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# Prediction models of calorific value of coal based on wavelet neural networks

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#### ABSTRACT

New prediction models based on wavelet neural networks (WNNs) have been proposed to estimate the gross calorific value (GCV) of coals. The input sets for the prediction models are involved of the proximate and ultimate analysis components of coal and the oxide analyses of ash. The coal samples, which have been employed to develop and verify the prediction models, are from United States Geological Survey (USGS) and China Huaneng Group. Some published methods have also been employed and redeveloped to make a comparison with the models proposed in this paper. The comparison reveals that the WNN models proposed here based on the proximate (ultimate) analysis components of coal, are consistently better than the published ones. The WNN models based on the oxide analyses of ash have higher accuracy in estimating the GCV of Chinese coals than US coals. Here we also analyze the possible reasons that could lead to the low estimated accuracy.

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#### 1. Introduction

Coal, which is an important petrochemical energy, is widely used in industrial production, such as electric power, iron and steel, chemical industry and so on. According to BP world energy statistics yearbook [1], the world proven reserves of coal were 891.53 billion tons up to 2014 and the reserves to production (R/ P) ratios in most regions of the world continued to decline (Fig. 1). This means that the utilization of coal resources has not subsided yet. In China, coal will occupy the dominant position in the energy supply structure for a long time, especially in the power generation industry (Fig. 2).

On the one hand, the calorific value (CV) as an indicator of the chemically stored energy in coal is an important parameter in the assessment of its value as a fuel [3,4], and potentially could be a basis for the purchase of coal [5]. On the other, determining gross calorific value (GCV) or higher heating value (HHV) experimentally by the essential apparatus become costly and time consuming [6]. Fortunately, in all thermal power plants, the proximate analysis, and ultimate analysis of coal are common practice to assess the quality of coals [7]. Thus, for many researchers, the present works have focused on developing a correlation which can estimate the GCV based on them [8]. Among the models

presented, most are based on linear regression method [6-32]. However, the relationships between the proximate and ultimate analysis and their GCV value are nonlinear and in the papers studying both linear and nonlinear regression approaches, the nonlinear-based models generally gave better prediction results [6,10-11,15,29,33-38]. Therefore, a few research works have focused on the development of nonlinear-based models between GCV and proximate or ultimate analysis of coals. For example, Huang et al. [37] proposed an artificial neural network (ANN) model to predict the heating value of straw samples. The ANN model could better deal with both linear and nonlinear relationship between the ash content and calorific value and showed the best accuracy (RMSE = 241 J/g) among the proposed models. Ghugare at al. [38] proposed two artificial intelligence (AI) formalisms namely GP and MLP neural networks for predicting the HHV of biomasses based on the constituents of the proximate and/or ultimate analyses. The prediction results revealed that the AI models were consistently better than that of their existing linear and/or nonlinear counterparts. Tan et al. [39] proposed a nonlinear model termed support vector regression (SVR) based on proximate analysis to estimate the higher heating value (HHV) of coals. A total of 167 Chinese coal samples and 4540 U.S. coal samples were employed to develop and verify the SVR-based correlations. The estimation results indicated that the average absolute errors from estimating the HHV of Chinese and U.S. coals were only 2.16% and 2.42%, respectively. Idoia et al. [40] evaluated the feasibility of



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Fig. 1. Reserves to production (R/P) ratios from BP world energy statistics yearbook [1,2].



Fig. 2. Fuels for power generation in China [1,2].

using artificial neural networks (ANN) and empirical correlations (Matlab 2013) to fit and estimate the gross calorific value of biomass from proximate analysis databases available in the literature. Starting from a database of 100 records and raising the database to 225 and thereafter to 350, it was possible to analyze the differences between basic fitting characteristics of ANNs and correlation models. Twelve HHV values of biomass available in the literature were used to verify the validity of the fittings. Ebru [9] proposed a new biomass higher heating value (HHV) prediction model using adaptive neuro-fuzzy inference system (ANFIS) approach. Its obtained coefficient of regression  $(R^2)$  and root mean square error (RMSE) are 0.8836 and 1.3006, respectively, in the testing phase. The results showed that sub-clustering based ANFIS model was an efficient technique to obtain high accuracy biomass HHV prediction. Ghugare et al. [41] proposed nonlinear models based on proximate and ultimate analysis for the prediction of HHV of coals by utilizing the computational intelligence (CI) based genetic programming (GP) formalism. The results of this modeling study indicated that each of the three GP-based models possessed an excellent HHV prediction accuracy and generalization capability. Qian et al. [42] proposed a simple prediction model based on ultimate analysis of biomass to predict higher heating value (HHV) via modifying reductance degree of the biomass. These models were easily applicable for they require only C, H or C, H, S contents (both on wt% dry biomass basis).

The framework of wavelet neural network (WNN) is constructed based on BP neural network. It replaces the sigmoid function with the wavelet transform function and combines translation factor and scaling factor to construct the wavelet basis. The threshold-controllable function in BP neural network, which is to carry on the horizontal fine adjustment to the weighted input vector after the input quantity, is realized by translation factor. The weight adjustment at different scales is realized by the scaling factor. Due to the combination of these two factors, the wavelet neural network can be used to approximate the objective function at different scales.

In this study, WNNs are introduced to develop the correlation between the proximate and ultimate analysis and GCV of coals from the top two largest coal consumption countries. Besides, oxide contents in the coal ash are also used to estimate the GCV of coals based on U.S. and Chinese coal samples respectively. Additionally, the proposed WNN models are compared with the published methods to show their advantages.

#### 2. Samples and methods

#### 2.1. Methods

#### 2.1.1. Topological structure of wavelet neural network

The topological structure of WNN is shown in Fig. 3. There are three layers in the wavelet neural network model: input layer, hidden layer and output layer. The input layer contains M (k = 1, 2, ..., M) neurons, the hidden layer contains K (j = 1, 2, ..., K) neurons and

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