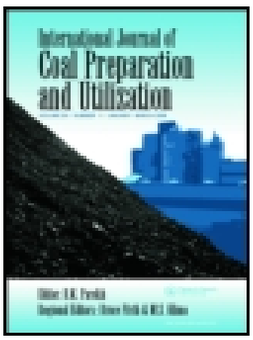

International Journal of Coal Preparation and Utilization

ISSN: 1939-2699 (Print) 1939-2702 (Online) Journal homepage: https://www.tandfonline.com/loi/gcop20

Estimation of Gross Calorific Value of Bituminous Coal using various Coal Properties and Reflectance Spectra

Nafisa Begum, Debashish Chakravarty & Bhabani Sankar Das

To cite this article: Nafisa Begum, Debashish Chakravarty & Bhabani Sankar Das (2019): Estimation of Gross Calorific Value of Bituminous Coal using various Coal Properties and Reflectance Spectra, International Journal of Coal Preparation and Utilization, DOI: 10.1080/19392699.2019.1621301

To link to this article: https://doi.org/10.1080/19392699.2019.1621301

INTERNATIONAL JOURNAL OF COAL PREPARATION AND UTILIZATION
https://doi.org/10.1080/19392699.2019.1621301

Estimation of Gross Calorific Value of Bituminous Coal using various Coal Properties and Reflectance Spectra

Nafisa Begum[a], Debashish Chakravarty[a], and Bhabani Sankar Das[b]

[a]Department of Mining Engineering, Indian Institute of Technology Kharagpur, Kharagpur, India; [b]Department of Agricultural and Food Engineering, Indian Institute of Technology Kharagpur, Kharagpur, India

ABSTRACT

In this study, the gross calorific value (GCV) of coal has been estimated using two types of coal analysis data. These are proximate data and spectral reflectance data in visible to near infrared range (wavelength: 400–2500 nm). The present study aims in developing two GCV prediction models and compare the accuracy of the predicted values using those models with the experimental value. Multiple linear regression (MLR) method is used to develop these models. In the first model, different properties of coal such as ash, moisture, and volatile matter contents are correlated with the GCV. Whereas in the second model, the GCV is predicted from the maximum absorption band depth at five different wavelength ranges. The performance accuracy has been evaluated using R^2, RMSE, and MAPE values of the two regression models. These two models yield R^2, RMSE, and MAPE values of 0.84, 2.26, 5.24 and 0.92, 1.6, 4.84, respectively. It has been concluded that the GCV predicted from the spectral reflectance data provides better accuracy than those predicted from the proximate data. Therefore, hyperspectral sensor based technology could be used for rapid determination of the GCV of coal with greater accuracy.

ARTICLE HISTORY
Received 6 April 2019
Accepted 13 May 2019

KEYWORDS
Coal; gross calorific value (GCV); proximate analysis; reflectance spectra; multiple linear regression

Introduction

In thermal power plants, coal as a fuel is assessed by its calorific value. Calorific value is expressed as the amount of heat released by a unit mass of coal upon its complete combustion. It is commonly termed as gross calorific value (GCV) and also known as higher heating value (HHV). GCV depends on rank, organic, and inorganic constituents of coal. In another way, GCV indicates the coal quality. Thus, several researchers have developed a number of linear and nonlinear model in order to estimate GCV from the proximate data of coal (Açikkar and SİvrİkaYa 2018; Majumder et al. 2008; Matin and Chelgani 2016; Mesroghli, Jorjani, and Chehreh Chelgani 2009; Patel et al. 2007).

The advantage of GCV prediction from other coal property data is that it could save the time and effort required for this experiment. Although, proximate analysis of coal also involves laborious laboratory experiments. In this context, imaging spectroscopy could be an option. At present, advancement in remote sensing has led the way for the development of hyperspectral sensors. It can very accurately give information on the chemical properties of an object. Thus, analysis of reflectance spectra of coal in visible to near-infrared range could serve as a tool for

CONTACT Nafisa Begum nafisa.geo@gmail.com Department of Mining Engineering, Indian Institute of Technology Kharagpur, Kharagpur, India

Color versions of one or more of the figures in the article can be found online at www.tandfonline.com/gcop

rapid determination of coal properties (Cloutis 2003; Wang et al. 2011; Kim, Lee, and Kim 2009; Bona and Andrés 2007; Andrés and Bona 2006; Wang et al. 2014).

Earlier researchers have already established that GCV can be calculated using conventional laboratory chemical analysis data as well as spectral analysis data. This study aims to estimate GCV from proximate data and spectral reflectance data by using multiple linear regression (MLR) and to comprehend the output obtained from these two regression models by comparing the calculated values of GCV with those experimentally derived values.

Methodology

Sample Collection and Preparation

Altogether, 43 coal samples of Oligocene and Permian age were collected from two different coal basins of North-eastern (Assam) and Eastern (West Bengal and Jharkhand) parts of India, respectively. These were of bituminous rank.

All coal samples were pulverized into three different grain sizes – 250 μm, 212 μm, and 74 μm to perform three different coal property analyses. GCV was determined by using Bomb calorimeter (Model Parr 660) following ASTM standard (D 5865-04) ("Standard Test Method for Gross Calorific Value of Coal and Coke 1" 2003). Ash, moisture, volatile matter, and fixed carbon (FC) contents of these samples were determined from the proximate analysis, following ASTM (D3172) standard (Standard 2002).

Spectral Data Recording

A total of 43 reflectance spectra were collected using ASD FieldSpec® within the wavelength range of 350–2500 nm and spectral resolution of 3 nm at 700 nm and 10 nm at 1400/2100 nm. The powdered sample of grain size less than 74 μm (Carlos, Alciaturi and Escobar 1996) was taken into a flat container and kept within the FOV of the sensor. The spectral data have been recorded in a dark room taking an average of 30 scans for each sample.

Spectral Data Pre-Possessing

At the initial wavelength range (350–400 nm), the instrument gave erroneous reflectance value. Thus, reflectance value from 400 to 2500 nm range was considered for this study. Before analysis, the reflectance spectral data were corrected using Savitzky–Golay digital filter in order to increase the signal-to-noise ratio without significantly distorting the spectra. After that continuum removal is applied to each laboratory spectra to normalize the reflectance spectra so that the absorption features could be compared from a common baseline. A convex hull was fit over the top of each spectrum using straight-line segments that connect local spectra maxima (Clark and Roush 1984). The continuum could be removed by following this formula (Equation 1):

$$S_{cr} = (S/C) \tag{1}$$

where S_{cr} is the spectra after continuum removal, S is the laboratory spectrum without any processing and C is continuum curve (Kokaly, Clark, Swayze, Livo, Hoefen, Pearson, Wise, Benzel, Lowers, Driscoll, and Klein 2017).

Multiple Linear Regression

The MLR method had been adopted to estimate the GCV value of coal. In this purpose, two different predictive models had been generated. In Model 1, the GCV had been estimated from the coal proximate data whereas in Model 2, the GCV had been calculated from the Vis-NIR (400–2500 nm) spectral analysis data. The prediction performance of the models was computed on three parameters. These are R^2, RMSE, and MAPE (Açikkar and SİvrİkaYa 2018). The formulae of these parameters are given in Equation (2–4).

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (f_i - \bar{y})^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \tag{2}$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - f_i)^2} \tag{3}$$

$$MAPE = \frac{1}{n} \sum_{i=1}^{n} \frac{|y_i - f_i|}{y_i} \tag{4}$$

where y_i denotes experimentally derived GCV, $\bar{y}$ is mean value of experimentally derived GCV, f_i represents predicted GCV and n is number of samples.

Model 1

The predictor variables are ash (A), moisture (M), and volatile matter (VM) of coal-derived from laboratory experiment on as received basis (Table 1). In proximate analysis, FC content is calculated from other variables [FC% = 100 – (A + M + VM). Therefore, it is not necessary to select FC content as a predictor variable because all these four parameters are in a closed system where the addition of all four parameters gives 100% (Hower 2006).

Model 2

Coal samples are showing prominent absorption feature at five wavelength intervals mainly due to the presence of moisture, different minerals, and functional groups. The maximum absorption band depth at each interval for each sample is measured and those absorption band depth is taken as predictor variable for Model 2. Further discussion on this model is made in the following sections.

Table 1. Proximate data of coal (as received basis) along with the GCV data.

Coal property	Minimum	Maximum	Mean	SD
Ash	0.90	52.90	14.44	14.27
Moisture	0.35	9.02	2.20	1.93
Volatile matter	12.97	45.93	34.01	11.64
Fixed carbon	24.01	62.79	49.35	7.91
GCV (mJ/kg)	13.65	34.09	28.32	5.51

Results and Discussion

Results

An increasing trend in the spectral reflectance values of coal in 400–2500 nm range can be observed in Figure 1. All coal samples show a broad absorption feature at 500–800 nm range and small absorption band at 1890–1950 nm, 2180–2230 nm, 2300–2340 nm, and 2440–2480 nm wavelength range. The generalized MLR formula was used for Model 1 (Equation 5) and Model 2 (Equation 6):

$$predicted\,\mathrm{GCV\ (MJ/kg)} = \mathrm{B} + A_1X_1 + A_2X_2 + A_3X_3 \tag{5}$$

$$predicted\,\mathrm{GCV\ (MJ/kg)} = \mathrm{B}' + A_1'Z_1 + A_2'Z_2 + A_3'Z_3 + A_4'Z_4 + A_5'Z_5 \tag{6}$$

where $X_1, X_2$and X_3 represent ash, moisture, and volatile matter content of coal; Z_1, Z_2, Z_3, Z_4 and Z_5 are the absorption band depth at wavelengths W_1 (500–800 nm), W_2 (1890–1950 nm), W_3 (2180–2230 nm), W_4 (2300–2340 nm), and W_5 (2440–2480 nm), respectively, B and B' represent regression constants and $A_1, A_2, A_3, A_1', A_2', A_3', A_4', A_5$ represent regression coefficients. The regression results of two models are given in Table 2.

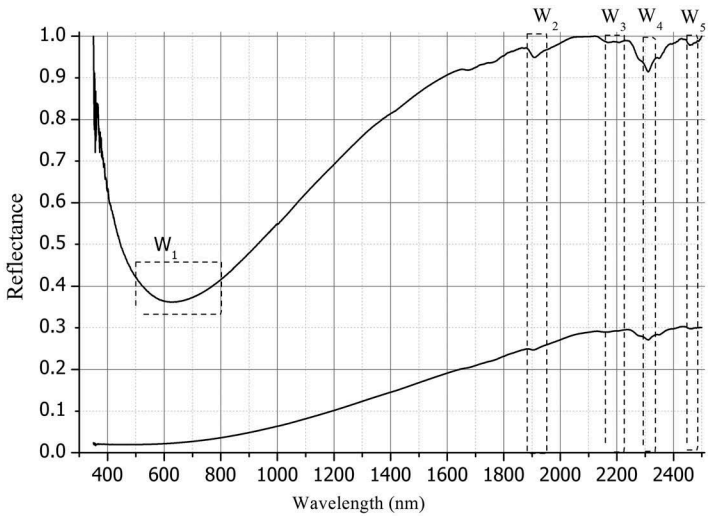

Figure 1. Mean spectral reflectance curve of bituminous coal. Lower reflectance curve is without any spectral preprocessing while the upper curve is after continuum removal.

Table 2. Results of the two regression models.

Model name	R^2	RMSE	MAPE (%)
Model 1	0.843	2.27	5.24
Model 2	0.92	1.64	4.85

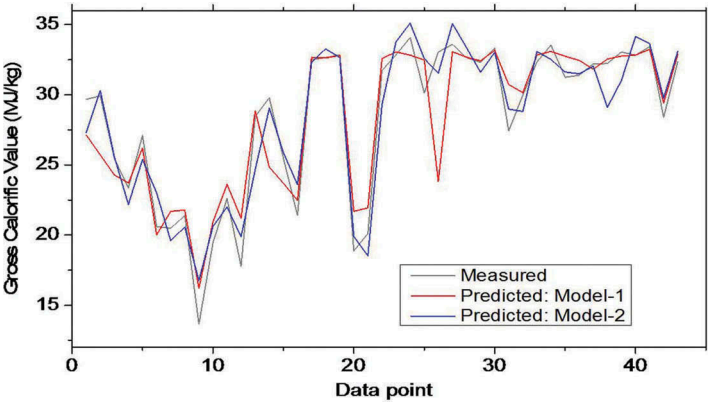

Figure 2. Comparison of GCV value derived experimentally with those estimated from regression models.

Discussion

The results obtained from two different models are shown in Table 2. It was observed that Model 2 gave a higher correlation coefficient (R^2 = 0.92) value and lower error value (RMSE = 1.64, MAPE = 4.85) compared with Model 1 (R^2 = 0.84, RMSE = 2.27, MAPE = 5.24). In Figure 2, experimentally derived GCV was plotted with those estimated from two regression models. Except in a few data points such as point 6, 38, 39, 42, and 43, estimated GCV from Model 2 gives closer value to the true value than those estimated from Model 1. In reflectance spectroscopy, the nature of absorption feature is governed by the chemical composition and atomic structure of the studied material (Meer, Yang, and Lang 2002). Therefore, spectroscopic data provide more information on the chemical properties of coal compared with a single proximate analysis which gives information on four parameters viz., ash, moisture, volatile matter, and FC content. This might be the reason of improvement in correlation coefficient and error values in Model 2.

Conclusions

Several researchers have estimated GCV from the organic and inorganic constituents of coal using different linear and nonlinear regression methods. In this study, the linear regression method had been selected because it is less complicated and easy to use. Like the earlier researches, this result also demonstrates that GCV could be well estimated from both proximate data as well as Vis-NIR analysis data. Although the rapid determination of GCV from reflectance spectra gives more accurate value than those estimated from proximate data. Analysis of reflectance spectra has more advantage on the conventional laboratory-based chemical analysis as it is nondestructive and takes no time to acquire the spectra and small amount of sample is required. Therefore, in thermal power plants, hyperspectral sensor could serve as a useful tool for estimating GCV. Although, there are certain limitation of this work. The sample number is few and all coal is of same rank and the spectra were recorded in laboratory condition. Thus, the study does not consider many other problems faced in thermal power plant while handling a huge amount of coal. Therefore, all these parameters should be considered before implementation. In future the

study team intends to carry out extensive studies including different coal ranks belonging to geologically different ages.

Acknowledgments

The authors gratefully acknowledge the financial support from the Department of Science and Technology, Government of India.

Disclosure statement

No potential conflict of interest was reported by the authors.

References

Açikkar, M., and S. Osman. 2018. Prediction of gross calorific value of coal based on proximate analysis using multiple linear regression and artificial neural networks. *Turkish Journal of Electrical Engineering & Computer Sciences* 26:2541–52. doi:10.3906/elk-1802-50.

Andrés, J. M., and M. T. Bona. 2006. ASTM clustering for improving coal analysis by near-infrared spectroscopy. *Talanta* 70 (4):711–19. doi:10.1016/j.talanta.2006.05.034.

Bona, M. T., and J. M. Andrés. 2007. Coal analysis by diffuse reflectance near-infrared spectroscopy: Hierarchical cluster and linear discriminant analysis. *Talanta* 72 (4):1423–31. doi:10.1016/j.talanta.2007.01.050.

Carlos, E., M. E. Alciaturi, and V. R. Escobar. 1996. Prediction of coal properties by derivative DRIFT spectroscopy. *Fuel* 75 (4):491–99. doi:10.1016/0016-2361(95)00246-4.

Clark, R. N., and T. L. Roush. 1984. Reflectance spectroscopy: Quantitative analysis techniques for remote sensing applications. *Journal of Geophysical Research: Solid Earth* 89 (B7):6329–40. doi:10.1029/JB089iB07p06329.

Cloutis, E. A. 2003. Quantitative characterization of coal properties using bidirectional diffuse reflectance spectroscopy. *Fuel* 82 (18):2239–54. doi:10.1016/S0016-2361(03)00209-6.

D3172. Standard practice for proximate analysis of coal and coke. 2002. *Annual Book of ASTM Standards* 1–2. doi:10.1520/D3172-07A.2.

Hower, J. C. 2006. Letter to the editor. *Fuel* 85:1307–08. doi:10.1016/j.fuel.2005.11.011.

Kim, D. W., J. M. Lee, and J. S. Kim. 2009. Application of near infrared diffuse reflectance spectroscopy for on-line measurement of coal properties. *Korean Journal of Chemical Engineering* 26:489–95. doi:10.1007/s11814-009-0083-0.

Kokaly, R. F., R. N. Clark, G. A. Swayze, K. E. Livo, T. M. Hoefen, N. C. Pearson, R. A. Wise, W. M. Benzel, H. A. Lowers, R. L. Driscoll, et al. 2017. USGS spectral library version 7. *USGS Spectral Library Version 7: U.S. Geological Survey Data Series 1035* 61. doi:10.3133/ds1035.

Majumder, A. K., P. Rachana Jain, A. Banerjee, and J. P. Barnwal. 2008. Development of a new proximate analysis based correlation to predict calorific value of coal. *Fuel* 87 (13–14):3077–81. doi:10.1016/j.fuel.2008.04.008.

Matin, S. S., and S. Chehreh Chelgani. 2016. Estimation of coal gross calorific value based on various analyses by random forest method. *Fuel* 177:274–78. doi:10.1016/j.fuel.2016.03.031.

Meer F., H. Yang, H. Lang. 2002. Imaging Spectrometry And Geological Applications. In: Meer F. D., Jong S.M.D. (eds.), *Imaging Spectrometry. Remote Sensing and Digital Image Processing*, vol 4. Springer, Dordrecht. doi:10.1007/978-0-306-47578-8_7.

Mesroghli, S., E. Jorjani, and S. C. Chelgani. 2009. Estimation of gross calorific value based on coal analysis using regression and artificial neural networks. *International Journal of Coal Geology* 79 (1–2):49–54. Elsevier B.V. doi:10.1016/j.coal.2009.04.002.

Patel, S. U., B. Jeevan Kumar, Y. P. Badhe, B. K. Sharma, S. Saha, S. Biswas, A. Chaudhury, S. S. Tambe, and B. D. Kulkarni. 2007. Estimation of gross calorific value of coals using artificial neural networks. *Fuel* 86:334–44. doi:10.1016/j.fuel.2006.07.036.

ASTM International. *D5865-13 Standard Test Method for Gross Calorific Value of Coal and Coke.* West Conshohocken, PA, 2013. doi: 10.1520/D5865-13

Wang, S., X. L. Feng, J. Zhou, and X. M. Wang. 2011. Fourier transform near infrared spectroscopy analysis of power plant coal quality. *Advanced Materials Research* 236–238:799–803. doi:10.4028/www.scientific.net/AMR.236-238.799.

Wang, Y., M. Yang, G. Wei, H. Ruifen, Z. Luo, and L. Guang. 2014. Improved PLS regression based on SVM classification for rapid analysis of coal properties by near-infrared reflectance spectroscopy. *Sensors and Actuators, B: Chemical* 193:723–29. Elsevier B.V. doi:10.1016/j.snb.2013.12.028.