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Evaluation of moisture content and higher heating value of bagasse using Fourier transform near infrared spectroscopy

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Abstract

The objective of this project was to evaluate of energy characteristics of bagasse using a Fourier transform near infrared spectroscopy (FT-NIRS) scanned in reflection mode at wavenumbers of 1000-2500 nm. There are 28 new bagasse samples and 28 old bagasse samples. The models were established by partial least square (PLS). Five difference pretreatments were raw spectra, first derivative, second derivative, standard normal variate and baseline offset. The best results for prediction moisture content and higher heating value were first derivative and standard normal variate, respectively. The models of moisture content and higher heating value showed the coefficients of determination (R^2) of validation set were 0.972 and 0.883, standard error of cross validation (SECV) were 2.171 and 259.441, bias were -0.017 and -0.184 %db, ratio of prediction to deviation (RPD) were 5.255 and 2.693, respectively. The model of ash showed the coefficients of determination (R^2) which was 0.372. The models of moisture and higher heating value had excellent accuracy while ash models were poor.

Keywords: Bagasse, Fourier transform, Near-infrared spectroscopy, Spectral pretreatment

1. Introduction

At present, there is a high demand for energy. Most of the energy being used still comes from fossil energy, which is about to run out. which in the future will not enough to meet demand, so we must find other sources of energy to use instead of fossil energy. Biomass is another type of renewable energy source. which is a waste material from the agricultural sector Especially Thailand is an important source of sugarcane cultivation. Therefore, there is material left over from the sugar production process, namely bagasse, which is a by-product of sugarcane juice extraction. By giving a high heat value approximately 4510 kcal/kg or 18,942 kJ/kg [1], objectives for using bagasse in thermal energy production. To produce superheated steam for use in generating electricity and transmitting electricity. Therefore, the efficient production of heat and electricity must have important factors: Quality of bagasse The quality of bagasse is assessed by energy properties such as moisture content, high heat value. and ash value Humidity value is considered an important factor in the bagasse combustion process. Because humidity directly affects combustion, high humidity makes burning difficult. This is because some energy is required to evaporate the water. and results in lower temperatures in the combustion chamber This results in problems in the production of electricity and heat. Resulting in decreased combustion efficiency. Ash is a solid substance in bagasse that cannot be burned. It is considered an unwanted part. The amount of ash affects the combustion efficiency. The higher the ash, the lower the heat energy. In commercial terms, biomass with high ash content will have a lower selling price. The calorific value is the energy obtained from combustion. Calorific value is useful in estimating the amount of raw materials to be used each day. and evaluate the amount of steam produced Including the electricity that can be produced as well. Commercially, biomass with a low calorific value should also have a low price. Currently, the measurement of these properties in bagasse power plants, the method is to look with the naked eye or randomly measure from bagasse piles. The reason is that measuring these properties takes a long time. and the price per sample is expensive make current control burning pot. It is still based on experience alone which may cause control errors. Therefore, a rapid method of measuring the thermal properties of bagasse is important and will help make work easier. At present, the Near Infrared Spectroscopy (NIR) technique is used to analyze the energy properties of biomass. Posom et al [2] used the near-infrared technique in the wavelength range of approximately 12500-4000 cm.$^{-1}$ Evaluating the high heat and moisture content of giant acacia wood pellets. Posom and Sirisomboon [3] evaluated the high heat, volatile matter, fixed carbon, and ash values of crushed bamboo using near-infrared spectroscopy techniques. year the results of the experiment found that This technique can evaluate the quality of biomass very well. and can be used in place of standard methods Biomass quality monitoring using NIR spectroscopy can be quickly analyzed. Does not destroy the sample Save cost per sample and does not use chemicals, causing no pollution and being environmentally friendly.

Therefore, this research aims to evaluate the energy properties of bagasse. High heating value, humidity and ash content Using near infrared spectroscopy, which is a rapid method for evaluating the energy properties of bagasse within 3-5 s/sample. If the equation for predicting the energy properties is obtained, it can be measured. It takes time to measure quickly. This makes it possible to predict situations that will occur during combustion. This makes it possible to make corrections in a timely manner, including being able to evaluate the amount of bagasse used to manage electrical energy production. Therefore, testing to determine the energy properties of bagasse is extremely important.

2. Materials and methods

2.1 Sample preparation

Fifty-six samples of bagasse used in the test came from Kaset Phol Sugar Factory. Udon Thani Province by random method from the bagasse pile. The bagasse samples were divided into 2 groups: 28 samples of new bagasse, 150 g each, and 28 samples of old bagasse, 150 g each. They were baked to reduce humidity to 0% by baking in an oven at a temperature. 105 °C until constant weight Divide the bagasse samples that have been dehumidified into a foil tray, totaling 56 samples. Bagasse humidity is adjusted by dividing the solution into 7 types, 1 box of each type. Place the bagasse in the foil tray into a box with All 7 types of solutions and then wait for humidity adjustment for 2 months.

2.2 Spectral measurement

FT-NIR spectroscopy machine, model MPA, Bruker, Germany, as shown in Figure 1.

Figure 1 FT-NIR spectroscopy machine, model MPA, Bruker, Germany.

The samples were scanned with Fourier transform infrared spectroscopy in backscatter measurement mode. (reflectance) at the wavelength range 1000 - 2500 nm, scanning resolution 16 cm^{-1} In one spectral measurement of each bagasse sample, 32 replicates were measured, and to average each bagasse sample, spectra were measured 3 times. The bagasse samples were divided into scanning cups. Then use the Bruker OPUS program to record the data.

2.3 Determination of humidity value

Put the bagasse samples into the oven, model Memmert Universal oven UF110, Germany, using a temperature of 105 C.° for 24 hours and then leave the bagasse samples in a desiccant (Desiccators) as shown in Figure 2 to keep the humidity constant. Then, the bagasse samples were weighed and the values recorded.

Figure 2 Dehumidifying jar

2.4 Determination of high heat value and ash

Take a sample of bagasse and press it into pellets. The weight was approximately 0.5 g (1 part compressed into 2 pellets) and then taken to determine the heat and ash values with the IKA bomb calorimeter, model C 200, as shown in Figure 3.

Figure 3 IKA bomb calorimeter, model C 200.

2.5 Calculation of energy properties of bagasse determined using standard methods

2.5.1 Find the moisture content as in Equation 1.

$$Moisture\ \%\ d.b = \frac{A-B}{B} x100 \quad (1)$$

2.5.2 Find the calorific value of biomass fuel using a bomb calorimeter as in Equation 2.

$$H_O = (C \times \Delta T - QExt1 - QExt2)\ /\ m \quad (2)$$

2.5.3 Find the ash content as in Equation 3.

$$Ash\ content\ \% = \frac{D}{B} x100 \quad (3)$$

2.6 Data analysis

2.6.1 Data customization before analysis (Pretreatment of spectral data) 1) first derivative 2) second derivative 3) Vector normalization and 4) Baseline offset.

2.6.2 Create equations (Calibration test)

2.6.2.1 Cross Validation is a method for estimating the error value of the model. Or the basic method of cross validation is sampling (Resampling), starting with dividing the data set into parts. and take some parts from that data set to examine.

2.6.2.2 Partial Least Squares (PLS) regression **a**s in equation 4.

$$Y = aX + b \quad (4)$$

2.6.3 Equation test (Validation test) includes Coefficient of determination $(R)^2$**,** Standard Error of Calibration (SEC), Standard Error of Prediction (SEP), Ratio of standard deviation of reference data in validation set to SEP; RPD and Average of difference between actual value and NIR value (bias).

3. Results and Discussion

3.1 Results of adjusting the moisture content of bagasse As shown in picture 4

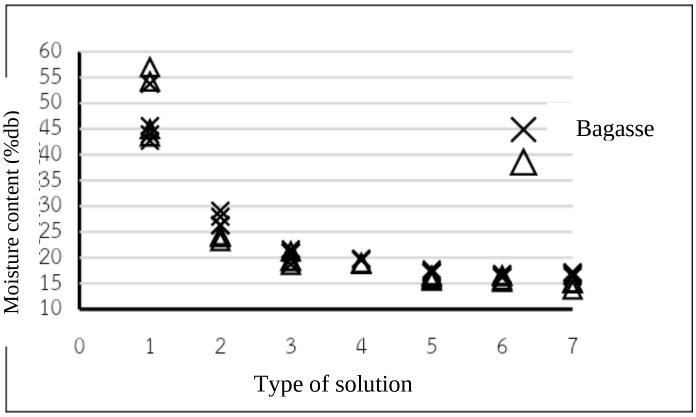


Figure 4 Moisture values of bagasse with all 7 types of solutions

where

Type 1 is CH3COOH solution. Type 2 is MgCl2 solution.
Type 3 is KNO3 solution. Type 4 is K2CO3 solution.
Type 5 is NaCl solution. Type 6 is NaNO2 solution.
Type 7 is KCl solution.

From Figure 4, it was found that the moisture values of new bagasse and old bagasse were adjusted using CH solution.$_3$COOH (acetic acid) had the highest moisture content, which was 56.9 %db, and bagasse whose moisture was adjusted using MgCl.$_2$ It had the second highest moisture content at 29.1 %db for bagasse whose humidity was adjusted using KNO solution.$_3$, K_2CO_3, NaCl, $NaNO_2$ The moisture content was 21.6, 19.8, 17.2, 16.8 %db, respectively. The solution used to adjust bagasse moisture that gave the lowest moisture value was KCl, which gave a moisture value of 13.7 %db. This different humidity value was used in Creating an equation to predict humidity values High heat and bagasse ashes continue.

3.2 Statistical values of humidity, heat, and ash

From Table 1, it shows the maximum, minimum, average, standard deviation, and data ranges of moisture, high heat, and ash. In the initial experiment, the plan was to use a total of 56 bagasse samples, but due to an error during Humidity adjustment This caused damage to 4 bagasse samples due to fungus. As a result, a total of 52 samples were left for testing. It was found that the highest humidity value was 59.6 %db and the lowest humidity value was 13.8 %db. For the high heat value, the highest value was 15667 J/g and the highest heat value had the lowest value equal to 13300 J/g. The highest value of ash value was equal to 11.7% and the lowest value of ash value was equal to 2.7%.

Table1 Statistical values of humidity, high heat, and ash values of all 52 bagasse samples.

Parameter	**Max**	**Min**	**Mean**	**SD**	**Range**
moisture (%db)	56.9	13.8	23.4	11.4	43.2
high heat (J/g)	15667	13300	14848.4	698.8	2367
ashes (%)	11.7	2.7	4.9	1.7	9.1

3.3 Internal relationship between high heat value and humidity value and high heating value and ash value

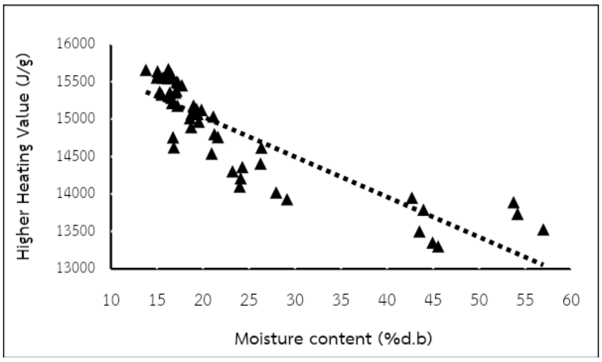


Figure 5 Relationship between high heat value and humidity value

Figure 5 shows the internal relationship between high heat values and humidity values. It can be seen that the high calorific value decreases with increasing humidity. Because biomass with a high moisture content has a low dry matter percentage, there will be less combustible parts, which will reduce the high calorific value as well [4]. The relationship between high heat and humidity is in the form of an exponential function. The correlation coefficient is 0.858, which indicates the internal relationship between these two values are high. It shows that the high humidity in the bagasse will result in a lower energy value for burning the bagasse. Therefore, reducing the humidity in biomass is another way to increase energy in biomass.

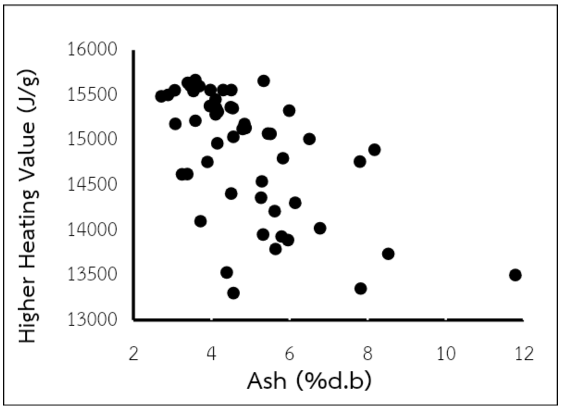


Figure 6 Relationship between high heating value and ash value

From Figure 6, it can be seen that the high heat value and the ash value are not related. Because the bagasse taken as a sample was adjusted for humidity, the values were not the same. Therefore, the proportion of moisture in the bagasse is higher than the proportion of ash that is in the small amount of bagasse. This makes it impossible to clearly see how the ash is related to the high heat. It shows that the moisture factor in bagasse has a greater effect on the heating value than the ash factor [4].

3.4 Creating equations to predict humidity values High heating value and ash

3.4.1 Results of modeling to predict humidity values

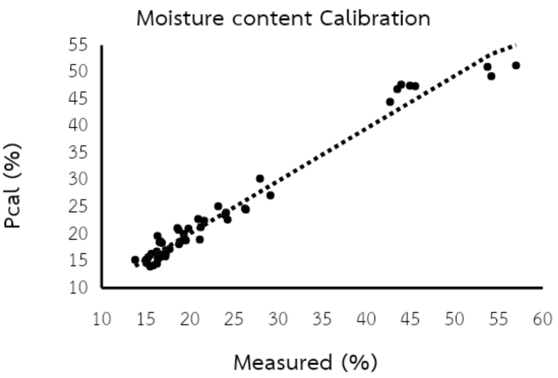
Table 2 Results of modeling and testing of models for predicting humidity values. high calorific value and ash values by comparing different spectral data enhancement techniques.

Table 2 Results of modeling and testing of models for predicting humidity values. high calorific value and ash values by comparing different spectral data enhancement techniques.

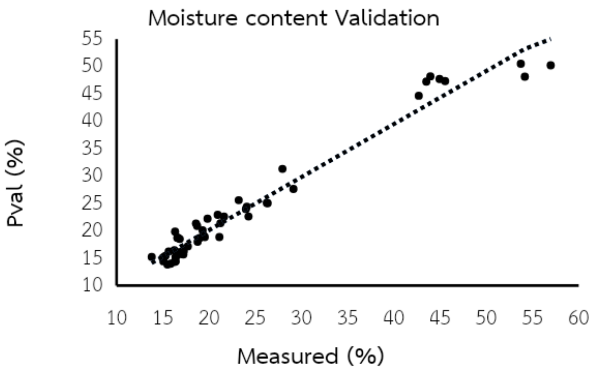
Parameter	Data improvement techniques	Calibration Set			Validation Set			
		F	R^2	SEC	r^2	SEQ	bias	RPD
MC	Raw spectra	5	0.960	2.261	0.948	2.580	-0.001	4.421
	SD1	3	0.972	1.900	0.963	2.171	-0.017	5.255
	SD2	4	0.971	1.930	0.962	2.207	-0.002	5.168
	SNV	5	0.954	2.415	0.938	2.811	0.017	4.058
	BASELINE	5	0.967	2.041	0.959	2.286	-0.024	4.990
HHV	Raw spectra	7	0.830	284.981	0.756	342.115	12.685	2.042
	SD1	6	0.823	290.980	0.749	346.388	4.535	2.017
	SD2	5	0.805	305.280	0.736	386.710	4.948	1.807
	SNV	3	0.883	199.374	0.859	259.441	-0.184	2.693
	BASELINE	6	0.771	330.922	0.684	388.917	-7.066	1.797
ASH	Raw spectra	3	0.350	1.334	0.225	1.457	-0.021	1.147
	SD1	2	0.349	1.335	0.264	1.420	-0.006	1.177
	SD2	2	0.363	1.321	0.273	1.411	-0.010	1.184
	SNV	3	0.301	1.384	0.194	1.486	-0.010	1.125
	BASELINE	3	0.372	1.312	0.279	1.406	-0.039	1.189

where
F : number of PLS factors use in calibration equation
R^2 : coefficients of determination of calibration set
r^2 : coefficients of determination of validation set
SEC : standard error of calibration
SECV : standard error of cross validation
bias : average error of validation
RPD : ratio of validation of deviation
HHV : Higher Heating Value
MC : Moisture content
SD1 : 1st Derivative
SD2 : 2nd Derivative
SNV : Standard normal variate
BASELINE : Baseline offset

From Table 2, the results of modeling and testing of the model for predicting humidity values are shown. The result is R.^{2} r^2 SEC, SECV bias, and RPD, respectively. It can be seen that spectral enhancements with different techniques give similar results in moisture estimation. Spectral improvement with technique 1st Derivative gave the best results compared to other techniques. Figure 6 shows the relationship between the moisture values obtained from predictions and from standard methods using spectra in the wavelength range of 1000-2500 nm for the bagasse calibration and validation sets by the technique. that are appropriate for evaluating humidity are Spectral improvement with technique 1st Derivative, with a coefficient of determination of 0.972, which indicates good prediction accuracy and can be used for quality assurance [5-6].



(a) Bagasse Calibration set



(b) Bagasse Validation Set

Figure 6 Bagasse Calibration and Validation set

3.5 Regression coefficients of humidity values

The regression coefficient is also known as the weighting factor for each wavelength value. It is a value that indicates how much each wavelength affects the modeling and prediction value. If the absolute value of the regression coefficient at any wavelength is high, it indicates that the vibration of any bond That wavelength affects the modeling and prediction value. Figure 7 shows the regression coefficient of Spectrum 1.st Derivative for moisture evaluation The peak at wavelength around 1430 nm is related to the first order overtone vibration of the O-H bond, and the wavelength of 2266 nm is related to the O-H +C-C bond, while the wavelength of 1705 nm is related to the vibration of the C-H bond in starch, and at wavelength 1923 nm is related to the O-H bond of water molecules [7].

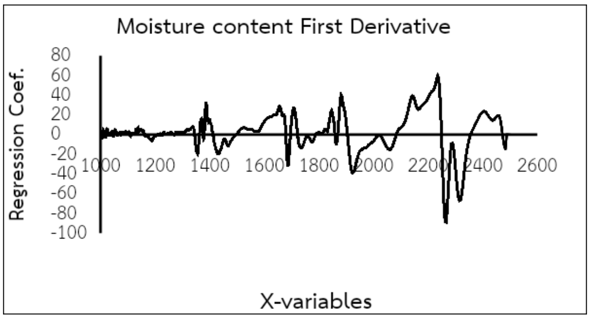
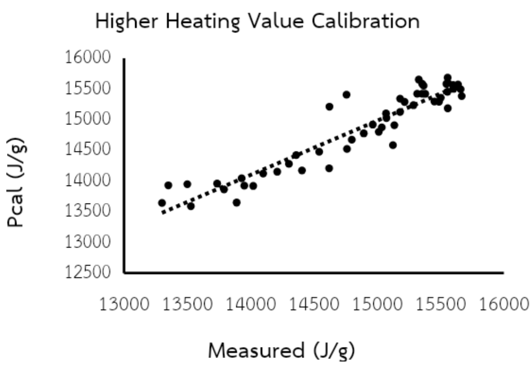
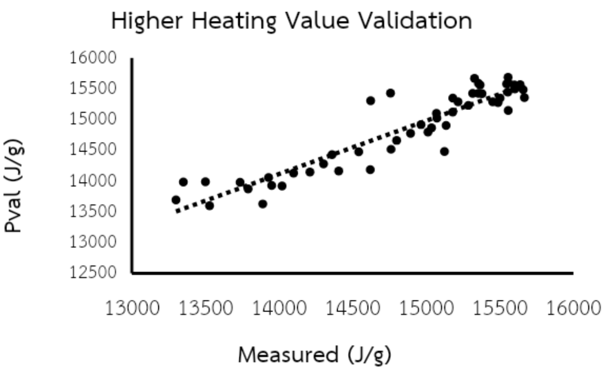


Figure 7 Regression coefficients of the spectra updated with Technique 1.st Derivative for humidity prediction models

From Table 2, results of modeling and testing of models for predicting high heating values are shown. which has the result value is R^2 r^2 SEC SECV bias and RPD respectively. From the results it can be seen that for the high heat estimation Spectral enhancement using various techniques gave similar results. However, improving the spectrum with SNV gave the best results compared to other techniques. Figure 8 shows the relationship between the high heat values obtained from the prediction and the standard method of spectra at the wavelength range of 1000-2500 nm of bagasse. Calibration set and validation set. The techniques that are suitable for evaluating high heat values are the spectral enhancement using the SNV technique gave a coefficient of determination of 0.883, which indicates quite good prediction ability and can be used for quality assurance evaluation as well, but should be used for work that does not require high resolution [5-6].



(a)Bagasse Calibration set



(b)Bagasse Validation Set

Figure 8 Bagasse Calibration and Validation set

3.5 Regression coefficients of high heating values

Figure 9 shows the regression coefficients of the SNV spectrum for estimating the calorific value. The peaks at wavelengths around 1406, 1583 nm are due to the first order overtone vibrations of the O-H bond and at the wavelength 2128 nm are the 2 x O-H vibrations. The wavelength at 1895 nm is related to the O-H bonds of water molecules [7].

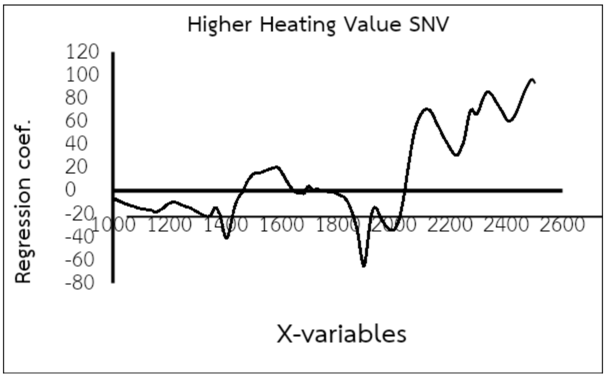
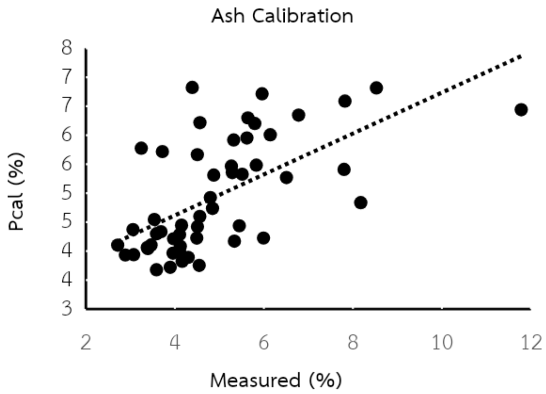
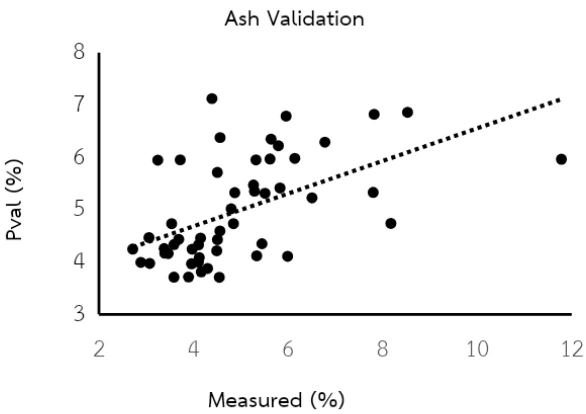


Figure 9 Regression coefficients of SNV-enhanced spectra with wavelengths for high-calorie analysis.

From Table 2 shows the results of modeling and testing of the model for predicting ash values. which has the result value is R^2 r^2 SEC SECV bias and RPD respectively. From the results it can be seen that for the evaluation of the ashes Spectral enhancement using various techniques gave similar results. But improving the spectrum with the Baseline offset technique gave the best results compared to other techniques. Figure 10 shows the relationship between the predicted ash values and the values obtained from the standard spectral method in the wavelength range of 1000-2500 nm. Bagasse Calibration Set and Validation Set. The techniques that are suitable for evaluating high heat values are the spectral enhancement using the Baseline Offset technique yielded a coefficient of determination of 0.372, indicating an inaccurate prediction ability. and is not recommended for use in quality assurance. The reason why an equation for predicting ash cannot be created may be because ash is an inorganic solid that does not react with infrared light. (no wave absorption occurs) [8-9].



(a) Ash calibration set



(b) Ash validation set

Figure 10 Ash calibration and validation set

4. Conclusions

From creating an equation to predict the moisture value, high heat, and ash value of bagasse adjusted for moisture with all 7 types of solutions using the partial least squares (PLS) regression method, it was found that the prediction of moisture value and high heat results in highly accurate predictions.

4.1 Results from the prediction of high heating values

From the results of the calibration equation using the improvement technique for Different spectra with data having a high heat range between 13300 - 15667 J/g found that a total of 5 spectra were compared. Raw spectra, 1st Derivative, 2nd Derivative, Baseline offset gives the R value.[2] The high value is in the range of 0.771 - 0.830 and the SECV value is in the range of 342.115 - 388.917. But for improving the spectrum with the SNV technique, it gives the best results in predicting the high heat value of bagasse by giving the R value.[2] is 0.883 and gives a low SECV value of 259.441, so it is accurate for predicting the high heat value of bagasse.

4.2 Results from predicting humidity values

From the results of the calibration equation using various spectral enhancement techniques with the data range for humidity values between 13.8 – 56.9 %d.b, it was found that there were 5 spectra that were compared. It was found that the Raw spectra, 2nd Derivative, SNV, Baseline offset gives R value.^{2} The high is in the range of 0.954 - 0.971 and the SECV value is in the range of 2.207 - 2.811, but for improving the spectrum with technique 1st Derivative gives the best results in predicting the moisture content of bagasse by giving the R value.^{2} is at 0.972 and gives a low SECV value of 2.171, so it is accurate for predicting the moisture content of bagasse within a sugar factory.

4.3 Results of the ashes prediction

From the results of the calibration equation using different spectral enhancement techniques, The data range for ash values was between 2.7 - 11.7 %. It was found that there were 5 spectra that were compared, including Raw spectra, 1st Derivative, 2nd Derivative, SNV, Baseline offset gives R value.^{2} Low values were in the range of 0.301 - 0.372 and high SEP values were in the range of 1.406 - 1.486. Due to the small coefficient of determination, they were not yet accurate enough for predicting bagasse ash values. A solution may be to increase the number of samples in the analysis with a larger range of differences.

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