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Prediction of elemental composition of coal using proximate analysis

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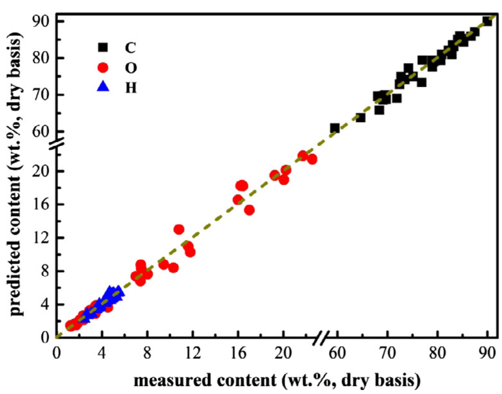
HIGHLIGHTS

- Select data points of four different rank coals.
- Understanding the relation between ultimate analysis and proximate analysis.
- Validate the fitted correlations with another set of data.
- Offer a valuable tool to set up a coal-thermal-conversion-process model.

GRAPHICAL ABSTRACT



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ABSTRACT

Ultimate analysis is an important property for fuel utilization. The experimental determination of ultimate analysis is sophisticated, long time consumed, and expensive, on the contrary, the proximate analysis can be run rapidly and easily. A variety of correlations to predict the ultimate analysis of biomass using the proximate analysis have been appeared, while there exists a few number of correlations to estimate the elemental compositions of coal using proximate analysis in the literature but were focused on the predicted model or dependent on the heating value of coal. According to the proximate analysis of four different ranks of coal, this study proposes a series of correlations which are classified to predict carbon, hydrogen, and oxygen compositions through using 300 data points and validated further by another set of 40 data points. These correlations have the R^2 of 0.95, 0.91, and 0.65 corresponding to the measured contents of C, H, and O in anthracite, 0.93, 0.83, and 0.67 of C, H, and O in high-rank bituminous, 0.86, 0.61, and 0.71 of C, H, and O in subbituminous, and 0.92, 0.67, and 0.66 of C, H, and O in lignite, respectively. The main merit of the correlations is the ability to estimate elemental composition of different rank coals using the proximate analysis and thus offers a valuable tool to set up a coal-thermal-conversion-process model.

1. Introduction

Utilization technique of coal is a major concern because of severe environmental pollution and energy inefficient. To suggest the clean and efficient utilization method of coal is essential. Physicochemical properties of coal are critical parameters for the

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utilization technology. For example, the higher heating value (HHV) that defines coal's energy content is an important parameter for designing the combustion system and evaluating pollution compliance [1]. The ultimate analysis of coal is either a necessary factor to investigate the whole process of chemical conversion and to predict the flow rate of flue gas and air quality in coal combustion [2]. While the proximate analysis is a fuel property which gives the chemical composition of coal and confirms the reasonable use of coal. Focusing on the ultimate and proximate analyses, it is possible to predict a large number of fuel parameters. Even if there is no direct cause-effect link between composition and properties, the systematic transformations accompanying coalification often permit correlations [3].

Several relationships were developed using ultimate and proximate analyses in the past. Chelgani et al. [4] developed a prediction method to estimate coal grindability using multiple regression and artificial neural network models, taking the data of the proximate and ultimate analyses. A similar study was conducted to compute Hardgrove grindability index for Kentucky coals [5]. Neavel et al. [6] proposed the simplest equation to estimate the volatile matter, using ultimate analysis data for low-rank coals. Correlations was also generated by Chelgani and his colleagues [7]. The goal in that work was to simultaneously predict vitrinite maximum reflectance and higher heating value of coal using ultimate analysis. A work used the combination of proximate and ultimate analyses with a neural network approach and multivariate regression analyses to predict maceral composition for Indian coals [8]. Attempts have been made to correlate ^{13}C NMR chemical structural analyses with coal properties such as the elemental composition and volatiles content [9]. By means of a semi-empirical method, Ko et al. [10] evaluated the complex relationship between the potential maximum amount of tar and elemental analysis. The ultimate and proximate analyses are the essential elements to estimate heating value of fuel. Various correlations for predicting higher heating value using ultimate and proximate analyses of solid fuel were reported [11–13]. Channiwala et al. [1] had developed the relationship to determine higher heating value based on ultimate analysis of solid, liquid and gaseous fuels. Similarly, Parikh et al. [14] and Komilis et al. [15] had estimated the heating value of biomass and municipal solid waste (MSW) from proximate analysis data, respectively. All the existing works show that it is possible to estimate the element composition of fuels with the help of proximate analysis, which requires only common equipment and can be implemented by any of efficient scientists or engineers.

Knowledge of proximate analysis thus can be used to determine element composition of fuels [2,16–19]. Vakkilainen et al. [16] developed a correlation to estimate the relationship between element composition and proximate analysis of black liquor. While Parikh et al. [17] and Shen et al. [18] proposed correlations to compute the ultimate analysis of biomass using proximate analysis. The data considered by Parikh and his co-workers are the contents of carbon, hydrogen, oxygen, volatile matter, and fixed carbon, neglecting the effect of ash content on the element composition. Considering this, adding the ash composition, Shen and his colleagues developed new correlations to estimate the carbon, hydrogen, and oxygen contents with a better estimation compared to those proposed by Parikh et al. [17]. Recently, Nhuchhen [2] distinguished raw and torrefied biomass, and then developed new correlations to estimate the contents of carbon, hydrogen, and oxygen using proximate analysis. For the municipal solid waste, there also exists a correlation to predict the element composition from proximate analysis [19]. However, there were no correlations to estimate the ultimate analysis of coal using the proximate analysis except the correlation proposed by Li et al. [20], which considered the effect of heating value on element composition. The content of nitrogen in coal is less to 0.5–1.8%, being haphazard with the degree of coalification. And the content of sulfur varies with depositional conditions when coal is formed. The nitrogen and sulfur compositions are thus not considered in this paper.

The main objective of this study is to develop the correlations for predicting the contents of carbon, hydrogen, and oxygen of coal using proximate analysis.

2. Methods

2.1. Collection and selection of suitable data

The coal ranks are wide and the properties vary with the coal rank to a great degree. Thus a great many original proximate and ultimate analyses of different rank coals, such as lignite, subbituminous, high-rank bituminous, and anthracite, were chosen from *Properties, classification and utilization of China coal* [21], and messages of 300 materials whose proximate and ultimate analyses are listed in Table S1, were gotten in for the sake of the correlations derivation, comprising 66 data for lignite, 74 data for subbituminous, 94 data for high-rank bituminous and 66 data for anthracite. In addition, 40 data were applied for correlations validation, as listed in Table 1. The boundary of C, H, and O in data utilized for the correlations validation and derivation are the same.

2.2. Methodology for fitting correlations

The proximate analysis on a dry basis includes fixed carbon, volatile matters and ash. The ultimate analysis includes carbon, hydrogen, and oxygen and so on. The volatile matters content shows the yield of volatile organic compounds after heating when under prescribed conditions. Undergoing a variety of chemical reactions, most of the mineral have shift and formed ash in the condition of high temperature. The formed ash also includes the unreacted mineral. And the fixed carbon is the residue after deducting the ash from the coke button. Both the volatile matters and fixed carbon contain carbon, oxygen along with hydrogen. However, the determination of fixed carbon content on a dry basis is closely related with the ash and volatile matters contents, it is reasonable to assume a relationship between the ultimate and proximate analyses.

According to the above analysis, it can be seen that carbon, hydrogen and oxygen compositions are proportional to the relative contents of fixed carbon, volatile matters and ash, respectively. Therefore, it is supposed that carbon (C, wt.%), hydrogen (H, wt.%) and oxygen (O, wt.%) are separately a function of fixed carbon (FC, wt.%), volatile matters (VM, wt.%), and ash (ASH, wt.%). The proximate and ultimate analyses are based on a dry basis herein.

Firstly, each dependent variable (i.e., C, H, and O) was plotted as opposed to each independent variable (i.e., FC, VM, and ASH), which allowed a rapid screening to decide the relative dependence on each independent variable and enabled a visual detection of correlation forms. Secondly, an individual nonlinear correlation was created for each independent variable, and a pseudo R^2 value was computed to decide the contribution of each correlation. All kinds of equation patterns were tested, yet experience indicated that a quadratic polynomial lead to the optimum matching for parameters. Thirdly, according to the separate polynomial correlation, the pattern of the correlation was deduced between each element composition and the combination of the proximate analysis. The detailed steps are described in the following example for element C of subbituminous.

A case study for element C of subbituminous

From the plots of element C of subbituminous versus each independent variable in Fig. 1. it was showed the content of C depends observably on the value of ASH, VM, and FC. Then the patterns of the optimum matching equations from the three plots (element