PREDICTION OF HIGHER HEATING VALUE OF VARIOUS BIOMASSES USING THE EQUATION FOR THE HYDROTHERMAL CARBONIZATION METHOD ON BANANA BUNCHES

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ABSTRACT

Biomass thermal conversion relies on accurate estimation of fuel Higher Heating Value (HHV), traditionally obtained via costly bomb calorimetry. This study develops four new HHV correlations for homogeneous biomass processed via hydrothermal carbonization (HTC), using both proximate and ultimate analyses. Multiple linear regression was employed to generate these correlations, with a focus on homogeneous biomass. Rigorous benchmarking against open literature models revealed the superior accuracy of our proximate-based correlation (HHV = 967.171 - 8.684 Ash - 9.299 VM - 9.913 FC). These new correlations offer significant advantages: cost reduction through eliminating expensive calorimetry, and enhanced process efficiency by enabling precise thermal modeling and resource allocation. This research addresses the limitations of existing models, contributing to more reliable and cost-effective biomass utilization for sustainable energy production.

Keywords: *biomass, hydrothermal carbonization, higher heating value, proximate analysis, ultimate analysis.*

ABSTRAK

Konversi termal biomassa bergantung pada estimasi akurat nilai kalor yang lebih tinggi (HHV) bahan bakar, yang secara tradisional diperoleh melalui kalorimetri bom yang mahal. Penelitian ini mengembangkan empat korelasi HHV baru untuk biomassa homogen yang diproses melalui karbonisasi hidrotermal (HTC), menggunakan analisis proksimat dan ultimat. Regresi linier berganda digunakan untuk menghasilkan korelasi ini, dengan fokus pada biomassa homogen. Pembandingan yang ketat terhadap model literatur terbuka mengungkapkan akurasi superior dari korelasi berbasis proksimat kami (HHV = 967,171 - 8,684 Abu - 9,299 VM - 9,913 FC). Korelasi baru ini menawarkan keuntungan yang signifikan: pengurangan biaya melalui penghapusan kalorimetri yang mahal, dan peningkatan efisiensi proses dengan memungkinkan pemodelan termal yang tepat dan alokasi sumber daya. Penelitian ini membahas keterbatasan model yang ada, berkontribusi pada pemanfaatan biomassa yang lebih andal dan hemat biaya untuk produksi energi berkelanjutan.

Kata Kunci: biomassa, karbonisasi hidrotermal (HTC), nilai kalor tinggi, analisis proksimat, analisis ultimat.

1. INTRODUCTION

The relentless growth in global energy demand, coupled with the accelerating depletion of fossil fuel reserves, poses a major threat to both the security of our energy supply and sustainable economic growth. Addressing this urgent challenge necessitates a worldwide shift towards alternative and renewable energy sources, as well as a diversification of our fuel resources. Biomass stands out as a sustainable and promising choice due to its potential for balanced CO_2 emissions. However, unlocking the full potential of biomass and other organic wastes for energy generation hinges on a comprehensive understanding of their physical, chemical, and thermodynamic properties (AlNouss et al., 2020; Islam et al., 2015; Rajput, 1996).

An essential metric for energy analysis in any system is the fuel's Higher Heating Value (HHV). Its determination has traditionally relied on expensive and complex bomb calorimeters, which present constraints in terms of time and resources (Putra et al., 2022; Sobek and Werle, 2020; Kang et al., 2012). To address these limitations, researchers have developed correlations that allow HHV estimation based on the results of proximate and ultimate analyses. Although ultimate analysis offers direct data on the fuel's elemental composition, it involves specialized laboratory facilities and significant resource investment.

Proximate analysis provides a more accessible and economical way to assess biomass properties. It quantifies essential components like fixed carbon (FC), volatile matter (VM), and ash (ASH) in solid fuels, representing the non-volatile, gaseous, and unburnable fractions, respectively. This method reveals key biomass constituents, including fixed carbon content, volatile matter, ash content, and fuel moisture (Shaaban et al., 2014). The relative ease and cost-effectiveness of proximate analysis explain the growing preference for using correlations based on these values to estimate the HHV of fuels. Early pioneering work established a robust linear relationship between total calorific value (GCV) and fixed carbon content in biomass, yielding an impressive correlation coefficient of 0.9997. Further studies by Gonzalez and Cordoba (1997), as well as Jimenez and Gonzalez (1991), delved into the combined impact of fixed carbon and volatile materials on HHV.

To capture more complex relationships, multiple regression analysis, within a least-squares fitting framework, has been applied to create HHV correlations. These often focus on lignocellulosic feedstocks and specifically include both fixed carbon and volatile carbon content (Friedl et al., 2005a). Researchers like Xiaorul et al. (2023) have even used artificial neural network (ANN) based correlations for HHV, taking into account that diverse elemental compositions in materials like black anthrax create non-linear effects. Additional correlations based on the least-squares method combine proximate analysis results, including water content, and demonstrate reasonable accuracy with modest average error rates (Erdoğan, 2021; Chen et al., 2017). Despite the proliferation of these correlations, accuracy must be ensured through robust error analysis. Importantly, Yin (2011) highlights that simply creating new correlations isn't enough and offers a new correlation specifically factoring in volatile matter and fixed carbon content.

A key area for potential refinement in these correlations is the exploration of hydrothermal carbonization (HTC). HTC converts organic materials like banana bunches (BB) into solid fuel. Notably, variations in HTC parameters (temperature, time, and solid-to-water ratio) could influence the accuracy of existing HHV estimation correlations. The suitability and efficiency of different biomass sources for energy production hinge on reliable HHV determination methods. This research therefore aims to investigate the relationship between HTC process parameters and the HHV of banana bunches. It will then assess the accuracy of

existing HHV correlations for hydrothermally carbonized banana bunches. The ultimate goal is to refine current correlations or develop new models tailored to these materials, boosting our ability to predict their HHV and improving their assessment for energy generation.

2. METHOD

Experimental of Hydrothermal Carbonization

Hydrothermal carbonization (HTC) was employed to convert banana bunches into solid fuel. The experiments were conducted in a 1-liter reactor where banana bunches were subjected to high temperatures (180°C and 200°C) and pressure. Process duration (15, 30, and 45 minutes) and banana bunch to water ratio (1:1, 1:2, and 3:2) were systematically varied. Each trial used 200g of banana bunches. These conditions promote hydrolysis, dehydration, and polymerization of the organic components (cellulose, hemicellulose, and lignin) leading to the formation of carbon-rich hydrochar. Constant stirring (100 rpm) ensured homogenous mixing, and a shutoff valve facilitated safe pressure release.

Once this process is complete, the materials produced are filtered before being analyzed to determine their instantaneous, final, and calorific properties. Evaluation of ash, volatile matter, and fixed carbon content (proximate analysis) in solid products was carried out using Leco TGA-601. To achieve this, the sample was subjected to 102°C for 24 hours in an oven and then cooled in a desiccator filled with silica gel, according to ASTM-E871 instructions. Moisture content was determined according to ASTM-E871 by calculating the difference between initial and final weight. Meanwhile, the ash ratio was established according to ASTM-E1755 standard by burning the dry sample at 575°C for 5 hours in a furnace. Volatile content was determined by burning the sample at 950°C for 7 min, also following ASTM-E872 protocols. The fixed carbon fraction is calculated as the percentage remaining after the completion of the entire analysis. For the ultimate analysis, the determination of carbon (C), hydrogen (H), and nitrogen (N) content was carried out using the Elementar Vario Macro instrument, and the oxygen (O) content was calculated by difference. Finally, the total calorific value (GCV) was measured using a Leco AC500 bomb calorimeter.



Figure 1. The scheme of the experimental apparatus of the HTC process

Energy yield represents the proportion of initial energy present in biomass remaining after carbonization. When biomass carbonizes, some energy-rich components are preserved, while less energy-rich components are lost. Therefore, the overall energy content of biomass will decrease, even though the energy density increases. The concept of energy efficiency is of considerable practical importance, especially when biomass serves as a source for energy Reka Lingkungan – 83

conversion processes. Energy efficiency provides a quantitative measure of the energy retained in biomass after torrefaction, and its definition can be summarized as follows:

$$Energy \ yield = \frac{mass \ of \ hydrochar \ x \ HHV}{mass \ of \ biomass \ x \ HHV}$$
(1)

Data Collection

Tables 1 and S1 present a comprehensive dataset comparing reference HHV data, test results, reference HHV prediction formulations, and newly developed BB HHV prediction formulations. These formulations are based on both proximate and ultimate analyses of various biomass sources, including agricultural biomass, vegetables, food crops, and solid waste. This dataset is notably diverse and valuable for comparative HHV modeling studies. To derive correlations, regression analysis was performed on five data points: proximate analysis components (VM, FC, Ash) and ultimate analysis components (C, H, O, N, S). From this analysis, four new correlation formulations were generated, comprising two based on proximate analysis and two on ultimate analysis. Finally, a total of 550 data points were used to assess the accuracy of the newly developed BB prediction formulations against established reference formulations.

Table 1. The summary of pu	blished correlation to	predict the HHV of biomass
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Model	Equation Model	Analysis	Unit	References
Model 1	HHV = 19.914 – 0.2324 Ash	Proximate	MJ/kg	Nhuchhen and Abdul Salam, 2012
Model 2	HHV = 0.3536 FC + 0.1559 VM - 0.0078 Ash	Proximate	MJ/kg	Erol and Ku, 2010
Model 3	HHV = -10.8141 + 0.3133 (VM+FC)	Proximate	MJ/kg	ÖzyuğUran and Yaman, 2017
Model 4	HHV = 0.1846 VM + 0.3525 FC	Proximate	MJ/kg	Jimenez and Gonzalez, 1991
Model 5	HHV = 10.982 + 0.1136 VM - 0.2848 Ash	Proximate	MJ/kg	Yin, 2011
Model 6	HHV = 0.879 C + 0.3214 H + 0.056 O - 24.826	Ultimate	MJ/kg	Elneel et al., 2013
Model 7	HHV = 0.2949 C + 0.8250 H	Ultimate	MJ/kg	Yin, 2011
Model 8	HHV = -0.763 + 0.301 C + 0.525 H + 0.064 O	Ultimate	MJ/kg	Ebeling and Jenkins, 1985
Model 9	HHV=0.441 C - 0.043 O	Ultimate	MJ/kg	Putra et al., 2022

The Estimation Errors

Researchers have extensively explored and documented numerous correlations to predict the Higher Heating Value (HHV) of biomass based on proximate and ultimate analysis results. Table 1 summarizes some of these published correlations, which often use linear and nonlinear functions. A key metric for evaluating their effectiveness is the R-squared value (the Pearson regression coefficient). R-squared ranges from 0 to 1; values above 0.5 suggest a valid correlation, and those above 0.7 are generally considered to indicate a strong

correlation. Calculation of R-squared, requiring regression analysis of multiple variables, can be performed using software like IBM SPSS version 26.

To assess newly developed correlations, two primary statistical parameters are applied: Average Absolute Error (AAE) and Average Bias Error (ABE). AAE measures how closely the calculated HHV aligns with the measured value – a lower AAE demonstrates higher accuracy. ABE reveals whether the correlation tends to overestimate (positive ABE) or underestimate (negative ABE) the HHV within the sample population. The ideal correlation will have a minimal absolute ABE value (Putra et al., 2022).

$$AAE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{HHV_{Calculated} - HHV_{measured}}{HHV_{measured}} \right| \times 100\%$$
(2)
$$ABE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{HHV_{Calculated} - HHV_{measured}}{HHV_{measured}} \right| \times 100\%$$
(3)

3. RESULTS AND DISCUSSION

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Hydrothermal Carbonization of Banana Bunches

Table 2 presents the results of converting banana bunches via the HTC process, varying temperature, time, and feedstock-to-water ratio. The table shows that temperature and processing time significantly affect the HHV (High Heating Value) and hydrochar yield. Higher temperatures and longer times result in higher HHV and hydrochar yields. This indicates that the HTC process at higher temperatures and times produces hydrochar with better quality, i.e., higher energy content and greater quantity.

Davamatava	Formulation						
Paremeters	BB (Ref.)	А	В	С	D	Е	
Temperature (°C)	-	180	200	200	200	180	
Solid to water ratio	-	1,5	1,5	1	2	1,5	
Time (Minute)	-	15	30	15	45	45	
		Pr	oksimat (wt%,dry)		
Ash content	88,8	8,85	7,62	11,96	6,94	6,95	
Volatile matter (VM)	11,0	61,12	64,74	62,6	62,66	64,73	
Fixed Carbon (FC)	0,20	30,03	27,64	25,85	29,83	28,31	
		U	ltimat (w	rt%, dry)			
Carbon (C)	37,93	47,4	46,97	44,56	48,86	48,54	
Hydrogen (H)	4,46	5,7	5,92	5,66	5,78	6	
Nitrogen (N)	1,87	0,8	0,77	0,68	0,77	0,83	
Sulfur (S)	0,37	0,07	0,08	0,08	0,07	0,07	
Oxygen (O) ^a	55,37	37,18	38,64	37,06	37,58	37,61	
Nilai Kalor (MJ/kg)	15,50	24,4	15,50	24,86	28,48	23,86	

d by difference

Statistical Analysis

A thorough analysis of publications on fuel heating value estimation through proximate analysis led to the proposal of several correlation models, including those based on proximate, non-volatile proximate, and ultimate analyses (Table 1). Initial correlations focused on linear effects for simplicity. This study assessed the reliability of these models using both reference data and banana bunch data. Proximate and ultimate basis models for banana bunches were then compared with those derived from the proposed correlations. Analysis was conducted using IBM SPSS version 26 and Microsoft Excel on 5 distinct data sets (see Table 2). The principle behind determining constant terms was minimizing the sum of squared errors between estimated and actual higher heating values. The correlation with the lowest error among all proposals was considered the most suitable. Finally, selected correlations were examined for non-linear effects that could potentially reduce error rates further, taking into account variations in neighboring data and their impact on heating value.

Linear Regression Analysis

Table 2 presents the composition of hydrothermally carbonized BB biomass, demonstrating the variation across five laboratory test data sets. This data informed the creation of new HHV estimation correlations. Assuming HHV has a linear relationship with its constituents, linear regression analysis was applied to derive four new correlations: two based on proximate analysis, and two based on ultimate analysis. Notably, the first proximate correlation uses VM, Ash, FC, and constants, while the second utilizes only VM, Ash, and constants. Similarly, the first ultimate correlation incorporates C, H, N, O, S, and constants, while the second uses C, H, N, S, and constants. IBM SPSS version 26 and Microsoft Excel were used in analysis.

To ensure validity, it's imperative that any regression model meets classical assumptions. These were carefully tested:

- *Normality Test:* This assesses whether the data distribution is normal. Normal P-P plots and histograms were analyzed for proximate formulations A and B (Figs. S1, S2). Data for ultimate formulations C and D was inconclusive through these visualizations. A normal distribution is a key assumption for many statistical tests.
- *Multicollinearity Test:* Examines correlations between independent variables. High correlation (multicollinearity) is undesirable. Value Inflation Factor (VIF) calculations (Tables S3, S4, S5) found VIF values below 10 for proximate and ultimate analyses, indicating no multicollinearity. However, Table S2 revealed possible multicollinearity due to a VIF above 10.
- *Heteroscedasticity Test:* Scatterplots of standardized predicted values (ZPRED) and studentized residuals (SRESID) were created for proximate formulations A and B (Figs. S3, S4). As no distinct patterns arose and points scattered above and below the zero line, heteroscedasticity was ruled out. Unfortunately, ultimate formulation data was incompatible with this test.
- *Autocorrelation Test:* Examines whether the dependent variable correlates with itself across lagged values. The Durbin-Watson (d) statistic is key; values between the upper bound (du) and lower bound (4-du) suggest no autocorrelation. This assumption was met for both proximate and ultimate analyses (Tables S4, S5, S8, S9).

In model development, a regression analysis using all factors identified four key equations (Equations 10, 11, 12, 13 in Supporting Information; detailed in Table 3). Equations 10 and 11 differ regarding the inclusion of the FC variable; Equations 12 and 13 differ with respect to the S and O variables. Initial analysis provided R² values (Pearson regression coefficient).

Values above 0.5 are considered valid, with those above 0.8 preferred. Notably, R^2 and Adjusted R^2 (which accounts for additional model variables) improved dramatically from values below 0.8 to above 0.95 when equation constants were set to zero. All variables yielded significant p-values below 0.005, affirming their importance within the model.

Model	Equation model	Based on	Unit	R	Adj. R ²	SE	Sig. F	p- value
Model 10	HHV = 967.171 – 8.684 Ash – 9.299 VM – 9.913 FC	Proximate	MJ/kg	0.983	0.866	0.664	0.232	<0.005ª
Model 11	HHV = 52.654 -0.389 Ash – 0.379 VM	Proximate	MJ/kg	0.526	0.637	2.321	0.819	<0.005 ^a
Model 12	HHV = 1.828 C - 5.862 H - 46.366 N + 1.222 O - 37.194	Ultimate	MJ/kg	1.000	0.847	0.000	0.000	<0.005ª
Model 13	HHV = 2.441 C - 7.383 H - 36.914 N + 266.624 S - 38.333	Ultimate	MJ/kg	1.000	0.875	0.000	0.000	<0.005ª

Table 3. Summary	y of developed HHV correlation models and their regression
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statistics

Comparison of New Correlations with Existing Literature Equations for HHV Estimation Using Banana Bunch Data

To validate the newly developed correlations, Table 3 data points were used to predict HHV values and compare them against well-established reference equations (Models 1-9), as shown on Table 4. It's important to note that published correlations were specifically validated for biomass and its derived fuels (like hydrochar). Calculated deviations, absolute errors, and biases for all biomass samples within Table S1 reveal the newly developed ultimate correlation (Equation 10) as the most accurate among all existing correlations. Compared to published correlations, our new equation delivers the lowest AAE and ABE values for both proximate and ultimate-based analysis (Figure 2). Notably, for proximate-based analysis, Equation 4 yielded the lowest AAE (0.83) and ABE (0.98) of all literature equations evaluated. Notably, this literature equation uses agricultural residues with some similarity to our material—though it doesn't specifically consider the hydrothermal carbonization process.



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Figure 2. AAE and ABE (with respect to experimental HHV) of the correlations. It refers to 13 correlations developed from proximate analysis and ultimate analysis.

These results, showing the lowest AAE and ABE values obtained, validate the efficacy of our newly developed correlations. Interestingly, ultimate-based correlations didn't outperform proximate-based ones, echoing findings from Fiedl et al. (2005b), Qian et al. (2016), and Yin (2011). Figure 2 visually contrasts the significant reduction in AAE and ABE values achieved by our developed equations (Models 10, 11, 12, 13), highlighting their superiority over literature-based references.

Table 4. Results Comparing HTC Data with All Formulation								
			HHV BB Data					
Model	Based on	Type of raw material	Absolut deviation MJ/kg	Bias deviation	Absolute average error percentage	Bias error		
Model 1	Proximate	Wood, Agricultural Waste, and Fruit	7.473	-0.7305	1.652	0.9706		
Model 2	Proximate	Vegetables, Fruits and Cakes	5.560	-0.6884	1.229	0.9781		
Model 3	Proximate	Herbal Plants, Wood and Fruits	7.567	-0.6820	1.672	0.9702		
Model 4	Proximate	Agricultural Residues, Wood and Flowering Plants	3.772	-0.6883	0.834	0.9852		
Model 5	Proximate	Residual, Wood and Food Waste	9.672	-0.6171	2.138	0.9619		
Model 6	Ultimate	Oil Pahn Fronds	7.556	-0.6941	1.670	0.9703		
Model 7	Ultimate	Residual, Wood and Food Waste	6.686	-0.6816	1.478	0.9737		
Model 8	Ultimate	Forest Residues, Food, and Field Crops	6.497	-0.6842	1.436	0.9744		
Model 9	Ultimate	Municipal Waste, Food, Sewage sludge,	6.193	-0.5896	1.369	0.9756		
Model 10	Proximate	New Formulation A (Banana Bunch)	0.023	-0.0170	0.005	0.9998		
Model 11	Proximate	New Formulation B (Banana Bunch)	0.010	-0.5738	0.008	0.9995		
Model 12	Ultimate	New Formulation C (Banana Bunch)	0.019	-0.0001	0.007	0.9996		
Model 13	Ultimate	New Formulation D (Banana Bunch)	0.020	0.0001	0.009	0.9990		

Comparison of Current Equations Using Literature Data

To assess the accuracy of our four newly developed equations (Formulations A, B, C, and D), we compared them against established proximate (Equations A and B) and ultimate-based (Equations C and D) HHV correlations from the literature. These published correlations were originally validated for diverse fuel mixtures across several conversion processes, suggesting limited accuracy outside their scope. However, this study demonstrates their broader applicability in specific cases (Table 5). We calculated absolute deviations, bias deviations, and errors from Equations 1-9 across all biomass samples in Table S1.

Based on this analysis, Formulation B performed best for proximate analysis when applying data from Model 2, with AAE and ABE values of 0.024 and 0.975, respectively. For ultimate analysis, Formulation D proved most accurate, yielding AAE and ABE values of 0.010 and 0.956. (See Table S1 for complete data). Figures 3 and 4 offer compelling insights. Figure 3 shows a pronounced R² difference of 0.457, resulting in divergent spike graphs between Formulations A and B. Similarly, Figure 4 exhibits substantial variation, highlighting the distinct impact of literature data across eight raw material-based models. Clearly, there are many other influencing factors yet to be investigated.

Our new correlations (Equations A, B, C, and D) effectively predict HHV for both hydrothermal carbonized biomass and mixed biomass fuels sourced from various thermochemical processes. Notably, published correlation equations also find some applications outside their original scope, depending on the biomass sample, conversion process, and analysis type (proximate or ultimate). The Supplementary Information further details calculated calorific values. Remarkably, our current research equations (PS) successfully predict literature-derived data, despite some remaining points warranting further accuracy improvement. This comparison reveals significant practical differences and the

Data Model based		ta ed References	Absolut deviation MJ/kg		Bias deviation		Absolute error persentase		Bias error	
	on	data HHV	For. A	For. B	For. A	For. B	For. A	For. B	For. A	For. B
Model 1	Proximate	Nhuchhen and Salam	18.01	3.39	5.7400	0.1042	2.824	0.532	0.3784	0.7404
Model 2	Proximate	Erol et al	14.55	1.89	2.9054	0.8003	0.185	0.024	0.8056	0.9748
Model 3	Proximate	Ozyuguran and Yaman	11.38	2.00	1.3768	-0.1993	0.187	0.033	0.8578	0.9750
Model 4	Proximate	Jimenez and Gonzales	8.47	25.53	45.5367	0.0032	0.054	0.164	0.9603	0.8804
Model 5	Proximate	Yin	15.67	2.87	10.9345	0.2233	0.490	0.090	0.6433	0.9348
			For. C	For. D	For. C	For. D	For. C	For. D	For. C	For. D
Model 6	Ultimate	Elneel et al	14.55	1.89	28.5289	14.2570	0.137	0.010	0.4113	0.9564
Model 7	Ultimate	Yin	11.38	2.00	22.8820	85.2502	-0.058	42.740	1.0428	32.4701
Model 8	Ultimate	Jenkins and Ebeling	1930.69	1508.58	110.2659	92.9760	56.345	44.026	52.9939	41.6264
Model 9	Ultimate	Putra et al	39.84	30.93	10.2883	24.2528	5.905	4.585	2.0953	0.1495

Table 5. Results Comparing Formulation H	ITC Banana Bunch	with Literature
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*For.A, B, C, & D = Formulation A, B, C, & D

potential for even broader future applications.



Figure 3. AAE and ABE (with respect to literature HHV) of the comparing 2 correlations from proximate analysis



Figure 4. AAE and ABE (with respect to literature HHV) of the comparing 2 correlations from ultimate analysis

5. CONCLUSION

Four new correlation models (Equations 10, 11, 12, and 13), based on both proximate and ultimate analyses, were developed through linear regression analysis to predict the HHV of hydrothermally carbonized biomass. Comprehensive investigations revealed that, in this context, proximate-based correlations hold the edge in accuracy compared to ultimate-based correlations. A key reason is that proximate analysis yields empirical compositions uniquely well-suited to predicting HHV for both carbonized biomass and biomass obtained

from diverse thermochemical processes. Remarkably, established correlations in the literature also demonstrated promising performance when tested against HHV data from hydrothermally carbonized biomass and other fuel sources. These newly developed correlations can directly improve process control and efficiency for industries relying on biomass or bio-derived fuels produced through hydrothermal carbonization or other thermochemical processes. The ability to accurately estimate HHV enhances resource allocation, energy balance calculations, and optimization of industrial processes. This research holds strong potential for future investigations. This exploration serves as a launchpad for several important areas of further research, including:

- Expanding the data set to test a wider range of raw materials and process parameters to fine-tune the accuracy and broader applicability of the correlation models.
- Delving into the specific compositional differences revealed by proximate analysis that are responsible for its superior predictive power in this case.
- Designing model refinements or integrating advanced computational techniques to improve the efficacy of ultimate-based correlations for specific contexts.

ACKNOWLEDGEMENT

This research was funded by the Indonesia Endowment Fund for Education (LPDP) No, PRJ-25/LPDP/2022, The Ministry of Finance, Indonesia, for funding this research.

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