



Study on the relationship between microscopic functional group and coal mass changes during low-temperature oxidation of coal



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ABSTRACT

It is important to have an in-depth understanding of the relationship between coal functional group and mass changes during low-temperature oxidation. This knowledge is necessary not only for detecting and preventing the spontaneous combustion of coal but also for reducing emissions of hazardous gases. Microscopic functional group changes of different classes of coal oxidation at temperatures below 230 °C were obtained from real-time measurements of the coal matrix via Fourier transform infrared (FTIR) spectroscopy equipped with in-situ reactor cells. Mass changes solely due to oxidation between coal and oxygen were obtained by subtracting the TG-N₂ curve from the TG-air curve. Experimental results show that the amount of carbonyl compounds exhibits a linear relationship with the coal mass. Based on two typical reactions of hydrogen elimination and oxygen addition involved in the oxidation process, the relationship between the changes in coal mass and in microscopic functional groups was explored. Experimental results show that with the increase in oxidation temperature, increasing the coal mass via oxygen-containing functional groups becomes more difficult, i.e., more oxidation events are required to increase the same unit of coal mass. The computational formula to find the amount of reactive hydrogen atoms in the coal matrix involved in low temperature oxidation was derived, and the amount of transferable active hydrogen in the three coals was calculated by this formula. This method for finding the amount of transferable active hydrogen determined by TG-FTIR may be promising for assessing the likelihood of coal spontaneous combustion.

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1. Introduction

Coal oxidation at low temperatures (i.e., <230 °C) is the major heat source responsible for the self-heating and spontaneous combustion of coal (Wang et al., 2003a; Yuan and Smith, 2009). Spontaneous combustion of coal caused by low-temperature oxidation is a key safety issue in mining, storage, and transportation of coal and has restricted and continues to severely restrict the development of the coal industry (Beamish et al., 2001; Beamish and Blazak, 2005; Carras and Young, 1994; Singh et al., 2007; Song and Kuenzer, 2014; Xue et al., 2010). In addition to safety problems, the oxidation of coal also significantly affects the molecular structure, elemental composition, and other properties of coal, thereby leading to the deterioration of its technological properties, such as carbonization and liquefaction (Cimadevilla et al., 2005; Mastalerz et al., 2009; Smędowski and Piechaczek, 2016; Zhang

et al., 2013). Both low-temperature oxidation and spontaneous combustion cause significant environmental problems, such as the emission of greenhouse gas (Carras et al., 2009; Gürdal et al., 2015; Pone et al., 2007) and hazardous trace elements (Zhao et al., 2008).

Low-temperature oxidation of coal is a complicated process that involves a series of reaction steps, including the attack of molecular oxygen on aliphatic hydrocarbon species, formation of intermediate complexes, and decomposition of unstable oxygenated intermediates to gaseous products and other species (Carras and Young, 1994; Wang et al., 2003a). As indicated by research results obtained previously, a series of migration and transformation reactions of active functional groups are involved in low-temperature oxidation of coal. These active functional groups include aliphatic C—H active components and contain C=O active components, such as quinones, ketones, aldehydes, acids, lipids, and acid anhydrides. Previous studies on the changes of functional groups during coal oxidation at low temperature typically use ex situ FTIR. This testing process requires the preparation of a series of coal samples oxidized under different temperatures and cannot test for changes in active groups online during coal reactions. Meanwhile, using ex situ FTIR, the coal sample must be blended with KBr powder before testing, which influences the coal structure and usually results

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in inexact data. In-situ FTIR technology can address these disadvantages and test the actual real-time changes of functional groups in coal oxidation. The aliphatic C—H active components are oxidized to form oxygenated compounds during low temperature oxidation of coal, leading to changes in coal composition and thus coal mass. It can be speculated that there should be a certain relationship between the evolution of aliphatic hydrocarbons and changes in coal mass.

Low-temperature oxidation of coal comprises a series of physical and chemical processes and many parallel reactions, such as the evaporation of water, oxidation reaction between oxygen and coal, and thermal decomposition of inherent oxygen-containing functional groups. The evaporation of water and thermal decomposition of inherent oxygen-containing functional groups lead to a decrease in coal mass, while chemical sorption of oxygen and formation of intermediate complexes due to coal oxidation bring about an increase in coal mass. The co-existence of these processes makes the study of the intrinsic reaction between oxygen and coal difficult, but the oxidation reaction between oxygen and coal is the main source for the self-heating and spontaneous combustion of coal (Li et al., 2016; Wang et al., 2016; Zhang et al., 2016c). The co-existence of coal and oxygen also gives rise to controversy between different studies. Some studies using TGA have shown an increase of the sample mass when coals were exposed to a heating ramp, suggesting a link between the mass change and oxidation characteristics of coal associated with the spontaneous combustion phenomenon (Avila et al., 2014a; Slovák and Taraba, 2010). Other similar studies did not identify these characteristics. Many investigators (Chen et al., 2015; Qi et al., 2016) have taken these processes only as a whole to study the mass change characteristics, while few studies (Zhang et al., 2016a) have been carried out to explore the intrinsic reactivity of low-temperature oxidation of coal. Low-temperature oxidation of coal in an air atmosphere involves the evaporation of water, oxidation reaction, and thermal decomposition of inner oxygen-containing functional groups. The heating of coal in a nitrogen atmosphere involves only the evaporation of water and thermal decomposition of inherent oxygen-containing functional groups. By subtracting the TG-N₂ curve from the TG-air curve, the common processes occurring in both atmospheres, i.e., water evaporation and thermal decomposition, are eliminated and the intrinsic oxidation reaction between oxygen and coal can be obtained. This research technique can be denoted as the TG profile subtraction method (Zhang et al., 2016a).

In this study, the in-situ FTIR method and TG profile subtraction method were introduced. The changes in active groups were obtained from real-time measurements of the coal matrix. TG profiles were obtained from real-time measurements of the change in coal mass. To investigate the effect of coal rank on changes in aliphatic hydrocarbon occurrence, three types of coal, namely, lignite, sub-bituminous coal, and bituminous coal, were used in this study. Therefore, the relationship between the changes in methyl and methylene groups and changes in coal mass was explored on the basis of the experimental findings. Furthermore, the amount of active hydrogen was obtained by TG-FTIR with the assumption that chemical reactions take place during low-temperature oxidation of coal, and a promising method to assess the proneness of coal spontaneous combustion was proposed.

2. Experimental

2.1. Coal samples

Three types of coal samples were investigated in this study. The geographic location of the mining area of the three coals is shown in Fig. 1. The Shendong Coalfield (denoted as SD), located east of the Mu Us Desert, is one of the most representative coalfields in northwest China. The Shendong Coalfield started production in 1986. Its coal seams are of the Jurassic period and are typically covered by a thin layer of bedrock. Large-scale longwall mining of the shallow coal seams used in this coalfield can disturb or even damage the overlying aquifers (Zhang et al., 2011) and thus can lead to the serious problem of leaking air in goaf. SD coal is subbituminous coal with a lower ignition temperature and higher reactivity. SD coal is highly susceptible to self-ignition due to its low rank with a low carbon content and high oxygen-containing function group content (Song et al., 2015). >350 coal fire areas were surveyed from 1998 to 2016. The Zaozhuang Coalfield (denoted as ZZ), located in the south of Shandong Province, is one of the largest production bases in the east of China. The Zaozhuang Coalfield started production in 1998. The coal seams are of the Permo-carboniferous period. The seam belongs to an extremely thick coal seam with an average thickness of 12.95 m. Fully mechanized slicing mining is used in this area. This mining method leads to a serious leaking air problem that can cause serious self-igniting phenomena in this coal mine. ZZ coal is gas coal with high volatile matter and high pyrite content. The shortest

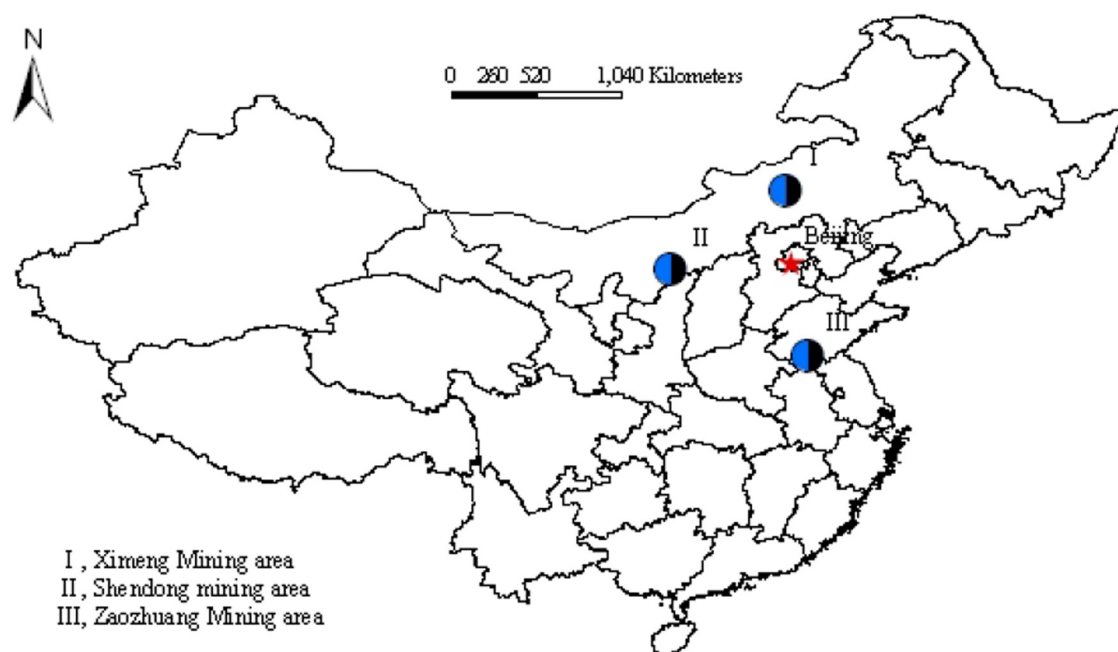


Fig. 1. Geographic locations of the mining areas of the three coal samples.

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