Applied Thermal Engineering 131 (2018) 221–229

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Research Paper

A new numerical method to predict the growth temperature of spontaneous combustion of 1/3 coking coal

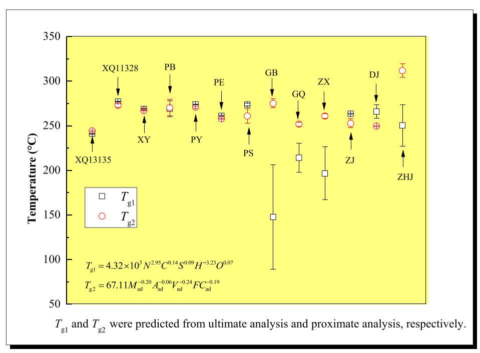
Yang Xiao [a,b], Hui-Fei Lü [a,b], An-Chi Huang [c], Jun Deng [a,b,*], Chi-Min Shu [c,*]

[a] School of Safety Science and Engineering, Xi'an University of Science and Technology (XUST), Xi'an 710054, PR China
[b] Shaanxi Key Laboratory of Prevention and Control of Coal Fire, XUST, Xi'an 710054, PR China
[c] Graduate School of Engineering Science and Technology, National Yunlin University of Science and Technology, Yunlin 64002, Taiwan, ROC

HIGHLIGHTS

- Growth temperature during spontaneous coal combustion is defined and evaluated.
- Apparent activation energy is calculated by the improved KAS method.
- The model predicts growth temperature based on ultimate and proximate analyses.
- The proximate analysis model exhibits little prediction error.

GRAPHICAL ABSTRACT



T_{g1} and T_{g2} were predicted from ultimate analysis and proximate analysis, respectively.

ARTICLE INFO

Article history:
Received 21 July 2017
Revised 11 November 2017
Accepted 2 December 2017
Available online 6 December 2017

Keywords:
Growthtemperature
Apparent activation energy
Kissinger–Akahira–Sunose method
Grey correlation analysis
Quasi-Newton method

ABSTRACT

Hazards caused by spontaneous coal combustion are of deep concern. To explore the process of spontaneous coal combustion, we focused on the key aspects of growth temperature (T_g) and the apparent activation energy (E_a), where T_g is associated with the E_a. We used four different heating rates to perform thermogravimetric (TG) experiments to calculate E_a values through an improved Kissinger–Akahira–Sunose method. The findings revealed a sudden change point in E_a values (that is, T_g), and comparisons between experimental data and calculated results demonstrated favorable agreement. The grey correlation analysis method was used to analyze the relationship between the samples' T_g and intrinsic properties. A quasi-Newton method and general global optimization model were adopted to derive a predictive relationship for spontaneous coal combustion. The results are beneficial and crucial for elucidating the mechanism of spontaneous coal combustion, which could facilitate a thorough understanding of this process and help provide proactive loss prevention measures.

1. Introduction

Spontaneous coal combustion is an extremely complex physical and chemical reaction between coal and oxygen, resulting in the gradual accumulation of heat that eventually produces favorable conditions for combustion. It occurs frequently during mining and transportation. In underground coal mines, coal dust combustion and explosion may cause gas explosions that are more severe

* Corresponding authors at: School of Safety Science and Engineering, Xi'an University of Science and Technology (XUST), Xi'an 710054, PR China (J. Deng); Graduate School of Engineering Science and Technology, National Yunlin University of Science and Technology (YunTech), Yunlin 64002, Taiwan, ROC (C.-M. Shu).

E-mail addresses: dengj518@xust.edu.cn (J. Deng), shucm@yuntech.edu.tw (C.-M. Shu).

https://doi.org/10.1016/j.applthermaleng.2017.12.007
1359-4311/© 2017 Published by Elsevier Ltd.

Nomenclature

A	pre-exponential factor (min^{-1})
a	fitting parameters
b	fitting parameters
B	constant = 1.92
D	constant = 1.0008
E_a	apparent activation energy ($J\ mol^{-1}$)
$f(\alpha)$	differential mechanism function
$G(\alpha)$	integral mechanism function
m	number of performance characteristics
n	number of coal samples
$P(u)$	approximation of the integral temperature (K)
R	universal gas constant (8.314 $J\ mol^{-1}\ K^{-1}$)
r^2	correlation degree
T_g	growth temperature (°C)
T	absolute temperature (K)
T_1	pyrolysis temperature (°C)
T_2	ignition temperature (°C)
T_{g1}	ultimate analysis-predicted T_g value (°C)
T_{g2}	proximate analysis-predicted T_g value (°C)
t	time (min)
X	normalized experimental results
$X_0(j)$	ideal normalized results for the jth performance characteristics
y_{ij}	jth experimental results in the ith test

Greek letters

α	conversion
β	heating rate (°C min^{-1})
γ	grey correlation degree
ζ	grey correlation coefficient
Δ	difference value
ε	distinguishing coefficient

than initial one [1]. Not only do these accidents have an immense deleterious effect on the natural environment, but also result in human casualties, property loss, and social problems [2–5]. In China alone, 100–200 million tons of coal undergoes spontaneous combustion annually, accounting for 2–3% of global CO_2 emissions [6,7]. Numerous efforts have focused on understanding the mechanism underlying spontaneous coal combustion [8–11].

The combustion process is generally divided into three stages: Incubation, self-heating, and burning [12]. During the incubation period, heat accumulation slowly increases the temperature, followed by a rapid increase in temperature during the self-heating period. After the coal's ignition point is reached, burning ensues. The growth temperature (T_g) at which the process progresses to the self-heating period (i.e., the crossing-point temperature) is vital for predicting spontaneous coal combustion and improving safety in coal mines [13]. However, a definitive method for determining this threshold temperature is yet to be established.

Current research has mainly determined the susceptibility of coal to spontaneous combustion based on macroscopic phenomena, such as heating or oxygen consumption rates or indicator gas changes. Zhu et al. [14] explored changes in characteristic temperature and oxygen consumption rates during the spontaneous combustion of coal across various temperatures, and observed that the oxygen consumption rate changed markedly at approximately 150 °C. Wang et al. [15], via experimental tests of coal thermally decomposed, revealed the temperature thresholds for these oxygenated species were 50 and 70 °C. Wang et al. [16] put forward an accelerated oxidation stage (> 140 °C) at low temperature coal oxidation. Nalbandian [17] evaluated the self-heating propensity of coal, and demonstrated that a swift interaction with oxygen occurs at temperatures up to 180 °C followed by thermal decomposition at 180–250 °C. Sloss [18] conducted an overview of spontaneous coal combustion and determined that after the temperature increases beyond approximately 150 C, combustion accelerates promptly.

Although these findings are based on the macro-phenomenon of temperature change, the associated changes are clearly related to the intrinsic characteristics of coal and the underlying mechanisms that drive the spontaneous combustion reaction. During the heating process, bonds of molecules are broken and macromolecules are decomposed, yielding smaller and more reactive molecules and some charged radicals. Alterations in the coal internal structure affect its reactivity, which can be approximated by its apparent activation energy (E_a). In theory, E_a is a key parameter for identifying the T_g of spontaneous coal combustion and is used to implement safety measures for avoiding such combustion. In recent years, more characteristics of ignition temperature have been studied, and generally ignition temperature of coal is solved by kinetics [19–22]. Wang et al. [23] studied the kinetics and reactivity at the ignition temperature, concluding that the key quality groups affect the ignition temperature of coal. However, there is little attention to the temperature (T_g) before the ignition. Predicting T_g can in advance control the coal spontaneous combustion to eliminate the resource loss.

We examined coal samples from the Huainan mining area in Anhui Province, Eastern PR China, which is one of the country's 14 large-scale coal bases [24]. The oxidative decomposition of coal was analyzed to determine the T_g of its spontaneous combustion using E_a calculations at different conversion degrees, and to analyze the relationship between the samples' T_g and intrinsic properties. The results provided valuable information on spontaneous coal combustion and fire control measures as well as facilitating proactive safety management in coal mining and improving economic efficiency.

2. Experimental and methods

2.1. Coal samples

Coal samples were obtained from the Huainan mining area in Anhui Province, Eastern PR China (Fig. 1). This area has rich and high-quality coal reserves that account for 74% of the total reserves in Anhui Province. Although the coal type varies, it is generally prone to spontaneous combustion. Seven samples were collected: Xie Qiao 13,135 (XQ13135), Xie Qiao 11,328 (XQ11328), Xie Yi (XY), Pan Bei (PB), Pan Yi (PY), Pan Er (PE), and Pan San (PS). The samples were ground to a particle size of 0.074–0.150 mm. Proximate analysis is an experimental method for substantiating moisture, ash, and volatile content; it was performed here under air-dried conditions. Ultimate analysis was also used to determine the ultimate composition of coal, and air-drying was again used as the standard [25]. The results of ultimate and proximate analyses are presented in Table 1. Notably, the samples had low ash and sulfur content, with high volatile matter content, which is a 1/3 coking coal. Six delayed test coal samples were used to verify the accuracy of the prediction equation derived from the seven coal samples: Gu Bei (GB), Gu Qiao (GQ), Xin Zhuangzi (XZ), Zhu Ji