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The application of kinetics based simulation method in thermal risk prediction of coal

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ABSTRACT

Coal spontaneous combustion is one of the major natural disasters faced in coal mines. The accurate prediction of the thermal risk of coal is of great importance. However, there isn't a widely accepted approach to get the oxidation process of coal that under adiabatic condition or in a specific environment under mine at present. To demonstrate whether the advanced kinetics simulation method could be employed to obtain the accurate oxidation process of coal for determining the coal's thermal risk in the mine design phase and mining phase, DSC experiments were conducted by C80 micro-calorimeter to get the heat behavior of coal, based on which the kinetic parameters can be solved and the oxidation process of coal can be predicted.

The results showed that the kinetics based simulation method was successfully used to predict the adiabatic temperature rise process of coal for risk prediction. The deviation between the predicted curve and tested curve that obtained by adiabatic test is small enough to be accepted. Kinetics based simulation method is a promising candidate, instead of adiabatic test, to assess the propensity of coal to spontaneous combustion, which can play an important role in the design phase of the mine and mining area. Moreover, through establishing the heat balance equation of residual coal and with the aid of kinetics based simulation method, the oxidation process of coal that in the suffocation zone of the gob was also accurately predicted. According to the index t_{70} (the time required for coal to reach 70 °C) and v_{min} (the lower limit of the advancing speed of the working face) obtained from the predicted curve, the thermal risk of coal was predicted to guide the further adjustment of the advancing speed of the working face, the amount of the injected mud and the determination that whether to add other fire prevention measures. Kinetics based simulation method, be of great practical importance in risk prediction of coal that in the gob, can be also used as a convenient tool to guide the safe production in the actual mining process.

1. Introduction

As an energetic substance and important energy resource, coal can react with oxygen at ambient temperature and produce large amounts of heat, which will lead to a temperature rise and thermal runaway described as spontaneous combustion if the heat can not be timely dissipated. The spontaneous combustion of coal resulting into mine fire is of interest in the world's major coal-producing countries, as it can cause huge casualties, economic losses and serious environmental pollution (Li, 1998). Therefore, it's essential to predict the thermal risk of coal and prevent it from catching fire. In practice, the risk predict of coal to spontaneous combustion should be performed in two stages, mine design phase and the mining phase.

In the mine design phase, the choice of roadway layout, the determination of the mine ventilation system type and daily technical measures to prevent and extinguish the fire due to spontaneous combustion, etc. all should be performed according to the thermal risk degree of coal. Several methods originated in different countries of the world, such as adiabatic oxidation method (Beamish, Barakat, & George, 2000, 2001; Ren, Edwards, & Clarke, 1999; Vance, Chen, & Scott, 1996), Crossing Point Temperature (CPT) method (Bagchi, 1965; Mahidin, Usui, Ishikawa, & Hamdani, 2002; Nandy, Banerjee, & Chakravorty, 1972; Sujanti, Zhang, &

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Chen, 1999), activation energy method (Liu, Wang, & Sun, 1999; Semsogut & Cinar, 2000), absorption of flowing oxygen method (Qi, Qian, & Luo, 1993) etc., can be available to assess the propensity of coal to spontaneous combustion, which is one of the intrinsic properties of coal and means the degree of difficulty for spontaneous combustion. However, none of them has been widely recognized as each method has its shortcomings that difficult to overcome. The adiabatic oxidation method, by contrast, is the most scientific and widely recognized method, as it allows the coal to raise its temperature only relying on absorbing all the heat generated by the oxidation itself, simulating the in-situ oxidation characteristics of coal. The reasons why the adiabatic oxidation method has not been widely applied yet are the long test time due to the very little heat production at initial oxidation stage and the difficulty to achieve an ideal adiabatic condition and standard test condition. Now, a new method, instead of the adiabatic oxidation test, is urgent needed to get the adiabatic oxygen process of coal.

In the mining phase, the risk degree of coal to spontaneous combustion is an important reference index for the technical staff to determine the lower limit of the advance speed of working face or consider what auxiliary fire prevention measures should be taken to ensure the safe production. Nevertheless, in a specific environment under mines, the oxidation temperature rise process of coal is associated with numerous factors of the environment which the coal in, such as the ambient temperature, air flow rate, air humidity, etc. Because of its complexity, we still haven't proposed a reliable way to get the oxygen process of coal which in a special environment with such influential factors until now. In China, the technical staff can only rely on experience and statistics of the actual situation to develop the fire prevention measures, which will produce large errors and greatly weakened the safety factor of production activities.

However, the advanced kinetics based simulation method (Roduit et al., 2005; Roduit, Dermaut, et al., 2008; Roduit, Folly, et al., 2008), enjoying grow favor in the field of the thermal stability analysis, is expected to become an important means to solve these problems at present, as it can accurately predict the reaction rate and reaction progress of the substances under various temperature mode, such as isothermal, non-isothermal, stepwise, etc. The kinetic based simulation method was successfully applied to predict the reaction progress of the coupling reaction of aniline with cyanamide at different constant temperatures, finding that the first reaction step of the decomposition reaction is a non-self-accelerating effect and the second is a strong self-acceleration type (Roduit, Dermaut, et al., 2008). The reaction rates of a sulfide-mineral sample under different temperature models was predicted using advanced kinetics simulation method, which supports an autocatalytic behavior of the sample during oxidation reaction (Iliyas, Hawboldt, & Khan, 2010). The adiabatic behavior (time to maximum rate under adiabatic conditions and self-accelerating decomposition temperature) of Cyclohexanone peroxide was simulated to analyse its thermal hazard according to the kinetics based simulation method (Zang, Qian, Huang, & Shu, 2013). The reaction rate and reaction progress of MWCNTs (multi-walled carbon nanotubes) were accurately simulated based on the kinetics based simulation method (Weng et al, 2013). The T_{D24} (the environment temperature when the time to maximum rate is 24 h) of the expired military propellant was derived by means of kinetics simulation to evaluation the thermal and pressure hazards (Yu, Chen, & Peng, 2012). But, unfortunately, there is scarcely any report about applying the advanced kinetics simulation method into the thermal risk predicted of coal up to now. In the study, the main attention was paid to demonstrate whether the advanced kinetics simulation method could be employed to obtain the accurate oxidation process of coal for determining the risk of coal to spontaneous combustion in the mine design phase and mining phase.

2. Materials and methods

2.1. Sample characteristics

Two Chinese coals of different ranks, one lignite from YI Ma mine and one anthracite from KA Bu-liang mine, were collected for this study. To facilitate expression, the two coals are expressed as YM and KBL respectively in later statements. After being tightly wrapped in the sampling sites, the fresh coal samples were sent to the laboratory as quickly as possible and stored in the freezer. Before the experiment, the inner core of the coal lump was crushed in a glovebox, which can provide an oxygen-free environment to prevent the coal from pre-oxidation in the process. At last the coal with particle size ranging from 0.074 to 0.096 mm was chosen for testing. There proximate analyses are given in Table 1.

2.2. Numerical tool

According to the advanced kinetics simulation method, the kinetic parameters (activation energy and pre-exponential factor) should be first determined and then the oxidation temperature rise process of coal that in adiabatic condition or under temperature programming with any heating rates could be predicted. As could be available in many papers, the theory of advanced kinetics simulation method (AKTS; Roduit, Dermaut, et al., 2008) isn't been elaborated here. The AKTS, one kind of advanced thermokinetic software packages, was chosen to data processing according to the advanced kinetics simulation method (AKTS). Simultaneously, during the data processing, the Friedman isoconversional method (Friedman, 1964; Iliyas et al., 2010) was used to determine the kinetic parameters.

2.3. Test equipment and procedure

According to the advanced kinetics simulation method, the thermal behavior of coal under at least three different heating rates for every coal sample is needed to get the accurate value of kinetic parameters.

To accurately test the heat generated during the low-temperature oxidation process of coal, DSC experiments were conducted by C80 micro-calorimeter (Fig. 1) that produced by Setaram, France. The gas circulating reaction pool was chosen to allow air to pass through, so that the oxygen could be available for coal sample throughout the test.

To ensure the complete elimination of external moisture, 1000 mg of the crushed coal was dried in a vacuum oven under nitrogen at 40 °C for 24 h. After drying is completed, the coal was transferred to the reaction cell of the micro-calorimeter and the switch of the gas cylinder was turned on to enable oxygen passing through the reaction cell and reference cell with a constant flow rate of 80 ml/min. Once this was achieved, it need to open the switch of the computer and accessory device and the data acquisition software "Date Acquisition" with entering the experiment

Table 1
Proximate analyses of the coal samples.

Coal samples	Proximate analysis, wt% (air-dry basis)				$Q_{net,ad}$, MJ/kg
	Moisture	Ash	VM	FC	
YM	12.15	6.82	33.67	47.36	29.00
KBL	1.12	6.86	11.76	80.26	32.93