A Proposed Equation for Predicting the Heating Value of Thai Bagasse

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Abstract

Several empirical equations, such as those by Dulong and Demirbas, have been widely used to estimate the higher heating value (HHV) of fuels from their elemental composition. However, when applied to Thai bagasse, these models exhibited substantial errors, with average deviations exceeding 10% from laboratory-tested values. To address this, 47 sets of elemental composition data for bagasse were compiled from Environmental Impact Assessment (EIA) reports of biomass power plants in Thailand. Two regression-based predictive models tailored to Thai bagasse were developed and evaluated. The performance of the developed models was evaluated against six established equations from international studies using four statistical indicators—Mean Absolute Error (MAE), Mean Bias Error (MBE), Average Bias Error (ABE), and Average Absolute Error (AAE). These indicators were selected to assess both the unsystematic bias and the overall predictive accuracy of the models. The proposed models demonstrated marked improvements, reducing MAE by 3.74% compared to the best existing equation. Model 1 ($HHV = 17.137 - 0.161 \times Mc$) yielded MBE = −0.061 MJ/kg, MAE = 0.52 MJ/kg, ABE = +0.0171%, and AAE = 5.75%, while Model 2 ($HHV = 1.496 + 0.157\ C + 0.19\ O$) achieved MBE = +0.037 MJ/kg, MAE = 0.37 MJ/kg, ABE = +0.98%, and AAE = 4.12%. These results confirm that the developed models provide significantly improved HHV prediction accuracy for Thai bagasse, which provides better fuel management for bagasse-based power plants.

Keywords: Thai bagasse, heating value, prediction accuracy, elemental composition, moisture content

Introduction

Thailand, as a predominantly agricultural country, supports a wide range of agro-industries, including palm oil, rice, and sugar processing. Among these, the sugar industry plays a particularly significant role in both agricultural and industrial sectors. A major byproduct of sugar manufacturing is bagasse—the fibrous residue remaining after juice extraction from sugarcane—which typically contains 45-50% moisture (Zafar, 2023) and is widely utilized as a biomass fuel in sugar mills. Bagasse is commonly combusted in boilers to produce steam for process heating and electricity, both for in-house use and for sale to the grid. According to the Ministry of Energy (2023), sugar production in Thailand generates approximately 21 million tons of bagasse annually. The energy potential of this biomass is primarily determined by its heating value, which is influenced by both its moisture content and elemental composition.

Accurate estimation of the heating value is essential for biomass-based power plants, as it directly impacts boiler efficiency, combustion performance, and overall fuel management under varying load conditions. In Thailand, thermal power plants commonly use empirical equations such as those proposed by Dulong and Demirbaş to predict heating values for operational planning. Prediction models can be constructed through different approaches. For instance, Dulong's model (Francis, 1965) employs the gross heating value of each elemental component as coefficients, while more recent models, such as that of Junjun et al. (2023), utilize biomass bond dissociation energy to establish correlations. Nevertheless, these equations were originally developed for purposes other than bagasse application; Dulong's model was designed for coal, whereas Junjun's model targets a broad range of biomass types, and thus are not specifically calibrated to Thai bagasse. Practical observations indicate that applying widely used models such as Dulong's to bagasse-fired plants often produces substantial prediction errors, leading to inefficient fuel allocation and elevated operating costs. Therefore, the development of locally adapted predictive models is necessary to achieve higher accuracy for this particular fuel. Heating value, expressed as either Higher Heating Value (HHV) or Lower Heating Value (LHV), represents the total energy released during complete combustion, which relies on elemental composition and their moisture content. HHV includes the latent heat of vaporization of water formed during combustion, whereas LHV excludes it. HHV is typically measured using a bomb calorimeter, while LHV can be calculated from HHV using thermodynamic relationships (Miller, 2010; Barzu, 2013). Direct measurement, although accurate, is often time-consuming and costly (Sukru, 2012). Consequently, numerous empirical equations have been proposed to estimate heating values from physical and chemical properties, including proximate analysis, ultimate (elemental) analysis, and chemical composition. Among these, elemental composition-based models generally offer the most consistent accuracy because they directly reflect the fuel's combustion-related constituents (Mahmut, 2023; Sheng & Azvedo, 2005).

Biomass composition can vary significantly with geographical origin and environmental conditions (Stanislav, 2012; Erol, 2010; Garcia, 2014). Factors such as soil quality, climate, cultivation practices, and plant variety can influence the proportions of carbon, hydrogen, oxygen, nitrogen, and sulfur, even within the same biomass category. For Thai bagasse, these variations mean that applying generalized equations may not yield accurate results. Therefore, there is a practical and economic need for predictive models for the specific properties of locally produced bagasse. The present study addresses this gap by evaluating the performance of existing heating value prediction models on Thai bagasse by developing regression-based models from Environmental Impact Assessment (EIA) reports of sugar mills and biomass power plants in Thailand. The objective of these proposed models is to improve prediction accuracy, thereby supporting more efficient fuel management and cost-effective operation in Thai biomass power generation.

Materials and Methods

Data Collection and Screening

This study utilized secondary data obtained from Environmental Impact Assessment (EIA) reports of sugar mills and biomass power plants across Thailand. The datasets included elemental composition (C, H, O, N, S), moisture content, ash content, and higher heating value (HHV) of bagasse samples. All 156 samples were initially reviewed and subsequently screened based on a series of quality control criteria to ensure data consistency and accuracy for model development. The screening process involved the following steps (Fig. 1).

Data Sources

Data were compiled from officially published EIA reports submitted to the Office of the Environment Policy and Planning. The reports provided laboratory-measured values for elemental composition and heating value, together with analysis methods and conditions.

Data Management

Some laboratory reports contained data of suboptimal quality due to typographical errors or improper formatting, where the reported analysis results were inconsistent with theoretical expectations or standard calculation procedures. In such cases, validation procedures were undertaken as described below.

Sulfur Content Reporting

Biomass typically contains low sulfur levels (usually <0.5%), yet some laboratories omit sulfur and report a value of zero. Since all biomass contains at least trace amounts of sulfur, and sulfur combustion is exothermic, thereby contributing to heating value, such omissions may compromise model accuracy. Therefore, all samples with zero sulfur content were excluded.

Inconsistency Reporting

Elemental composition and HHV can be reported on varying bases: as-received, dry, ash-free, or dry ash-free. Inconsistent bases within a single record (e.g., elemental data on a dry basis and HHV on an as-received basis) can lead to analytical errors. Only samples with internally consistent reporting bases were retained.

Incomplete or Inaccurate Data Totals

Samples where the sum of elemental composition deviated significantly from 100%, either falling short or exceeding it, were considered unreliable and excluded to preserve data integrity.

Unreasonable Element Values (Outliers)

Values falling outside typical bagasse composition ranges were flagged and removed. For example, bagasse oxygen content on a wet basis typically ranges from 18–25%, but some samples reported values as high as 60%, indicating likely errors.

Inconsistent Elemental Trends Across Bases

In certain records, elemental values on a dry basis were inexplicably lower than those on an as-received basis. This is technically invalid, as moisture removal should increase elemental percentages. Such samples were excluded. However, an exception was made in cases where H and O on the as-received basis included moisture content. In such scenarios, conversion to a dry basis may reduce H and O values accordingly, while increasing C, N, S, and ash content due to moisture elimination.

Use of Lower Heating Value (LHV)

Some datasets reported elemental composition alongside LHV instead of HHV. Since LHV is derived from HHV by subtracting the latent heat of water vaporization, and the conversion process can vary, back-calculation may introduce error. Only samples with directly measured HHV were included.

Zero Nitrogen Reporting

Although biomass contains low nitrogen levels, its combustion is endothermic and influences the net energy output. Zero nitrogen reporting neglects this factor and may affect model accuracy. Samples reporting zero nitrogen were excluded.

Redundant Moisture Reporting

Some as-received datasets embedded a portion of moisture within the %H and %O values, while also reporting moisture separately, resulting in double-counting. This redundancy leads to inflated H and O values, which can distort HHV estimation. Such samples were identified and excluded based on ASTM D standard interpretations.

Data Processing

To reduce moisture variation and improve comparability, all elemental composition data and higher heating value (HHV) values were converted to a dry basis using standard normalization formulas. This conversion is essential to eliminate the influence of moisture, which dilutes elemental concentrations and energy content, thereby obscuring the true relationship between elemental composition and HHV, by standardizing all data to a dry basis.

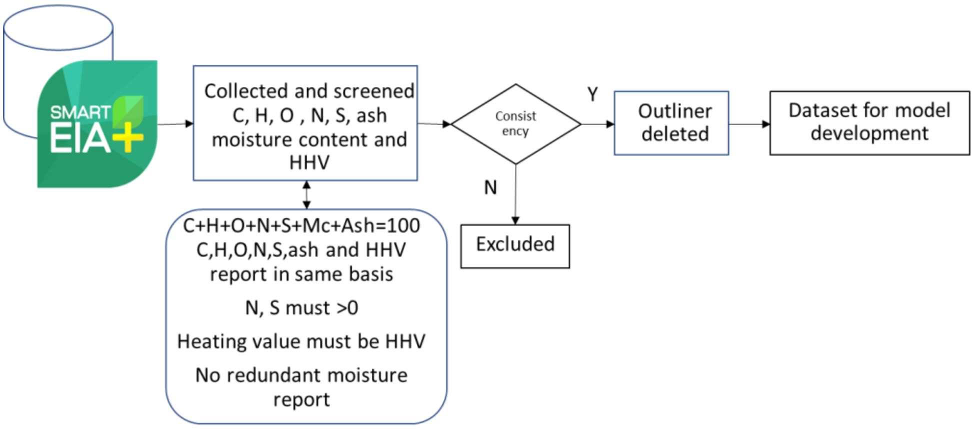

Figure 1 Logical Flow for Model Development

Model Development

After data preprocessing and conversion to a dry basis, statistical analysis was performed to identify suitable predictors for estimating the higher heating value (HHV) of bagasse. Pearson correlation analysis was conducted to assess the relationships between each elemental variable (C, H, O, N, S, and ash) and HHV. Corresponding *p*-values were used to evaluate the statistical significance of each correlation, with variables showing $p < 0.05$ considered statistically significant.

Only elemental variables with significant correlations to HHV were selected for inclusion in the regression model. These selected variables were then used to develop multiple linear regression (MLR) models, with HHV as the dependent variable and elemental composition as the independent variable.

In addition to developing regression models from the collected dataset, a selection of existing empirical equations based solely on ultimate analysis was compiled for comparative purposes. These models were chosen based on their widespread use and frequent citation in biomass energy research. The selected models were applied to the same dataset as shown in Table 1 to evaluate their performance against the regression models developed in this study. This comparison was conducted to assess how well generalized equations based on ultimate analysis predict the HHV of Thai bagasse and to highlight the potential improvements gained by using a localized regression approach.

After data screening and quality control, 47 samples from the EIA report passed quality screening.

Developed Model Validation

To ensure the prediction accuracy of the developed model, 6 other bagasse samples were used to validate

Statistical Evaluation Metrics

To assess the predictive accuracy of both the developed and existing models, several statistical indicators were employed

Mean Absolute Error (MAE)

$$MAE = \frac{1}{n}\sum_{i=1}^{n} |HHV_{cal} - HHV_{measured}| \quad (1)$$

Mean Bias Error (MBE)

$$MBE = \frac{1}{n}\sum_{i=1}^{n} (HHV_{cal} - HHV_{measured}) \quad (2)$$

Average Bias Error (ABE)

$$ABE = \frac{1}{n}\sum_{i=1}^{n} \left(\frac{HHV_{cal} - HHV_{measured}}{HHV_{measured}}\right)\times 100 \quad (3)$$

Average Absolute Error (AAE)

$$AAE = \frac{1}{n}\sum_{i=1}^{n} \left|\frac{HHV_{cal} - HHV_{measured}}{HHV_{measured}}\right|\times 100 \quad (4)$$

Table 1 selected higher heating value prediction model

Model	Form	Unit	Citation
Dulong (1)	$HHV = [0.338\ C + 1.44\ (H - \frac{O}{8})]$	MJ/kg	Francis, 1965
Dulong (2)	$HHV = [0.31\ C + 1.32\ (H - \frac{O}{8}) + 0.09\ S]$	MJ/kg	Francis, 1965
Demirbas	$HHV = [33.5C + 142.3H - 15.4O - 14.5N]\times 10^{-2}$	MJ/kg	Demirbas, 1997
Parr	$HHV = 8080C + 34500H + 2250S$	kcal/kg	Francis, 1965
Sheng and Azevedo (1)	$HHV = -1.3675 + 0.3137C + 0.525H + 0.064O^{*}$[1]	MJ/kg	Sheng and Azevedo, 2005
Sheng and Azevedo (2)	$HHV = 0.3259C + 3.4597$	MJ/kg	Sheng and Azevedo, 2005

[1]O* calculated by O* = 100-(C+H+Ash)

Results

The performance of the developed multiple linear regression model was evaluated using four statistical indicators: MAE, MBE, ABE, and AAE. The results were also compared with widely cited empirical models.

Each metric provides a distinct perspective:

MAE measures the average magnitude of the absolute differences between predicted and actual HHV values. It does not indicate whether the model over- or underestimates, but a lower MAE reflects better overall predictive accuracy.

MBE captures the average signed difference between predicted and actual values, showing whether the model systematically overestimates (positive MBE) or underestimates (negative MBE). It helps identify consistent directional bias.

ABE similarly retains the direction of the error, but expresses the average signed deviation without squaring or taking the absolute value. It is often used interchangeably with MBE in some studies, and confirms whether the model is consistently biased in one direction.

AAE represents the average of the absolute percentage errors, providing a relative measure of model accuracy across different sample scales. It allows easier comparison between models when the range of HHV values varies.

General Observations

As the graphical analysis in Fig. 2 shows, the two regression models developed in this study outperformed all existing empirical equations in terms of predictive accuracy. Model (2) from this study, which included multiple elemental variables, exhibited the lowest MAE (0.38 MJ/kg) and AAE (4.12%), indicating a close agreement between predicted and actual HHV values across the test dataset.

In contrast, traditional empirical models, particularly Parr and Sheng & Azevedo (1), showed relatively poor performance. Parr's model exhibited the highest overall error, with an MBE of +3.05 MJ/kg, indicating a consistent overestimation of HHV. The absolute average percentage error (AAE) for Parr was also the highest at 32.64%, which makes it unsuitable for the accurate prediction of Thai bagasse heating values.

Evaluation of Bias (MBE and ABE)

MBE reflects the direction and magnitude of the prediction error. Negative values suggest that the model underestimates HHV, while positive values indicate overestimation. The proposed Model (1) produced an MBE of −0.06 MJ/kg, while Model (2) showed an MBE of +0.037 MJ/kg. Both values are very close to zero, confirming that the developed models are statistically unbiased.

In contrast, Dulong (2) showed a substantial underestimation bias (MBE = −1.60 MJ/kg), while the Sheng & Azevedo (1) and Parr models overestimated HHV, with MBE values of +2.82 MJ/kg and +3.05 MJ/kg, respectively. Similarly, ABE, which also reflects directionality, shows that most empirical models introduced consistent directional errors. Notably, Sheng & Azevedo (1) and Parr had ABE values exceeding +30%, highlighting a systematic overestimation. On the other hand, the proposed Model (1) had a near-zero ABE of +0.017%, while Model (2) yielded a low ABE of +0.98%, further confirming their balanced predictive behavior.

Evaluation of Magnitude of Errors (MAE and AAE)

MAE quantifies the average size of prediction errors, regardless of their direction. The proposed models showed substantially lower MAE values compared to all other models. Model (1) achieved an MAE of 0.52 MJ/kg, while Model (2) reduced this further to 0.38 MJ/kg. For comparison, Dulong (1) reported an MAE of 1.02 MJ/kg and Demirbas (1997) reported an MAE of 0.73 MJ/kg. The highest MAE was observed for the Parr model at 3.05 MJ/kg. AAE, expressed as a percentage, allows for scale-independent comparison. Once again, the proposed models achieved the best results with AAE values of 5.75% (Model 1) and 4.12% (Model 2). These figures are significantly lower than the next best performer (Demirbas, AAE = 7.86%) and dramatically outperform Parr (AAE = 32.64%) and Sheng & Azevedo (1) (AAE = 30.95%).

Overall Improvement in Model Performance

These results clearly demonstrate that the newly developed models significantly enhance both the accuracy and reliability of HHV predictions for Thai bagasse when compared to traditional empirical equations. By explicitly incorporating moisture content and elemental composition specific to the regional characteristics of Thai bagasse, the models achieve error reductions of up to an order of magnitude in certain cases and effectively correct the systematic biases inherent in classical models. Such improvements are critical for enabling more precise fuel quality assessments and supporting more efficient operational decision-making in thermal power plants that rely on bagasse as their primary fuel.

Models validation

To assess the generalization ability of the developed models, six independent bagasse samples were used for validation. The statistical indicators obtained from this evaluation are summarized in Table 2-3. The graphical analysis of different models are presented in Fig.2.

Both models performed well, producing low error values across all metrics. Model 1 showed an average Mean Bias Error (MBE) of −0.240 and a Mean Absolute Error (MAE) of 0.240, indicating that the predictions were close to the laboratory values with only a slight underestimation trend. The Absolute Bias Error (ABE) and Average Absolute Error (AAE), expressed as percentages, averaged 2.759%, reflecting a relatively small deviation from the measured HHV values. These results confirm that Model 1 can provide reliable estimates of bagasse HHV.

Model 2, meanwhile, demonstrated even stronger performance. The average MBE was nearly zero (−0.006), suggesting that systematic bias was effectively minimized. The MAE was also very low at 0.101, while the ABE averaged just 0.014% and the AAE averaged 1.201%. These results highlight Model 2's excellent predictive accuracy and consistency with experimental values.

Table 2 Statistical Results of Each Model

Model	Form	MBE (MJ/kg)	MAE (MJ/kg)	ABE (%)	AAE (%)
Dulong	$HHV = [0.338\,C + 1.44\,(H-\frac{O}{8})]$	-0.90	1.02	-9.54	10.92
Dulong (2)	$HHV = [0.31\,C + 1.32\,(H-\frac{O}{8}) + 0.09\,S]$	-1.60	1.61	-17.02	17.15
Demirbas	$HHV = [33.5C + 142.3H - 15.4O - 14.5N]\times 10^{-2}$	-0.47	0.73	-4.97	7.86
Parr	$HHV = 8080C + 34500H + 2250S$	+3.05	3.05	+32.64	32.64
Sheng and Azevedo(1)	$HHV = -1.3675 + 0.3137C + 0.525H + 0.064O$*	+2.82	2.82	+30.95	30.95
Sheng and Azevedo (2)	$HHV = 0.3259C+3.4597$	+1.86	1.88	+20.51	20.70
Developed model (1)	$HHV = 17.137-0.161\times M_c$	-0.061	0.52	+0.017	5.75
Developed model (2)	$HHV = (1.496+0.157C+0.19O)$	+0.037	0.37	+0.98	4.12

Table 3 validation statistical result of developed models

Model	MBE(MJ/kg)	MAE (MJ/kg)	ABE (%)	AAE (%)
Developed model (1)	-0.240	0.240	-2.759	2.759
Developed model (2)	-0.006	0.101	0.014	1.201

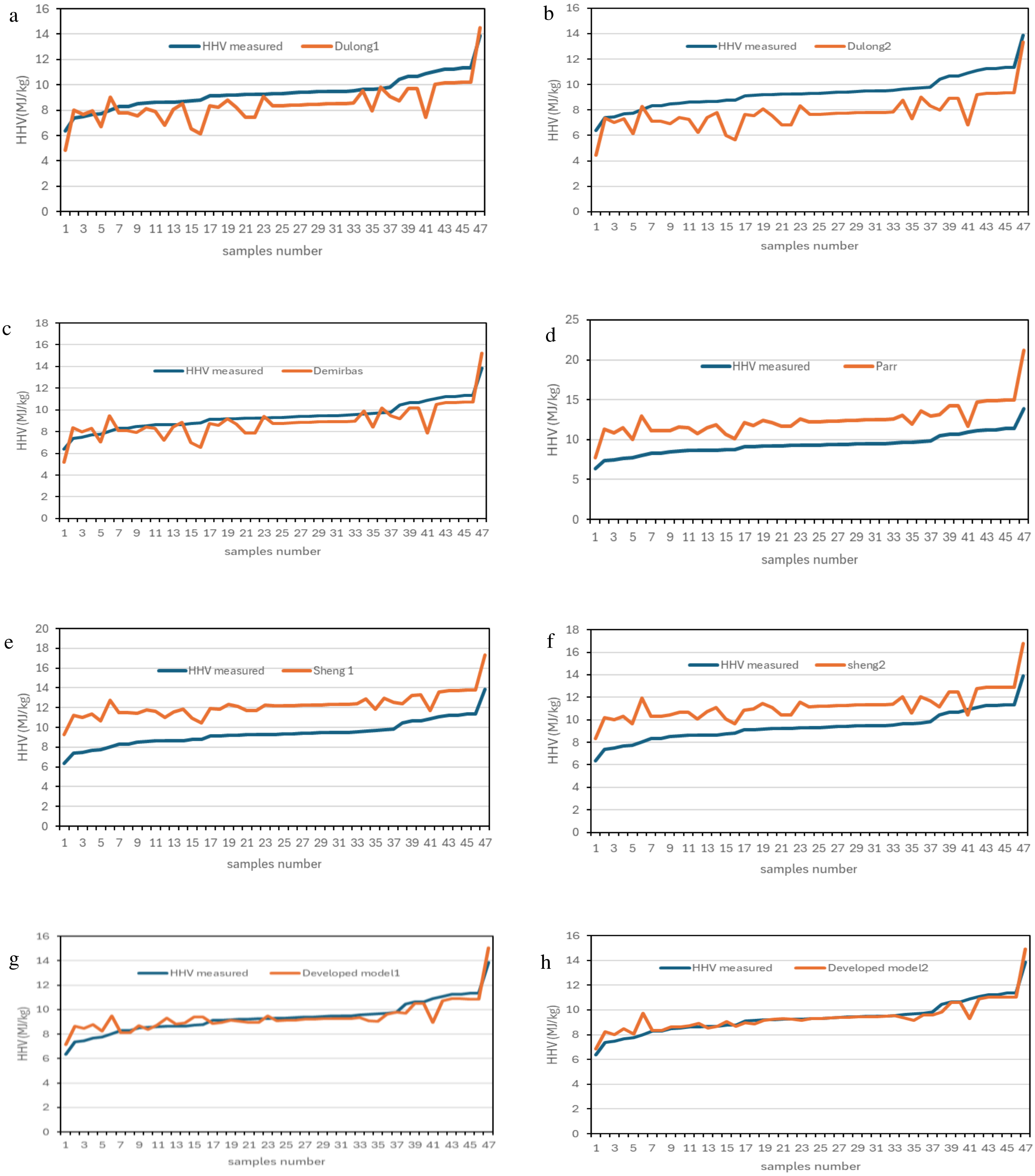

Figure 2 graphical analysis of different models a) Dulong1 b) Dulong2 c) Demirbas d) Parr e) Sheng1 f) Sheng2 g) Developed model1 h) Developed model2

Discussion

The statistical results presented in the comparison table reveal that the MBE and MAE, as well as the ABE and AAE, produce identical values for certain models. This pattern suggests the presence of a systematic bias, where errors consistently occur in one direction across all samples. In other words, these models tend to either overpredict or underpredict the higher heating value (HHV), rather than exhibiting random fluctuations.

For instance, both the Parr model and the Sheng & Azevedo (1) model consistently overestimate the HHV of Thai bagasse. This tendency is evident not only from the bias error values but also from the line graphs, where predicted values remain above the laboratory-measured values. Such systematic overprediction indicates that these models are not well-suited for Thai bagasse, likely due to regional variations in biomass composition that were not considered during their initial development. These results align with previous research emphasizing the importance of region-specific calibration for empirical models applied to diverse biomass types.

Similarly, the Dulong (1,2) and Sheng & Azevedo (2) models show weak predictive capability. While the Dulong models consistently underpredict, the Sheng & Azevedo (2) model overpredicts in more than 90% of the samples, both with inconsistent deviations. The absence of a clear, systematic trend highlights their limited reliability and poor generalizability when applied outside the datasets on which they were originally developed.

A notable strength of this study is the use of a relatively homogeneous dataset derived from bagasse samples processed under standardized milling practices common in Thai sugar mills. This uniformity, particularly in moisture content, contributed to reducing variability and strengthening model performance. Importantly, the regression model developed in this study explicitly incorporates moisture content as a predictor, which significantly enhanced its accuracy compared to the reference models. Even with minor variability, accounting for moisture proved to be critical in capturing its consistent influence on HHV and improving prediction reliability.

Nonetheless, several limitations should be acknowledged. The dataset, although regionally relevant, represents only a limited range of bagasse samples under specific processing conditions, which may constrain the applicability of the model to other bagasse sources with different characteristics. Furthermore, while linear regression proved effective in this study, it may not fully capture nonlinear interactions among compositional factors that influence HHV.

Future research could extend the dataset to include bagasse samples with broader compositional diversity, influenced by different milling processes or geographical regions. Incorporating advanced modeling approaches, such as machine learning algorithms, may further enhance predictive accuracy by identifying complex patterns within the data. Additional parameters—such as volatile matter or fixed carbon—could also be integrated to refine model performance. Validation with independent datasets and cross-regional comparisons would strengthen the robustness and broader applicability of the proposed predictive models.

The findings of this study are consistent with those of Sanchompu (2024), who also developed an HHV prediction model using regression analysis and reported high statistical reliability, reinforcing regression as a robust and effective approach. Likewise, Kikarncharoensin and Innet (2024) observed that applying models to biomass types on which they were not trained often results in substantial variability and reduced accuracy. This further emphasizes the necessity of developing models tailored to the specific characteristics of each biomass type to ensure stable, reliable, and industry-relevant predictions for fuel management and process optimization.

Conclusion and Suggestions

This study investigated the accuracy of existing empirical equations in predicting the higher heating value (HHV) of Thai bagasse and proposed a new model tailored to its specific properties. The bagasse samples were collected from Environmental Impact Assessment (EIA) reports in Thailand. Six widely referenced models were evaluated using statistical indicators such as MAE, MBE, AAE, and ABE. The results revealed that several commonly used equations produced substantial prediction errors when applied to Thai bagasse. In contrast, the proposed empirical model, developed through regression analysis, demonstrated significantly improved accuracy and reliability.

Accurate prediction of the heating value is critical for efficient fuel management in thermal power plants that use bagasse. With more precise HHV estimates, plant operators can optimize fuel feeding and combustion processes, ultimately reducing operational costs and improving energy efficiency. This underscores the practical significance of developing region-specific predictive models. Future research could extend this approach to other biomass types and explore machine learning techniques to further enhance prediction accuracy and support sustainable bioenergy development.

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Author Contributions

Author 1: Conducted the literature review, designed the methodology, performed data collection and analysis, and prepared the manuscript draft.

Author 2: Provided academic supervision, contributed to the development of the research framework, and reviewed and revised the manuscript.

Author 3: Provided technical guidance, verified the analytical methods, and contributed to the critical revision of the manuscript for important intellectual content.

Conflict of Interests

All authors declare that they have no conflicts of interest.

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