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Prediction of heating value of straw by proximate data, and near infrared spectroscopy

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ABSTRACT

Exploration of straw resources for energy production has been attracting agricultural scientists and engineers for decades. And the heating value of straw has always been the focus when initiating a straw-based biomass energy project. Nevertheless determination of heating values of straw needs delicate and expensive calorimeter, and is time-consuming. It's quite desirable to develop quick and easy model predicting heating values of straw. In this study, we proposed three applicable models, first two are multiple linear regression (MLR) equations by contents of moisture, ash, and volatile matter, the other one is based on the near infrared spectroscopy (NIRS) technology. All the models provide satisfactory estimations of heating values of straw samples. The adjusted determination coefficients for MLR models were 0.9049 and 0.9039, and determination coefficients of calibration for NIRS model was 0.9604; When evaluated on independent validation, the determination coefficients were 0.8595, 0.8524 and 0.8946, respectively. The results indicated that both MLR models and NIRS model have the potential to predict the heating values of straw, while the NIRS model presented better accuracy.

1. Introduction

Biomass resources consumption for energy production had gained its popularity since the common awareness of energy crisis, increasing pollution [1] and carbon dioxide emission caused by fossil fuel combustion [2]. Abundance of straw from agricultural production interested scientists and engineers to explore efficient approaches in straw utilization for energy conversion. Power and heat production, gasification, ethanol fermentation and pyrolysis liquefaction of are the dominating technologies nowadays. Whatever the conversion technologies adopted, heating value is the straightest index should be concerned because it directly expresses how much energy can be obtained from the biomass resources. From engineering's view, it is the most important properties for design calculations or numerical simulations of conversion systems for biomass.

Determination of heating value usually was accomplished by interpreting absorbed heat from complete combustion in a calorimeter. This approach of analysis needs delicate and expensive calorimeter. Several formulae calculating heating value of biomass fuel by regression from ultimate analysis were introduced [3–8]. These equations are believed to be more accurate than correlations based on proximate analysis, but the instrument for ultimate analysis costs even more than calorimeter method. Literatures [9–13] correlating heating values and lingocellulosic contents were also presented frequently. While estimation of heating value from proximate analysis is found to be a cheaper and more achievable procedure. Reported models predicting heating value by proximate analysis were found in literatures. In Demirbaş's [14] research, the heating values of 7 species of biomass shells were correlated with their lignin, fixed carbon, and volatile material contents. Results indicated a high significant correlation between the heating values of the fruit shells and the lignin, fixed carbon, and volatile material contents. Sheng and Azevedo [13] reviewed existing regression models and proposed a new correlation to estimate heating value from the current proximate data. The proposed correlation between the heating values and dry ash content (wt%) of biomass could be conveniently used to estimate the heating values from proximate analysis. Other studies [15–17] contributed their equations to predict heating values of various biomass samples.

Different species of Biomass resources differ in characteristics and perform differently during energy conversion. Equations that using one documented data for one entire species of biomass were found not applicable for practical industrial use, because the cited proximate data of a specified biomass resource sometimes was not representative due to variation of sorts. Since predictive models already exist for other biomass resources, the present study focussed on model development for straw samples exclusively. In this paper, two of the most widespread biomass resources, rice straw and wheat straw, were collected in China. Proximate analyses of large

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Fig. 1. Origins of straw samples.

number of straw samples were conducted to estimate heating values through MLR models.

Near infrared spectroscopy (NIRS) is another method expanding its applicability in agricultural, food and pharmaceutical industry. Little sample preparation, simultaneous determination of multi-components made NIRS a rapid and cost-effective quantitative analysis technique. Alciaturi et al. [18] evaluated near infrared spectroscopy as a method for the determination of heating value of coal. Fifty-five samples (mainly bituminous coals) were analyzed in laboratory and the results correlated with second derivative spectra data. Andres and Bona [19] collected spectra from 142 coal samples of different origins in absorbance, reflectance and Kubelka–Munk units. The resultant spectra were correlated to heating value using partial least squares regression (PLS). By contrast, few researches were conducted using the NIRS technology as a predictive tool for determination of heating value of biomass resources. Related researches are imminently demanded for the development of biomass industry. Considering the necessity and feasibility this paper examined the feasibility of predicting heating values of straw samples by NIRS as a tentative study. The straw samples represented most of the range in heating value of straw around China. The variability was broad to ensure a wide range of heating values, thus better applicability of NIRS model.

2. Materials and methods

2.1. Samples

Two hundred and twenty two ($n = 222$) straw samples, which consist of 172 rice straw samples and 50 wheat straw samples, were collected from 24 provinces/municipalities around China. Mainly harvested in the year of 2005 and 2006, the samples covered different species, soil types and climates and the origins are mapped in Fig. 1. The straws were cut into 4–5 cm long, then one half of the samples were used for spectra collection and the other half for reference analysis.

2.2. Laboratory analyses

The Foss NIRSystems 6500 scanning monochromator (NIRSystems, Silver Spring, MD, USA), which is able to collect spectra from 400 to 1098 nm with a silicon detector and from 1100 to 2500 nm