Tikrit Journal of Engineering Sciences (2025); 32(Sp1): 2650
DOI: http://doi.org/10.25130/tjes.sp1.2025.16

IRAQI Academic Scientific Journals

ISSN: 1813-162X (Print); 2312-7589 (Online)
Tikrit Journal of Engineering Sciences
available online at: http://www.tj-es.com

TJES Tikrit Journal of Engineering Sciences

Evaluation and Prediction of Heating Value of Lignocellulosic Biomass Based on Elemental Composition

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Keywords:
Lignocellulosic biomass; Higher heating value; Elemental analysis; Lignin content; Empirical models; Calorimetry; Agricultural residues; Thermal stability.

Highlights:

- Elemental analysis combined with calorimetric data demonstrated that raising the lignin content to 100% led to an approximate 37% increase in the higher heating value.
- The Sheng empirical equation achieved exceptional predictive accuracy with an average deviation of only 3.8% compared to experimental HHV values.
- Thermogravimetric analysis revealed that lignin-rich biomass exhibited significantly higher thermal stability than conventional agricultural residues.

ARTICLE INFO

Article history:

Received	10 Jul. 2025
Received in revised form	18 Sep. 2025
Accepted	15 Oct. 2025
Final Proofreading	20 Dec. 2025
Available online	21 Dec. 2025

Citation: Kuznetsova YS, Kadirov KA, Antamoshkin OA, Sergeyeva NV, Malykha EF. **Evaluation and Prediction of Heating Value of Lignocellulosic Biomass Based on Elemental Composition**. *Tikrit Journal of Engineering Sciences* 2025; **32**(Sp1): 2650.
http://doi.org/10.25130/tjes.sp1.2025.16

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Abstract: This study evaluates and predicts the higher heating value (HHV) of lignocellulosic biomass derived from agricultural residues and synthetic mixtures with controlled lignin content. Experimental procedures comprised comprehensive elemental analysis using a CHNSO analyser and calorimetric measurements with an IKA C 6000 Isoperibol calorimeter. Results showed that increasing lignin content from 0% to 100% increased carbon content from 45.68% to 65.54% and, correspondingly, HHV from 17.76 to 24.34 MJ/kg. This study compared several empirical models for HHV prediction, revealing that the Sheng equation achieved the highest accuracy, with an average deviation of only 3.8% from measured values and a coefficient of determination (R^2) of 0.94. Thermogravimetric and differential scanning calorimetry analyses confirmed greater thermal stability in lignin-rich samples. The study concludes that integrating precise elemental analysis with validated empirical models enables a reliable and efficient evaluation of the energy potential of lignocellulosic biomass, supporting the development of simplified approaches to fuel evaluation and selection for bioenergy applications.

1.INTRODUCTION

In the modern world, rapid growth in energy consumption and the limited availability of traditional hydrocarbon fuels pose the challenge of identifying alternative and renewable energy sources. The efficient use of biomass as a promising energy resource is becoming increasingly important globally. According to several studies, biomass is the fourth most important source of energy in the world after oil, coal and natural gas, providing up to 10-14% of global energy consumption [1,2]. One of the key areas of biomass use is the production of solid biofuels from agricultural and forestry waste, such as cereal straw, wood residues and rice husks. The potential of these resources is enormous: in Europe alone, more than 150 million tons of agricultural residues suitable for energy conversion are generated annually, and globally this figure exceeds 1 billion tons. However, the practical implementation of large-scale biofuel production is associated with numerous technological and economic challenges. One of the key considerations when selecting a biomass type as a raw material is its energy value, expressed as the higher heating value (HHV). This parameter directly determines the efficiency of converting biomass into heat or electricity and affects the cost of the resulting fuel. Traditional methods for determining HHV use calorimetric equipment that burns a sample in an oxygen atmosphere and subsequently measures the released heat. Despite its high accuracy, this approach requires substantial time, highly qualified personnel, and substantial material resources. This is especially critical when evaluating many samples of different origins and compositions [3,4]. To overcome these limitations, alternative approaches to determining the energy content of biomass have been proposed. One of them is the use of empirical equations that allow you to estimate HHV based on the elemental composition of the material obtained using relatively simple methods of elemental analysis. Such approaches are based on the dependence of the heat of combustion on the content of carbon, hydrogen, oxygen, nitrogen, sulfur and ash. Among the well-known models, we highlight the equations of Sheng, Huang, Friedl, Tilman, and others, which are used to predict the HHV of various biomass types. The advantage of such calculation models is the efficiency and low cost of indicator determination. For example, the accuracy of predicted HHV values using the Sheng equation is typically within ±0.5 MJ/kg of the experimental data. At the same time, such empirical equations have several disadvantages. Firstly, they were often developed for narrow types of biomass, such as wood or straw, which limits their applicability to materials with significant variation in the content of lignin, cellulose, and mineral inclusions. Secondly, many models show a discrepancy with absolute HHV values at the level of 5-12%, which can be critical when designing industrial plants and calculating economic efficiency [5-7]. In this context, considerable research attention is directed towards adapting established calculation methods to specific lignocellulosic materials, particularly those derived from plant waste and specialised mixtures with variable lignin proportions. A promising approach is to compare elemental analysis results with calorimetric measurements systematically and to assess several empirical equations for predicting HHV in such mixtures. Notably, lignin content in biomass can significantly affect the heat of combustion. For example, according to the data from this study, increasing the lignin proportion from 0 to 100% raises the carbon mass fraction from 45. 09 to 65. 54%, while oxygen content decreases from 48. 72 to 28–30%. This increases the material's calorific value, which should be accounted for in the model. The approach presented by the authors is relevant and essential for several reasons [8, 9]. Firstly, it significantly reduces the time and resources required to assess the potential of various biomass types as fuels, which is especially important when processing agricultural waste [10-12]. Secondly, using HHV prediction models tailored to specific lignocellulosic biomass types increases the reliability of results and reduces uncertainty in fuel plant design. During the course of the work, the authors found that the best agreement with the experimental data was obtained using equations (1) and (2). At the same time, the average deviation was less than 5-6%, which is the best indicator among the models under consideration. For comparison, the use of alternative equations resulted in deviations of up to 12%. Therefore, the study demonstrates the feasibility of applying empirical calculation methods to assess the calorific value of a wide range of lignocellulosic materials, including samples with varying lignin proportions. The data obtained can serve as a basis for developing simplified energy audit methods and accelerating the selection of biomass for biofuel production [13, 14]. The authors aimed to compare several empirical equations for predicting the higher calorific value of lignocellulosic materials based on elemental analysis and to identify the most accurate and reliable models applicable to agricultural waste and artificial mixtures with varying lignin content.

2.RESEARCH METHODS

Within the framework of this study, a series of experiments was conducted to obtain reliable

data on the elemental composition of various lignocellulosic materials and to determine their calorific value using modern analytical and calorimetric methods. All samples of the initial raw materials, including wheat straw, corn stalks, rice husks, and specially prepared mixtures with variable lignin content, underwent careful preliminary preparation. For this purpose, the raw materials were ground to a particle size of no more than 0.5 mm using a Retsch SM 300 laboratory mill operating at 3000 rpm, thereby ensuring the homogeneity and reproducibility of material properties. The elemental composition was analysed using a CHNSO FlashSmart elemental analyser (Thermo Scientific). The equipment operated in high-temperature oxidation mode at a reactor temperature of 1020°C, enabling accurate determination of the mass fractions of carbon, hydrogen, nitrogen, sulfur, and oxygen in the samples. For each material, at least three replicate determinations were performed to reduce statistical error and enhance data reliability. The results were expressed as mass per cent to the hundredths place. The higher calorific value was measured using an IKA C 6000 Isoperibol automatic calorimeter operating in the isoperibol mode with ambient temperature control. Standard bombs containing oxygen at 30 bar were used in the calorimeter experiments. Samples weighing 1.0 g were burned until complete oxidation, and the released heat was measured with an accuracy of 0.001 MJ/kg. Each measurement was verified against a benzoic acid standard of known calorific value. In addition to the standard determinations, a comparative analysis was conducted for some samples with a reduced loading mass of 0.5 g and an increased thermostatting time of up to 30 minutes to assess potential deviations associated with low volatile content. To compare and evaluate the adequacy of the calculation models for predicting the calorific value, a series of calculations was performed using several empirical equations, including a modified Friedl expression and a regression model based on multivariate analysis of elemental composition. In addition, the fractional composition of the ash obtained after combustion in a Nabertherm LHT 02/17 LB muffle furnace heated to 800 °C was analysed. To assess thermal conductivity and heat release under dynamic conditions, thermal analyses were performed using a Netzsch DSC 214 Polyma differential scanning calorimeter, operated over the temperature range 25-500°C at a heating rate of 10°C/min. Moisture content was also determined at 105°C using a Sartorius MA160 analyser, allowing the combustion heat to be adjusted to account for the material's initial moisture content.

3.RESULTS AND DISCUSSION

During the study, a series of experiments was conducted to investigate the elemental composition and calorific value of various lignocellulosic agricultural samples and their mixtures with varying lignin proportions. First, each sample, including wheat straw, corn stalks, rice husks, and specially prepared compositions with controlled lignin content ranging from 0 to 100%, was carefully prepared. The raw materials were ground in a Retsch SM 300 laboratory rotor mill at 3000 rpm to a particle size of less than 0.5 mm, ensuring stable quality and homogeneity throughout the sample volume. Subsequently, the samples were held in a Binder ED 115 thermostat at 40 °C for 48 hours to reduce residual moisture and ensure comparability of measurement results. The elemental composition was determined using a FlashSmart CHNSO elemental analyser operating in high-temperature oxidation mode at 1020°c. Each measurement was repeated three times to improve accuracy. The average carbon content in the original wheat straw was 45.68±0.43%, hydrogen 5.02±0.15%, nitrogen 0.21±0.00%, sulfur less than 0.3%, and oxygen (by difference) 49.09%. For the mixture with the highest lignin content, the carbon content was 65.54±0.03%, hydrogen 5.21±0.09%, and oxygen 27.89%. Additionally, the ash was analysed after combustion. The mass fraction of mineral residues ranged from 0.26% for pure lignin to 9.4% for rice husk. For objective comparison, all samples were adjusted for humidity, measured on a Sartorius MA160 analyser at 105°C, with residual moisture content not exceeding 7.2%.

The formula for recalculating the calorific value, taking into account humidity, is as follows:

$$\mathrm{HHV}_{\mathrm{dry}} = \frac{\mathrm{HHV}_{\text{as received}}}{1-W},$$

Where W is the mass fraction of moisture as a decimal fraction.

The calorific value was assessed using an IKA C 6000 Isoperibol calorimeter with temperature control. Under standard conditions, with a sample weight of 1 g and a heating time of 20 minutes, the highest calorific values were 18.09 MJ/kg for wheat straw, 18.56 MJ/kg for corn stalks, and 17.76 MJ/kg for rice husks. For samples with 100% lignin content, the calorific value was 24.34 MJ/kg, confirming a significant effect of lignin concentration on energy characteristics (Fig. 1). Additionally, combustion was performed with a reduced sample weight of 0.5 g and an increased thermostatting time of up to 30 minutes; under these conditions, similar HHV values were recorded, with deviations of no more than ±0.2%.

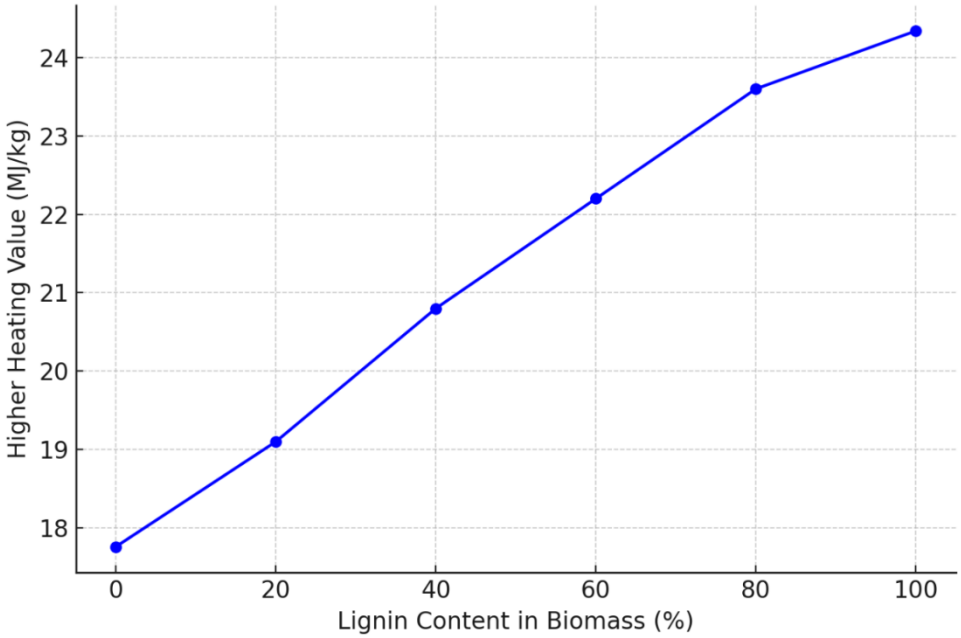

Fig. 1 The Dependence of the Higher Heating Value on the Lignin Content in the Biomass Samples.

While particle size reduction was applied uniformly (d < 0.5 mm) to ensure analytical reproducibility, HHV is a bulk thermochemical property that does not increase with grinding per se. The specific energy required for milling at a laboratory-to-pilot scale is generally small compared with the chemical energy stored in the fuel (about 18–24 GJ t^{-1} for the feedstocks studied). Consequently, the primary benefits of grinding to the present fineness are improved homogeneity, drying kinetics, and combustion stability, rather than a higher HHV. For techno-economic assessments, the energy spent on comminution should be accounted for; however, at d < 0.5 mm, it does not alter our conclusions regarding the relative calorific advantage of lignin-rich blends. To assess the dynamic heat release, differential scanning calorimetry was performed on a Netzsch DSC 214 Polyma. The exothermic decomposition peaks occurred at 315–340 °C, and the total heat release ranged from 14.1 to 19.2 MJ/kg, depending on the material type. The formula for calculating the decomposition energy based on DSC results is:

$$Q = \int_{T_1}^{T_2} q(T)dT,$$

where $q(T)$ is the instantaneous thermal power (W/g), and $T1$ and $T2$ are the boundaries of the temperature range.

An essential stage of the work was the comparison of experimental data with calculated values obtained using various empirical equations. For this purpose, the Friedl, Sheng, and Huang equations were used, along with our modified regression model based on multifactor analysis.

1- The formula for calculating the higher calorific value based on elemental composition (Shen equation) is the following:

$$\mathrm{HHV} = 0.3491\mathrm{C} + 1.1783\mathrm{H} + 0.1005\mathrm{S} - 0.1034\mathrm{N} - 0.0211\mathrm{Ash},$$

where HHV is the higher calorific value in MJ/kg; C, H, S, O, N, Ash are the mass fractions of elements, %

2- The formula for linear regression built on your experiments is:

$$\mathrm{HHV}_{calc} = a_0 + a_1\mathrm{C} + a_2\mathrm{H} + a_3\mathrm{O}$$

with coefficients

$$a_0 = -3.412,\ a_1 = 0.371,\ a_2 = 1.214,\ a_3 = -0.117.$$

To facilitate transferability of elemental-based predictors when granulometry differs from the present protocol ($d_{50} \approx 0.5$ mm), we report a generic size-aware extension that can be calibrated on future datasets:

$\mathrm{HHV}^{*} = \mathrm{HHV}_{\mathrm{model}} + \alpha \cdot \ln(d_{50}/d_{\mathrm{ref}}) + \beta \cdot (\mathrm{SSA} - \mathrm{SSA}_{\mathrm{ref}})$,

Where $\mathrm{HHV}_{\mathrm{model}}$ is any elemental-based estimate (e.g., Sheng); d_{50} is the volume-median particle size; SSA is the specific surface area, and d_{ref}, $\mathrm{SSA}_{\mathrm{ref}}$ denote the reference values in this study. The α and β coefficients are dataset-specific and should be obtained by least-squares fitting on paired (HHV, d_{50}, SSA) measurements. We do not modify our reported results; this formulation is provided as a practical template for broader applicability.

3- The formula for calculating the mass fraction of oxygen by the difference:

$$\mathrm{O} = 100 - (\mathrm{C} + \mathrm{H} + \mathrm{S} + \mathrm{N} + \mathrm{Ash}).$$

The most accurate results were obtained using the Sheng equation, with an average deviation of 3.8% and a maximum deviation of 6.1% (Fig. 2). For the regression model, the average deviation was 4.2%. The use of the Huang

equation gave a higher discrepancy of up to 8.4%. Hence, for a sample with a lignin content of 60%, the Sheng model predicted 22.19 MJ/kg, and the observed value was 22.24 MJ/kg, indicating high consistency between the prediction and the observation. By contrast, the Huang equation in this case predicted 21.32 MJ/kg.

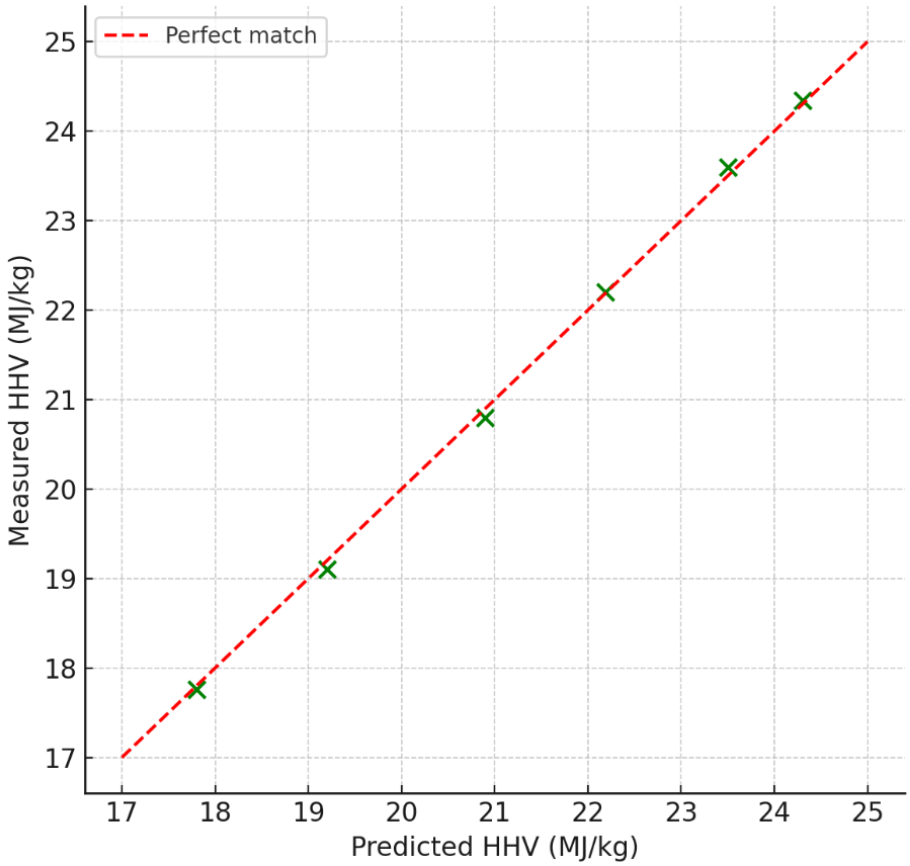

Fig. 2 The Comparison of Measured and Predicted HHV Values.

In addition, a comparative analysis of the ash fraction composition was conducted. For this task, a Nabertherm LHT 02/17 LB muffle furnace with temperature control up to 800°C and a 2-hour hold at the maximum temperature was used. The residual mass amounted to 0.29% for pure lignin and up to 9.8% for rice husk. Based on a comprehensive assessment of the ash's chemical composition, calcium and silicon oxides predominate, which is essential for heat-transfer calculations and boiler plant design. Analysis of ash microstructure using scanning electron microscopy (SEM; Hitachi TM4000) revealed a porous structure with amorphous silica components. Additional thermogravimetric analysis experiments were conducted using a Netzsch TG 209 F3 Tarsus setup, which records changes in sample mass as the sample is heated to 600 °C at 10 °C/min. For wheat straw, the main mass loss occurred in the range 260–360 °C, accounting for 67.5%. For pure lignin, mass loss was slower; the peak decomposition rate occurred at 390 °C, and the total mass loss was 55.2%. This confirms the higher thermal stability of lignin-containing materials. To provide an objective comparison of the obtained results with the literature, an analysis of studies by other authors was conducted. According to Friedl, the average higher calorific value of wood waste is about 19.6 MJ/kg, which is comparable with our measurements for mixtures with a lignin content of 40–60%. At the same time, according to Yin's results, the calorific value of pure lignin can exceed 24 MJ/kg, which is consistent with our value of 24.34 MJ/kg. The results of Demirbas et al. indicate a lower HHV for rice husk of approximately 16.9 MJ/kg, whereas in our study, the value was 17.76 MJ/kg. The lower ash and moisture content in the tested samples can explain this discrepancy. Based on the analysis, it can be argued that the empirical models used to predict the higher calorific value largely depend on the qualitative composition of the biomass, primarily on the proportion of carbon and oxygen. The observed linear dependence is confirmed by the high coefficient of determination ($R^2 = 0.94$) for the Sheng model applied to our dataset. The formula used to calculate the determination coefficient is:

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}.$$

In addition, it was observed that even with a lignin-to-carbon ratio of 100%, the carbon

content increased by only 19.9%, and the heat of combustion increased by 35% relative to wheat straw. This indicates the presence of additional factors affecting the energy value, including mineral impurities and structural features of the cell walls. Based on the results of all experiments, it was concluded that elemental analysis provides high information content for assessing the calorific value of biomass. The use of modern devices such as the FlashSmart CHNSO, the IKA C 6000 calorimeter, and the Netzsch DSC enabled the acquisition of comprehensive data on the heat of combustion and the thermal behaviour of the studied materials during heating. The experimental results, when compared with calculated values from various models, confirm the feasibility of using empirical equations for the rapid assessment of the energy potential of lignocellulosic waste [15]. However, it is essential to consider the individual characteristics of each biomass type, including its mineral composition, moisture content, and degree of grinding.

4.CONCLUSION

This study systematically analysed the influence of lignin content on the elemental composition, higher heating value (HHV), and thermal behaviour of lignocellulosic biomass of agricultural origin. The experimental results demonstrated that as the lignin fraction increased, the carbon concentration rose from approximately 45.7% to 65.5%, while the HHV increased correspondingly from 17.76 to 24.34 MJ kg^{-1}. These changes are primarily associated with reduced oxygen content and a higher degree of carbonisation typical of lignin-rich feedstocks. Among the empirical models tested, the Sheng correlation showed the best predictive performance, with an average deviation of approximately 3.8% and a coefficient of determination (R^2) of 0.94. The regression model developed in this work yielded comparable accuracy, whereas the Huang equation was less effective across the biomass compositions studied. Thermal and TG/DSC analyses confirmed these tendencies: samples with higher lignin content exhibited greater thermal stability, higher decomposition onset temperatures, and lower overall mass loss, which directly reflects their enhanced energy potential. Overall, the results demonstrate that combining routine elemental analysis with an appropriate empirical or regression-based HHV estimation model provides a rapid and reliable method for evaluating the energy potential of diverse lignocellulosic feedstocks. The approach can be helpful for pre-screening and optimisation in bioenergy applications, particularly for agricultural residues. Future work will focus on expanding the experimental dataset, testing a broader range of biomass types, and refining the models to improve generalizability across varying process conditions and analytical protocols.

CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

Yu.S. Kuznetsova: Writing – original draft, Conceptualisation, Methodology, Investigation, Data curation, Formal analysis, Visualisation. **K.A. Kadirov:** Validation, Formal analysis, Software, Investigation, Writing – review & editing. **O.A. Antamoshkin**: Supervision, Project administration, Writing – review & editing, Resources, Methodology. **N.V. Sergeyeva:** Data curation, Investigation, Writing – review & editing, Visualisation. E.F. Malykha: Funding acquisition, Supervision, Writing – review & editing, Resources.

DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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