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Evaluation of Models for the Prediction of higher Heating Value of Biomass Based on Proximate Analysis

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Research Article

Abstract

Biomass is a renewable and sustainable source of energy with little greenhouse gas emissions. The higher Heating value (HHV) of biomass is a significant parameter that is used in characterising fuel quality, class and type for energy application systems. Experimental determination of HHV is expensive, takes time and not always available. This brings the need for mathematical models for HHV prediction. In this research, proximate analysis and HHV of ten common biomass samples in Nigeria were determined. The biomass considered included rice husk, rice straw, corn cob, woodchips, groundnut shell, desert date, coconut shell, palm kernel, millet straw and sugarcane bagasse. Eight linear and five non-linear correlations with good performance from the literature were employed for predicting the biomass' HHV from proximate analysis data. The performance of the models was tested using statistical indicators. Model M1 and M7 were the best among all the tested models with average absolute error (AAE), average bias error (ABE), and root mean square error (RSME) of 3.8389%, 2.5002% and 0.8780 MJ/kg; and 3.8918%, 2.2301% and 0.8701 MJ/kg respectively. Other models also correlated relatively well with the experimental HHV with low error, though, some are good for specific biomass only. This research identifies the best models that have high accuracy and can be used for the prediction of the higher heating value of biomass samples from proximate analysis.

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Keywords
Biomass; Higher heating values; Models; Proximate analysis; Prediction

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1. Introduction

The potential for biomass to serve as a sustainable supply of energy has become a major research topic all over the world (Uzun *et al.*, 2017). The combustion of biomass as fuel has many environmental and economic advantages. Because, it is a cheap, clean and renewable source of energy (Erol *et al.*, 2010). The design of new biomass energy combustion/conversion systems requires knowledge of the fundamental characteristics of the biomass. Proximate analysis reveals characteristics of biomass in terms of ash content (A), fixed carbon (FC), and volatile matter (VM) (Keybondorian *et al.*, 2017). The higher heating value (HHV) of a fuel refers to the heat generated when a unit mass of fuel is completely burned, and it includes the latent heat of vaporization of water vapour generated when the fuel is burned. Fuel with a higher HHV has higher energy output (Xu and Jingqi, 2015). HHV is the most important parameter used to evaluate biomass fuel quality (Özyuğuran *et al.*, 2018). Higher heating value (calorific value) is experimentally determined using a bomb calorimeter. However, the experiment to measure HHV is time-consuming, expensive and not always available (Majumder *et al.*, 2008). The use of models for the prediction of HHV from biomass composition is a cost-effective and practical solution (Roy and Ray, 2020). In the models, HHV is the dependent parameter and the components of proximate analysis (fixed carbon, volatile matter and ash) are the independent parameters (Krishnan *et al.*, 2019). Most of the recent models rely on regression analysis for the prediction of HHV (Samadi *et al.*, 2019).

There are so many models developed for predicting the HHV of biomass from proximate analysis (Krishnan *et al.*, 2019; Roy and Ray, 2020). Cordero *et al.* (2001) proposed a correlation for the estimation of HHV in terms of VM and FC content. Demirbas (2003) proposed a correlation to calculate HHV in relation to its fixed carbon (FC), lignin (LC), and volatile material (VM). In another study, Sheng and Azevedo (2005) proposed a relation for the calculation of HHV in terms of only the ash content of biomass. Parik *et al.* (2005) developed a correlation for HHV determination from proximate analysis of 450 solid fuel samples, the equation demonstrated low error. Erol *et al.* (2010) proposed 13 new formulae for estimating the calorific values of 20 different biomass samples from their proximate analyses data. Yin (2011) proposed two linear correlations from ultimate and proximate analysis using Microsoft Excel, they

consider 44 biomass samples from agricultural by-products. Kwaghger *et al.* (2017) developed equations for estimating higher heating values of fuel woods using proximate and ultimate analysis. In similar studies, Özyuguran and Yaman, (2017) determined the proximate analysis of twenty-seven different biomass species of different categories. Eight equations were developed and tested for HHV prediction based on the proximate analysis.
Qian *et al.* (2020) developed two empirical correlations based on proximate analysis and ultimate analysis for HHV prediction for ten different kinds of biochars. The correlations were developed by stepwise multiple linear regression and multiple non-linear regression methods. The correlations developed showed good performance in HHV prediction. Recently, Park *et al.* (2022) used thermogravimetric analysis to obtain proximate analysis data for the prediction of calorific value. Garcia *et al.* (2014) developed HHV empirical correlations with MATLAB from ultimate and proximate analysis of 100 Spanish biomass solid fuel samples. It was concluded that the equations are not universal for various biomass and sometimes make large deviations due to the complex chemical and physical properties of biomass. From the models studied, it is obvious that most of the models are specifically good at predicting certain biomass but not all categories. There is need to evaluate the models so that one will identify the best model that is robust and can be used to estimate higher heating value for various biomass categories.
The objective of this study is to evaluate the best linear and non-linear models reported in the literature for predicting the HHV of biomass that are very common in Nigeria from the proximate analysis. Statistical indicators are used to evaluate the performance of such models in relation to experimental measurement. The statistical indicators used in this work include: average absolute error (AAE), average bias error (ABE), and root mean square error (RSME). Kieseler et al. (2013) stated that ABE and AAE are calculated for each correlation, they are used to arrive at conclusions from the comparative assessment of models.

2. Materials and Methods

2.1 Sample collection and preparation

In this study, ten different samples of biomass were collected. All of the biomass samples were collected from Bauchi state, which are readily available in Nigeria. The biomass considered in this research are: rice husk (RH), rice straw (RS), corn cob (CC), woodchips (WC), groundnut shell (GS), desert date (DD), coconut shell (CS), palm kernel shell (PK), millet straw (MS) and sugarcane bagasse (SB). The biomasses were collected from the residues and/or by-products of agricultural products. The biomass was kept in open trays and sun-dried. The sun-dried samples were milled and then sieved to pass through a screen that has openings of 250 µm grain size according to ASTM D2013-86 standard method. The milled and sieved samples were stored in air-tight sample bottles to avoid further interaction with air.

2.2 Proximate analysis and higher heating value determination

The proximate analysis on dry basis involves the determination of volatile matter, ash, and fixed carbon contents of the samples. The proximate analysis was carried out according to ASTMD1762-84 (2007) standards. The higher heating value otherwise known as the calorific value of the sample species is the heat liberated when a unit quantity of the fuels (sample) is burned completely. The HHV was determined according to ASTM D5865/D5865M (2019) using bomb calorimeter model Parr 6100.

2.3 Models for prediction of higher heating values

Correlations for estimating HHV based on proximate analysis usually consider the content of ash (A), volatile matter (VM) and fixed carbon (FC) as the independent variables. Correlations for the prediction of HHVs based on proximate analysis of biomass exist in many related literatures. In this research, thirteen models were considered, eight linear and five non-linear models. The models were selected from numerous ones based on their high performance as reported previously. The eight linear models used are the ones given by: Parikh *et al.*(2005); Kieseler *et al.* (2013); Sheng and Azevedo (2005); Soponpongpipat *et al.* (2015); Cordero *et al.* (2001); Yin (2011); Kwaghger *et al.* (2017); Özyuğuran and Yaman (2017). The five non-linear models used are the ones given by: Qian *et al.* (2020); Garcia *et al.* (2014); Erol *et al.* (2010); Dashti *et al.* (2019) and Xing *et al.* (2019) (see Table 1).
The predicted heating values are calculated by substituting the volatile matter (VM), ash (A), and fixed carbon (FC) contents obtained experimentally from the proximate analysis. This procedure was repeated for all the biomass samples using the correlations M1-M13 (Table 1) to obtain the predicted HHVs of each of the samples. The calculated higher heating values were then compared with the experimental heating values.

Table 1: Predictive Higher Heating Value Models Based on Proximate Analysis

Model No.	Equation	Reference
M1	$HHV = 0.3536FC + 0.1559VM - 0.0078(A)$	Parikh et al. (2005)
M2	$HHV = 0.4108(FC) + 0.1934(VM) - 0.0211(A)$	Kieseler et al. (2013)
M3	$HHV = -3.0368 + 0.2218(VM) + 0.2601(FC)$	Sheng and Azevedo (2005)
M4	$HHV = 18.297- 0.4128A + 35.8/FC$	Soponpongpipat et al. (2015)
M5	$HHV = 35.43 - 0.1835VM - 0.3543(A)$	Cordero et al. (2001)
M6	$HHV = 0.1905VM + 0.2521FC$	Yin (2011)
M7	$HHV = 0.6042FC + 0.4083VM + 0.24424A + 0.4107M -25.204$	Kwaghger et al. (2017)
M8	$HHV = -17.507 + 0.3985(VM) + 0.28755(FC)$	Özyuğuran & Yaman (2017)

M9	HHV = $(30.3(FC)^2 + 65.2(A)^2 + 55.4(FC) - 48.5(A) + 9.591)/1000$	Qian et al. (2020)
M10	HHV = $(1.83 \times 10^{-4} - 3.98(A^2) - 112.1(A))/1000$	Garcia et al. (2014)
M11	HHV = $-5.9 + 0.836(FC) - 0.0116(FC)^2 + 0.00209(VM)^2 + 0.0325(A)^2$	Erol et al. (2010)
M12	HHV = $-0.0038\ (-19.9812FC^{1.2259}-1.0298 \times 10^{-13}VM^{8.0664} + 0.1026A^{2.4231}- 1.2065 \times 10^7\ (FCxA^{4.6653}) + 0.0228\ (FCxVMxA) - 0.2511(VM/A)) - 0.0478(FC/VM) + 15.7199$	Dashti et al. (2019)
M13	HHV = $19.050+0.124FC-0.021VM-0.167A-0.001FC^2 + 0.000018VM^2 - 0.000055A^2$	Xing et al. (2019)

Footnote: HHV = Higher Heating Value (MJ/kg); FC = Fixed Carbon (%); VM = Volatile Matter (%); A = Ash (%).

2.4 Evaluation of the models

The predictive performance of the models was assessed in terms of statistical indicators. Correlation is said to be the best-fitted regression line, if the error of the estimation between the experimental and calculated tends to zero. In order to choose the most appropriate model, the average absolute error (AAE) (Equation 1), average bias error (ABE) (Equation 2) and root mean square error (RMSE) (Equation 3) were evaluated to select the best correlation.

The AAE quantified the proximity of the calculated HHV value to the experimental HHV value, with the lower AAE indicating a higher accuracy of the particular correlation; the positive ABE value meant that the average calculated value of HHV was higher than the measured one. The smaller absolute value of the ABE, the smaller the deviation of correlation (Qian *et al.,* 2020).

$$\text{AAE} = 1/\text{n} \sum_{i=1}^{n} \left| \frac{HHVcalculated - HHVexperimental}{HHVexperimental} \right| \quad (1)$$

$$\text{ABE} = \frac{1}{\text{n} \sum_{i=1}^{n} \left(\frac{HHVcalculated - HHVexperimental}{HHVexperimental} \right)} \quad (2)$$

$$\text{RMSE} = \sqrt{1/n \sum_{i=1}^{n} \left(HHV_{Calculated} - HHV_{Experimental} \right)^2} \quad (3)$$

Where: AAE is the Average absolute error, ABE is the Average bias error, and RMSE is Root mean square error

3. Results and Discussion

3.1 Experimental proximate analysis and HHV

The proximate analysis and experimentally determined higher heating value results for the different biomass samples are given in Table 2. The biomass analysed included rice husk (RH), rice straw (RS), corn cob (CC), wood chips (WC), groundnut shell (GS), desert date kernel (DD), coconut shell (CS), palm kernel shell (PK), wheat straw (WS), and sugarcane bagasse (SB). The proximate analysis (dry basis) indicates the fixed carbon (FC), volatile matter (VM) and ash content (A) of the biomass.

Table 2: Proximate Analysis and Experimental Higher Heating Values of Biomass Samples

Biomass	FC	VM	Ash	HHV(Exp)
Rice Husk	13.89	69.53	16.58	15.96
Rice Straw	15.28	67.44	17.28	15.84
Corn Cob	20.7	75.10	4.20	18.22
Wood Chips	16.77	79.11	4.12	18.65
Groundnut Shell	22.45	74.22	3.33	17.97
Desert Date	18.09	78.94	2.97	18.25
Coconut Shell	22.34	71.86	5.80	19.73
Palm Kernel	19.85	73.87	6.28	18.52
Wheat Straw	16.01	77.12	6.87	15.84
Sugarcane Bagasse	13.73	84.15	2.12	17.23

The results of the proximate analysis showed variation due to the changes in composition and properties of the different biomass materials. The fixed carbon varied from 13.73% to 22.45%, the volatile matter was in the range of 69.53% to 84.15%, and ash content was in the range of 2.12% to 17.28%. Groundnut shell and coconut shell contains 22.45 and 22.34% fixed carbon, which was higher than all the other samples. It was reported previously that coconut shell has 24.4 fixed carbon (Mamat *et al.,* 2015). Wood chips showed good HHV due to high volatiles and low ash content. Rice straw and rice husk have ash content of 17.28 and 16.58, which are higher than other samples. It was reported in literature that rice husk contains about 16.3 % ash (Vaskalis *et al.,* 2019). High ash content translates to the poor fuel quality while higher fixed carbon and volatiles is related to good quality of fuel (Özyuguran and Yaman, 2017). The higher heating values recorded were in the rage of 15.84 to 19.73 MJ/kg (Table 2). The result obtained is similar to what was reported previously, where, twenty-seven biomass samples were studied and the heating value was between 14.51 to 20.24 MJ/kg (Özyuguran and Yaman, 2017). In another study, the HHV of twenty samples was found to be between 15.41 to 19.52 MJ/kg (Erol *et al.* 2010). It was noted that samples with high ash content (rice husk and rice straw) gave the least higher heating value (Table 2). Usually Samples that have higher fixed carbon and lower ash content would reasonably give higher heating value (Ahmaruzzaman, 2008).

3.2 Prediction of higher heating values

The HHV value of a biomass sample is directly related to the fixed carbon, volatile matter and ash content of the biomass. Equations 1-13 given in Table 1 were used to predict the HHV of the biomass samples. All the equations contain at least one of the proximate analysis parameters (i.e FC, VM or A). Model M1-M8 are all linear, while model M9-M13, are non-linear. The experimental HHV obtained from calorimeter and the calculated (predicted) HHV results using linear models M1-M8 are plotted for all the biomass samples (Figure 1). The linear correlations showed some deviations with least AAE of 3.84% by M1 (Parik *et al.*, 2005 model) and highest of 23.52 % by M2 (Kieseler *et al.,* 2013 model). Model M7 (Kwaghger *et al.,* 2017) showed least ABE and RSME of 2.2301% and 0.8701 MJ/kg (Table 3). The result was similar to what Kwaghger *et al.* (2017) obtained on HHV prediction of wood samples, Average Bias Error of 0.0365 to 1.137% was obtained. The result obtained is close to that reported by Ahmaruzzaman (2008), where four HHV models were tested on chars from coke, plastics, biomass and coal samples, it was also found out that Parik *et al.,* (2005) was the best model in HHV prediction from proximate analysis. The model showed average absolute error of 3.07 and average bias error of 0.41%. The experimental HHV and the predicted HHV results obtained from non-linear models M9-M13 are plotted for all the biomass samples (Figure 2).

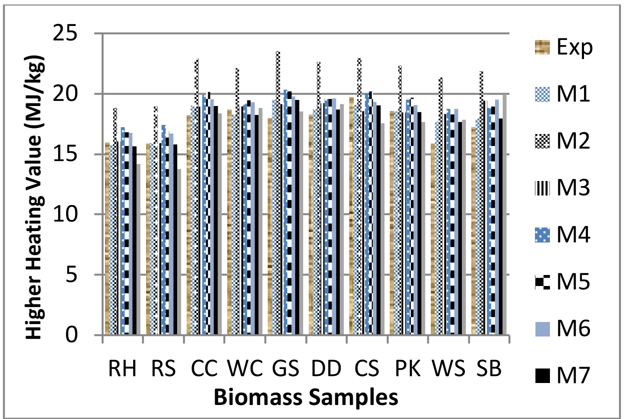

Figure 1: Experimental and predicted higher heating value of biomass using linear models

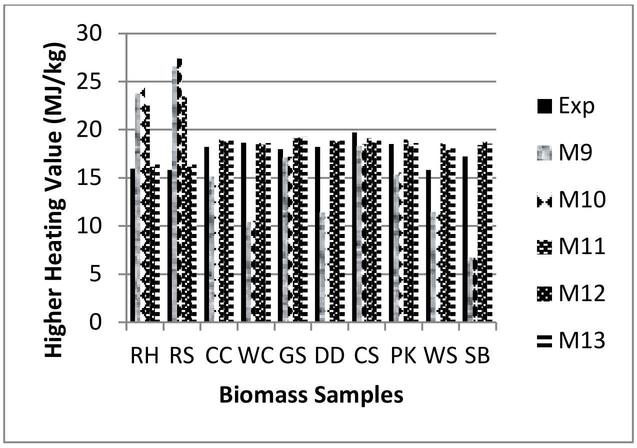

Figure 2: Experimental and Predicted Higher heating value of biomass using Non-linear models.

The non- linear correlations showed error between the measured and calculated HHV, (AAE) of 4.52 % by M9 (Qian *et al.,* 2020 model) and M12 (Dashti *et al.,* 2019 model) while highest was 33.69% by model M10 (Gacia *et al.,* 2014 model) (Table 3). Model M9 and M12 are closer to the experimental HHV (Figure 2), they also have the least error among the non-linear models (Table 3). Model M10 deviated much from the experimental HHV (Figure 2). In a similar study, the AAE of the best non-linear models tested was found to be between 1.7097 and 3.5339% (Erol *et al.,* 2010). In another study, empirical linear and non-linear correlations by Xing *et al.* (2019) gave RSME of 2.327 to 8.413 MJ/kg respectively.

Table 3: Comparison of the HHV prediction models based on statistical indicators for Linear Models

MODEL	AAE (%)	ABE (%)	RMSE (MJ/kg)	Reference
Linear Models				
M1	3.8389	2.5002	0.878	Parik *et al.,* 2005
M2	23.522	23.522	4.2244	Kieseler *et al.* (2013)
M3	5.2755	5.2755	1.2322	Sheng and Azevedo (2005)
M4	8.4703	8.4703	1.6267	Soponpongpipat *et al.* (2015)
M5	8.9953	8.9953	1.7501	Cordero *et al,* (2001)
M6	7.4993	7.085	1.5025	Yin, 2011
M7	3.8918	2.2301	0.8701	Kwaghger *et al.* (2017)
M8	7.8358	-0.1596	0.8701	Özyuğuran and Yaman (2017)

Table 4: Comparison of the HHV prediction models based on statistical indicators for Non-Linear Models

MODEL	AAE (%)	ABE (%)	RMSE (MJ/kg)	Reference
Non-linear models				
M9	4.5185	3.0082	0.9894	Qian *et al.* (2020)
M10	33.6887	-8.4538	6.8184	Garcia *et al.* (2014)
M11	13.4038	12.7176	3.3806	Erol *et al.* (2010)
M12	4.5185	3.0082	0.9894	Dashti *et al.* (2019)
M13	4.9308	4.0822	1.0546	Xing *et al.* 2019

Some models are generally good for all samples while some are specifically good in the estimation of HHV of some particular biomass only. Model M2 (Kieseler *et al.,* 2013) was far among the linear models in predicting accurate HHV for the biomass samples considered in this work (Figure 1 and 3). Similar observation was reported by Qian *et al.,* (2020), where Kieseler *et al.,* (2013) was used to predict HHV of biochars. It was concluded that the correlation of Kieseler *et al.* (2013) was biased ABE of 11.99%, therefore, it cannot be applied to the calorific value prediction of the biochar. Model M4 (Soponpongpipat *et al.* 2015) is specifically good in predicting HHV from proximate analysis for coconut shell (Figure 1 and 3) only. Model M6, (Yin, 2011) is good in predicting HHV for palm kernel shell (Figure 3). Model M1 by Parik *et al.*, 2005 and M7 by Kwaghger *et al.,* 2017 were generally better HHV estimators for almost all biomass samples (Figure 1 and 3). From the evaluation of statistical indicators that compared the calculated and the experimental HHV, it is found that the linear correlations showed better performance compared with that of the non-linear correlations. It was reported previously that that the addition of non-linear terms did not improved HHV models significantly (Özyuğuran *et al,* 2018).

Experimental and Predicted higher heating value of biomass using Non-linear models were compared (Figure 2 and 4). The statistical performance indicators for the non-linear models for HHV prediction from proximate analysis is given in Table 3. Model M10, the Garcia *et al.,* (2014) formula led to higher deviations for most of the biomass considered compared to the other non-linear models (Figure 2 and 4), though it predicted HHV for groundnut very well. Model M11 predicted other biomass very well except rice husk (RH) and rice straw (RS). The biomass had the highest ash content (Table 2), it could be that the model is good for biomass with low ash content only. Yin, (2011); Özyuguran and Yaman (2017) stated that for biomass with low calorific values (e.g. rice straw and rice husk), there is gap between the experimental and predicted values of HHV. Since some models are good to specific group of biomass, it was suggested that it will be reasonable to make biomass subclasses such as herbaceous samples, woody samples, agricultural residues, etc. and each subclass to be evaluated separately (Özyuguran and Yaman 2017). M9 (Qian *et al.,* 2020), M12 (Dashti *et al.*, 2019) and M13 (Xing *et al.,* 2019) were generally better non-linear HHV model estimators for almost all biomass samples (Figure 2 and 4).

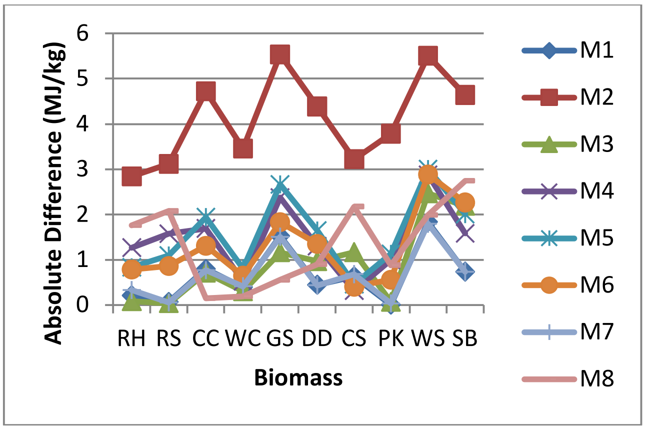

Figure 3: HHV Absolute difference for linear Models for different biomass samples.

The absolute difference between the experimental and predicted higher heating values of the ten biomass samples is depicted in Figure 3, for linear equations and Figure 4, for the non-linear equations. Model M2 (Kieseler *et al.,* 2013 model) is far from the actual HHV for all the biomass. Some models are good in predicting specific biomass, but not all the samples. Model M4 is good in predicting HHV of coconut shell, the absolute difference is 0.31523%. The experimental and predicted HHV are very close, but it deviates for other samples (Figure 3). Model M5 (Cordero *et al.,* 2001) fitted well for coconut shell only. Model M1 (Parik, *et al.*, 2005 model) and M7 (Kwaghger *et al.,* 2017 model) are better than other linear models with less absolute difference for most of the samples (Figure 3).

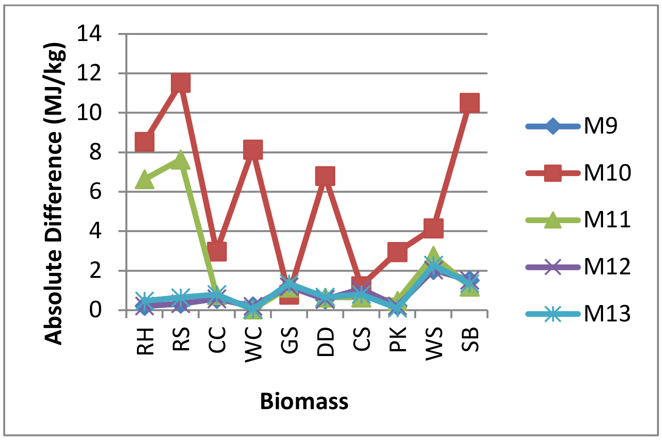

Figure 4: HHV Absolute difference for non-linear models of different biomass samples.

For the non-linear models, the absolute difference for Model M10 (Garcia *et al.* (2014) is much for most of the biomass samples except for groundnut shell and coconut shell (Figure 4). Therefore, the model can only be used in HHV prediction for biomass with relatively higher HHV. M11 (Erol *et al.*, 2010) is good in HHV estimation for all biomass except rice husk and rice straw (Figure 4), which are the two samples with the highest ash content (Table 2). Therefore, the model is not very good in HHV prediction of samples with high ash content. M9 (Qian *et al.* 2020), M12 (Dashti *et al.* (2019) and M13 (Xing *et al.* 2019) have less absolute difference (Figure 4) than other non-linear models for most of the biomass. Therefore, those models are the recommended non-linear models for HHV prediction from proximate analysis of biomass samples.

4. Conclusions

Evaluation of linear and non-linear empirical correlations for high heating value prediction of biomass samples from proximate analysis was carried out. The proximate analysis indicated that the biomass had different fixed carbon, volatile matter and ash content. The fixed carbon, volatile matter and ash content of the samples varied from 13.73% to 22.45%, 69.53% to 84.15%, and 2.12% to 17.28% respectively. Rice husk and rice straw have the highest ash content of 16.58 and

17.28% respectively. Eight linear and five non-linear predictive models were used in HHV prediction of the ten biomass samples. Statistical indicators such AAE, ABE and RMSE were used to evaluate the performance of the HHV predictive models and compared with the experimental values. Some model showed good performance to only specific biomass. For the linear models, Model M1 (Parik, *et al.*, 2005 model) with AAE, ABE, and RSME of 3.8389%, 2.5002% and 0.8780 MJ/kg; and M7 (Kwaghger *et al.,* 2017 model) with AAE, ABE, and RSME of 3.8918%, 2.2301% and 0.8701 MJ/kg are better than other linear models. Considering the non-linear models, M9 (Qian *et al.,* 2020 Model), M12 (Dashti *et al.* 2019 model) and model M13 (Xing *et al.* 2019 model) shows best performances with low AAE, ABE, and RSME. The non-linear models did not show superior performance than the linear HHV prediction models. The aforementioned models with better performance for the biomass samples considered in this work could be applied for HHV prediction for other different category of biomass.

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