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Ignition temperature and activation energy of power coal blends predicted with back-propagation neural network models

Jun Cheng *, Xin Wang, Tingting Si, Fan Zhou, Junhu Zhou, Kefa Cen

State Key Lab of Clean Energy Utilization, Zhejiang University, Hangzhou 310027, China

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ABSTRACT

Back-propagation (BP) neural network models were developed to accurately predict the ignition temperature and activation energy of 16 typical Chinese coals and 48 of their blends. Pearson correlation analysis showed that ignition temperature and activation energy were most relevant to the moisture, volatile matter, fixed carbon, calorific value and oxygen of coals. Accordingly, three-layer BP neural network models with five input factors were developed to predict the ignition characteristics of power coal blends. The BP neural network for ignition temperature gave a relative mean error of 1.22%, which was considerably lower than 3.7% obtained by the quadratic polynomial regression. The BP neural network for activation energy gave a relative mean error of 3.89%, which was considerably lower than 10.3% obtained by the quadratic polynomial regression. The accuracy of the BP neural network was significantly higher than that of traditional polynomial regression.

1. Introduction

Coal consumption in China was approximately 3.51 billion tons in 2014, and more than 50% of the total consumption was used for coal-fired power generation and industrial boilers. However, the uneven distribution and imbalance between the supply and demand of coal resources in China have led to the frequency change and instability of coal quality in many power plants and industrial boilers. Power coal blends make coal characteristics more consistent with the designed coal, thereby solving problems, such as high coal consumption, furnace slagging and excessive emission of pollutants in power plants that burn non-designed coal [1–3]. A strong nonlinearity of ignition characteristics exists between blended coal and parent coals, whereas the traditional weighted average method cannot accurately obtain the ignition characteristics of blended coal based on the properties of parent coals [4]. The most important thing is that many combustion experiments can be avoided if the ignition characteristics can be accurately predicted based on coal properties.

The neural network is a powerful nonlinear tool and has been widely used in the field of coal-fired power generation [5–10]. Li et al. [11] reported that the Hardgrove Grindability Index (HGI) can be estimated indirectly from the proximate analysis of coals in China through the generalised regression neural network (GRNN) method. The maximum error is less than 5 for GRNN, which is acceptable according to the China National Standard for the testing of HGI. Patel et al. [12] developed seven nonlinear models using the methodology of artificial neural networks (ANNs) to estimate gross calorific value (GCV) with a special focus on Indian coals. The results of the GCV estimation clearly suggest that all the ANN models possess excellent prediction accuracy. Yao et al. [13] applied the feed-forward back-propagation (BP) ANNs to predict hydrogen content in coal through proximate analysis from a diverse range of coals. The linear regression between the predicted and experimental values of the hydrogen content in coal produced a correlation coefficient of 0.937, with a mean squared error of 0.0087, and the mean relative error was 5.46%. Liukkonen et al. [14] modelled the formation of nitrogen oxides (NO_x) in a circulating fluidised bed (CFB) boiler through ANN. The results show that the ANN method is an efficient and productive visual method of modelling the CFB process and its emissions. Smrekar et al. [15] applied two ANN models through real plant data to predict the fresh steam properties of a brown coal-fired boiler in a Slovenian power plant. Both models showed good accuracy in predicting the real data not used for their training, and an improved model based on these two gave the average error of mass flow rate, pressure and temperature of 0.95%, 0.38% and 0.47%, respectively. Bekat et al. [16] predicted the amount of bottom ash formed in a pulverised coal-fired power plant through three-layer ANN modelling which used the one-year operating data of the plant and the properties of the coals processed. The R^2 (coefficient of

* Corresponding author. Tel.: +86 571 87952889; fax: +86 571 87951616.
E-mail address: juncheng@zju.edu.cn (J. Cheng).

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determination) values between the actual (bottom ash/coal burned) ratios and the model predictions were 0.988 for the training set and 0.984 for the testing set. Joo et al. [17] applied ANN with three input factors—flame temperature, length, and input airflow rate—to estimate the EINO$_x$ trends and to determine the effectiveness of the NO$_x$ mechanism. Yin et al. [4] reported the application of the BP neural network in predicting the coal ash fusion temperature of the ash compositions of some Chinese coals. The ignition temperature and activation energy of power coal blends have an important influence on coal combustion stability and efficiency. However, the application of the BP neural network in predicting the ignition characteristics of power coal blends based on coal properties has not been reported in the literature until now. In this study, the ignition temperature and activation energy of 16 typical Chinese coals and 48 of their blends were obtained through experiments on a thermogravimetric analyser. Pearson correlation analysis was adopted to quantitatively investigate the influence of coal properties on ignition temperature and activation energy. Moreover, the ignition temperature and activation energy of power coal blends were predicted using BP neural network models and traditional polynomial regression according to the results of Pearson correlation analysis.

2. Experiments and computation methods

2.1. Thermobalance experiments

The chemical compositions and ignition characteristics (see Table 1) of 16 typical Chinese coals and 48 of their blends were obtained by experiments. The air-dried coal samples were pulverized in a mill to particle size about 150 μm. The burning profiles were determined in a SINKU RIKO-5000RH thermogravimetric analyser produced in Japan. The test materials were placed in a platinum crucible, whose temperature was monitored by a thermocouple. The combustible mass of the coal sample was constantly maintained at (2 ± 0.1) mg. At an airflow of (50 ± 2) ml/min, the furnace temperature was increased from room temperature to 1000 °C at 40 °C/min. The weight of coal samples was monitored continuously by a thermobalance as a function of temperature, as shown in Fig. 1.

The ignition temperature is defined as follows: Firstly, a vertical line is made upwards through the differential thermogravimetric (DTG) peak point to meet the TG oblique line. Secondly, a tangent line to the TG oblique line is made to meet the extended thermogravimetry (TG) initial level line. Finally, the temperature at the intersection point is defined as the ignition temperature [18]. The TG curves are used to calculate the activation energy of the 16 typical Chinese coals and 48 of their blends based on the Doyle–Ozawa method. Activation energy is calculated using the following equation:

$$\ln[-\ln(1-\alpha)] = \ln\frac{AE}{\beta R} - 2.315 - 0.4567\frac{E}{RT} \quad (1)$$

where α is the sample conversion ratio, A is the frequency factor, E is the activation energy, β is the heating rate and R is the gas constant. A linear regression is fit to the data points on the graph of '$\ln[-\ln(1-\alpha)]$' versus '$1/T$' based on the TG curves at different sample conversion ratios. The line slope is used to calculate the activation energy of E.

2.2. Pearson correlation analysis

The coal ignition is the premise based on which the whole coal combustion process can be performed. Debate always exists on whether the ignition mechanism of pulverised coal particles is homogeneous, heterogeneous or heterohomogeneous. The homogeneous theory considers that the volatile matter of coal gathers at the surface of coal particles after pyrolysis and then forms the flame surrounding coal particles by co-combustion with oxygen in air. Only when the concentration of volatile matter is decreased can oxygen reach the surface of the particles and then form coke ignition. The heterogeneous theory considers that oxygen firstly diffuses into the surface of coke, after which it directly reacts with particles to catch fire. The temperature of the particles then increases rapidly, the pyrolysis of volatile matter intensifies, until finally combustion becomes acute. The ignition process of coal in the applications of practical engineering is complex. The calorific value of coal, moisture and external combustion conditions all have a significant effect on the continuous combustion of coal. Therefore, this study uses Pearson correlation analysis to quantitatively investigate the influence of coal properties on ignition temperature and activation energy. Moreover, the ignition temperature and activation energy of power coal blends are predicted using the BP neural network models and traditional polynomial regression according to the results of Pearson correlation analysis.

2.3. Topological structure of neural network models

According to the results of Pearson correlation analysis, the three-layer BP neural network models with five input factors—moisture, volatile matter, fixed carbon, calorific value and oxygen—were developed to predict ignition temperature and activation energy based on coal properties. The BP neural network model with five input factors for ignition temperature, which was similar to the model for activation energy, is shown in Fig. 2. Furthermore, the BP neural network models with other combinations of factors can be obtained by increasing or decreasing the number of input nodes.

In the three-layer BP neural network models developed in this study, the neurons between the upper and the lower layers were fully connected, whereas the neurons in the same layers were not connected. The output vectors of this layer were obtained from the calculation results of the transfer function for the input data in this layer. Afterwards, the output vectors reached the lower layer neurons via the connection between the upper and the lower layers and were then integrated with the threshold of the lower layer neurons to determine the input vector for the lower layer. Assuming that the number of nodes of the input (layer 1), hidden (layer 2) and output layers (layer 3) were n_1, n_2 and n_3, respectively, then the input IN^l and output OUT^l of the l layer neurons were both n_l dimensional vectors. in_i^l and out_i^l were the input and output of u_i^l, which were i neurons of the l layer. w_{ij}^l was the connection weights between u_i^l and u_j^{l+1}. $bias_i^j$ was the threshold for i neurons of the l layer. in_j^{l+1} for the hidden layer and output layer were calculated as follows:

$$in_j^{l+1} = \sum_{i=1}^{n_l} w_{ij} \times out_i^l + bias_j^{l+1} \quad (2)$$

The neurons of the input and output layers of the two neural network models used the linear transfer function; therefore, $out_i^l = in_i^l$. However, the neurons of the hidden layer used the hyperbolic tangent s-type transfer function, with the output of the hidden layer given as follows:

$$out_i^l = \frac{1-e^{-2in_i^l}}{1+e^{-2in_i^l}} \quad (3)$$

The Levenberg–Marquardt algorithm [19], which is particularly suitable in obtaining the minimum sum of error squares and has a fast operating speed, was used for the BP neural network models in this study. It is a hybrid algorithm, which combines the Newton