the model accuracy, some coefficients were observed, as shown in Table 4.

Table 4 Coefficients of the Linear Regression Model

Coefficients:	Estimate	Std. Error	t-value	Pr(>|t|)	
(Intercept)	5649.31	1546.893	3.652	0.00236	**
Concentration	77.108	25.301	3.048	0.00814	**
Temperature	61.623	6.048	10.189	3.90E-08	***
Signif. codes:	0="***"	0.001="**"	0.01="*"	0.05=" "	1=

The table shows the estimated coefficients for each variable in the linear regression model, together with the standard error, t-value and associated p-value. Significance levels are indicated by codes: *** for p < 0.001, ** for p < 0.01 and * for p < 0.05, while the absence of a symbol indicates that p > 0.05, which means that the coefficient is not statistically significant. These significance values reflect the strength of the relationship between the predictor variables and the response variable in the model; thus, coefficients with p less than 0.05 are considered statistically significant, indicating a strong association in the context of the fitted model.

In addition to providing the coefficients b_0, b_1 *and* b_2 of the equation, the regression summary included the standard error. Specifically, the standard error served as a measure of the distance between the observed values in the sample and the values predicted by the regression line. This error allows the construction of confidence intervals for the estimated coefficients, as shown in Table 5. The analysis contributed to the evaluation of the accuracy and reliability of the estimated coefficients within the context of multiple linear regression model.

Table 5 Confidence Intervals for Estimation Coefficients with 95% Confidence Level

Reliability	(Intercept)	Concentration	Temperature
2.50%	2352.19004	23.18087	48.73173
97.50%	8946.43695	131.0358	74.51399

The $t - value$ and the $P_r(|t|)$ are available, which are essentially used to accept or reject the null hypothesis $H_o: b_1 = 0$. When b_1 or b_2 is null, it will show the absence of a linear relationship. Asterisks (*) show the significance level of a variable for the linearity of the model. The concentration variable is highly significant, while the temperature is significant, reaffirming non-collinearity.

The analysis of $P_r(|t|)$ and confidence intervals can reject the null hypothesis (H_o) as the values show a high linear relationship. A relevant piece of information is the coefficient of determination R^2, which reaches 0.8829 with an adjusted R^2 of 0.8673. This shows that the model explains 88.29% of the variability in HHV based on temperature and oxygen concentration. Moreover, the value of R^2 is similar to the adjusted R^2, suggesting that the independent variables are relevant to the model.

3.3. ANOVA

In the analysis of variance represented in Table 6, the $F - value$ being greater than 1 rejects the null hypothesis, with a $p - value$ of $1.03x10^{-07}$, showing significance in the overall model. This is further supported by the significance of the $p - values$ of the independent variables.

3.4. Residuals

Analyzing the residuals, the linearity of the model can be easily observed. For example, plotting the residuals against the variable shows the distribution of values, including some outliers, as presented in Figure 4.

Table 6 Analysis of Variance (ANOVA)

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
Concentration	1	7134834	7134834	9.2882	0.008142	**
Temperature	1	79744907	79744907	103.813	3.90E-08	***
Residuals	15	11522387	768159			

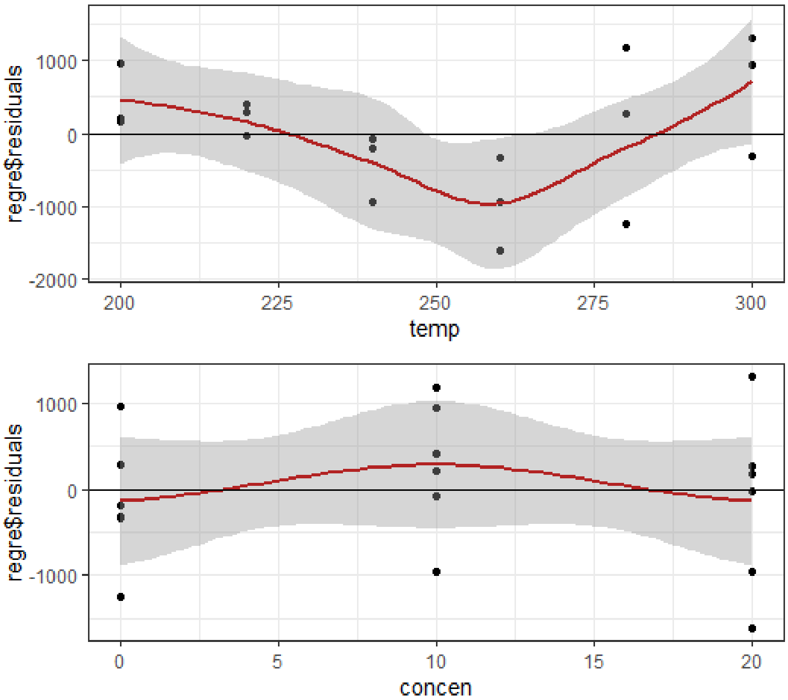

Figure 4 Distribution of residuals versus temperature and concentration to assess model linearity

Another method to assess the normality of the residuals is through a Q-Q Plot, as shown in Figure 5. This plot shows data distribution, indicating that the central data points are more closely related to the line compared to the ends, namely outliers.

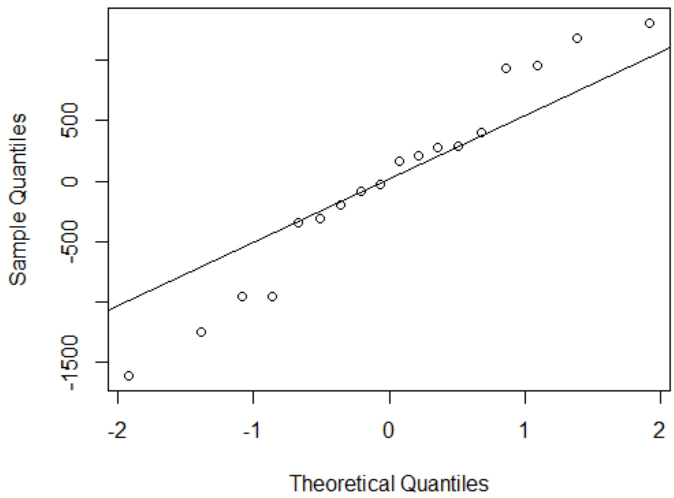

Figure 5 Q-Q plot to assess normality of residuals

Based on the results, an oxidative torrefaction process can predict the HHV with temperature and oxygen concentration at an 88.29% confidence level using the following model, as shown in equation 2:

$$HHV = 5649.313 + 77.108 * \text{concentration} + 61.623 * \text{temperature} \quad (2)$$

The results have significant practical implications for the biomass industry, providing an accurate predictive tool for optimizing the oxidative torrefaction processes of sugarcane bagasse. The ability to predict calorific value of bagasse based on temperature and oxygen concentration enables industry stakeholders to make informed decisions regarding optimal operating parameters to maximize energy efficiency and the quality of the final product. Furthermore, the results suggest essential areas for future research, such as exploring other process variables that can influence calorific value, as well as validating the proposed model in different industrial contexts and with several types of biomass. This line of future research can lead to further improvements in the efficiency and sustainability of energy production from biomass, significantly contributing to the transition towards cleaner and renewable energy sources.

Predicting the HHV of torrefied biomass is essential for assessing efficiency, energy use, and optimizing torrefaction processes to ensure the viability of biomass as a renewable energy source. However, the ability of this model to predict the HHV of other biomasses requires external validation using different experimental data to show broader applicability.

4. Conclusions

In conclusion, this research applied a multiple linear regression model to predict the HHV of sugarcane bagasse based on oxidative torrefaction using temperature and concentration as predictor variables. The results showed a significant relationship between HHV and temperature, while the correlation with concentration was weaker. The model showed good predictive capability, explaining 88.29% of the variability in HHV. The examination of coefficients showed that both temperature and concentration were significant variables in predicting HHV. The validity of the estimated coefficients was supported by confidence intervals and significance values. However, the unexplained portion, accounting for 11.71% could be attributed to factors such as insufficient samples or the presence of outliers. The regression assumptions were also satisfied, since F-test showed a p-value of $1.03x10{-}07$, and the model achieved a confidence level of 95%. Although the model showed accuracy in predicting HHV, there was a suggestion for improvement by including other relevant parameters such as volatile materials and moisture. Furthermore, the economic viability of oxidative torrefaction in the presence of oxygen to reduce costs was discussed. These results supported the application of oxidative torrefaction as an effective strategy to enhance the calorific properties of sugarcane bagasse, potentially driving more sustainable practices in energy generation from waste. The model presented in Equation 2 was developed based on data obtained from an experiment conducted within a 30 minute torrefaction period. Although the design was the experimental setup, its underlying principles and methodology could potentially be applied to other cases with similar conditions. Extrapolating the model to significantly different torrefaction durations or conditions could require additional validation and adjustment. The coefficients and relationships established in the model were not directly translated to scenarios beyond the scope of the original experimental design. Therefore, careful consideration and possibly recalibration of the model were recommended for application to other torrefaction durations or conditions to ensure accuracy and reliability.

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Conflict of Interest

The authors declare no conflict of interest.

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