



An experimental approach to selecting chemical inhibitors to retard the spontaneous combustion of coal



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HIGHLIGHTS

- Distribution of functional groups at coal surface has been analyzed.
- Change concentrations of functional groups at coal surface have been analyzed.
- Efficient experimental approach to selecting chemical inhibitors has been proposed.

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ABSTRACT

Because of the complex structure of coal, selecting an efficient chemical inhibitor to retard or prevent its spontaneous combustion remains a challenging task. In the present work, the distributions and concentrations of functional groups on coal surfaces were analyzed using *in situ* FTIR. The active functional groups and their oxidation processes were elucidated so as to develop an efficient approach to selecting effective chemical inhibitors. The validity of the experimental approach was demonstrated by measuring various performance metrics for samples with and without a chemical inhibitor, including crossing point temperature (CPT), oxygen consumption, carbon monoxide (CO) emission rates and changes in active functional groups. The results indicate that the chemical inhibitor chosen using the proposed approach effectively slows the oxidation of coal, thereby demonstrating the validity of the selection method.

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1. Introduction

Coal is a chemically reactive organic material; when exposed to air, it can combine with oxygen and generate heat. This reaction can lead to spontaneous combustion with the release of toxic gases [1,2], which may create both health and environmental hazards. Retarding the spontaneous combustion of coal is therefore highly desirable.

Chemical inhibitors are widely used to prevent or extinguish coal mine fires and have been applied effectively for these purposes. At present, a wide range of inorganic salts such as NaCl, MgCl₂ and CaCl₂ have been considered [3–6] for use in this role. These inhibitors, however, retard coal oxidation merely by creating a barrier to oxygen and by the adsorption of water. As a result, these compounds typically exhibit low efficiency and short active lifetimes. Recently, other chemical substrates that have been used to retard coal oxidation have been found to either decrease the rate

of formation of reactive species or to inhibit the free radical reactions associated with combustion. For example, Zhan et al. [7] reported that Na₃PO₄ plays a role in modifying the decomposition pathways of hydroxyl radicals, thereby improving the thermal stability of the coal. Wang et al. [8] studied the inhibiting effect of ionic liquids on coal oxidation; the liquids solvated various functional groups and attenuated the exothermic oxidation of coal. The results suggested that 1-butyl-3-methyl-imidazolium trifluoromethanesulfonate [Bmim][OTf] and 1-butyl-3-methyl-imidazolium acetate [Bmim][AC] are more effective than other ionic liquids in decreasing the oxidation rates of bituminous coals. The distribution of functional groups varies from one coal to the next [9,10], however, and studies of chemical inhibitors reported to date have neglected these variations in functional groups as well as the structural diversity of coal. Some of the chemical inhibitors also exhibit disadvantages, such as an unstable inhibitory effect when combined with certain types of coal. As a result, the selection of the optimal inhibitor for any given type of coal is still a challenging task and accordingly there is a need to develop an efficient approach to choosing chemical inhibitors for the purpose of retarding coal oxidation.

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Coals contain a wide variety of functional groups, including alkyl, aryl, carbonyl, carboxyl and hydroxyl moieties. Some of these groups are more active in the coal oxidation process than others and can trigger a series of exothermic reactions. The types and quantities of functional groups are therefore primary factors in determining the likelihood of spontaneous combustion in a particular coal [11–13]. Under actual combustion conditions, coal oxidation is subject to kinetic control and low-temperature oxidation kinetics studies of coal oxidation have recently been performed [14–16]. Certain active sites, the so-called *active groups*, are primarily responsible for the low-temperature oxidation of coal [11,17] because these groups react exothermically with oxygen, thereby supplying energy to the other functional groups that require higher levels of activation energy before undergoing oxidation reactions. According to chemical reaction theory, once the oxidation of the active groups is interrupted, no further energy will be generated and the subsequent oxidation of other groups will slow or halt entirely. Accordingly, determining the active sites and analyzing the processes by which they undergo oxidation is particularly important when selecting chemical inhibitors to retard coal oxidation. The analysis of the distribution and evolution of functional groups, the determination of the active functional groups and the prospects for removing active groups or slowing down their oxidation are thus important factors when choosing chemical inhibitors.

This paper describes an efficient approach to the selection of chemical inhibitors to retard coal oxidation. Herein, a process is described in which *in situ* FTIR is used to monitor the distribution and changing concentrations of functional groups, so as to obtain information concerning the active functional groups at the coal surface. The resulting data, together with existing literature, were subsequently used to analyze the oxidation processes of the active functional groups. On this basis, specific chemical substances that can either remove the active sites or prevent the oxidation process of active groups may be selected so as to allow the effective inhibition of coal oxidation. The optimal concentration of a selected additive was determined and the oxidation behaviors of coals blending with the additive based on the details of active groups were examined to verify the inhibition effect. In summary, an approach to selecting chemical inhibitors based on the results of *in situ* FTIR is proposed.

2. Materials and methods

2.1. Experimental materials and coal samples

Coal samples were collected from the Liangbaosi (LBS) Colliery in Shandong Province, the Pansan (PS) Colliery in Anhui Province and the Bulianta (BLT) Colliery in Neimeng Province. Table 1 summarizes basic characteristics of the coals. Lumps from the various coal samples were milled and sieved and fragments from 0.25 to 0.80 mm in size were used for the experimental investigations. Poly(ethylene glycol) (PEG) 200 (99% purity) was selected as the chemical inhibitor based on an assessment of the most suitable candidates.

Table 1
Properties of the coal samples.

Sample	Proximate analysis (air dried basis) (%)			
	M_{ad}	A_{ad}	V_{ad}	FC_{ad}
LBS coal	3.24	9.40	33.24	54.14
BLT coal	11.86	3.28	28.56	56.30
PS coal	1.62	24.86	27.45	46.18

2.2. Experimental procedures

The coal samples were dried in a vacuum oven overnight at 40 °C. PEG 200 was then blended with the raw coal particles in a beaker with mechanical stirring to produce coal samples containing 0, 1, 2, 5 or 10 wt.% of the PEG additive. All samples were stored in a desiccator prior to measurements.

The distributions and changing concentrations of the coal surface functional groups were determined *in situ* using a Nicolet 6700 Fourier transform infrared spectrometer. A KBr powder background was collected prior to sample analysis as a baseline reference. During analysis, each ground coal sample was placed into the reaction chamber and the dome installed, following which dry air flowed into the reaction chamber from its base, exiting from the top. A temperature controller was connected to the reaction chamber and the chamber was heated to 220 °C at a rate of 1 °C/min. The region from 650 to 4000 cm^{-1} was scanned with 4 cm^{-1} resolution, adding 64 scans per spectrum and applying a Kubelka–Munk conversion to the data. For each sample, a series of spectra were collected at 30 s intervals.

The cross point temperature (CPT), oxygen consumption during low temperature oxidation (40–70 °C) and the combustion gases were all measured using an experiment apparatus of our own design consisting of a spontaneous combustion simulation system, a gas chromatograph (to collect and analyze gas emissions) and a data acquisition system to record the temperature in real time. Each 50 g coal sample was placed in the reactor so as to ensure that there was sufficient airflow throughout the sample. Dry air with an oxygen concentration of 20.96% was allowed to pass through the sample for half an hour at a predetermined initial temperature to equilibrate the test system, following which the program-controlled temperature enclosure was set to run at a programmed temperature rise rate of 0.8 °C/min. During this process, dry air flowed into the reactor at a rate of 8 mL/min for 160 min and the temperature was continuously recorded while gas samples at the reactor outlet were analyzed at every 10 °C increase.

3. Results and discussion

3.1. Selecting a chemical inhibitor

The chemical reactions that take place between coal and oxygen are affected by the rank of the coal and it is therefore necessary to determine the distribution and changing concentration of functional groups on the coal surface. For this reason, coal samples were characterized by *in situ* FTIR after being dried in a vacuum oven at 40 °C for 24 h and before any treatment. The spectra of the raw (untreated) coal samples are shown in Fig. 1.

The spectra were resolved using the Fit Peaks program to identify individual peaks in cases in which peaks were superimposed. The absorption wavenumbers and peak areas of the main functional groups in the coal samples are summarized in Table 2. These results suggest that the surfaces of these coal samples contain significant quantities of alkyl, aryl and hydroxyl groups.

It is well-known that aryl groups are much more stable than are other moieties during the oxidation process and so, during this work, only changes in the concentrations of alkyl and hydroxyl groups were monitored by *in situ* FTIR. As noted, the spectra of coal samples during oxidation were collected by *in situ* FTIR; the 3D (Kubelka Munk-time-wavenumber) data obtained for raw LBS coal are shown in Fig. 2. The 3D data were analyzed to determine the peak intensity at specific wavenumbers as well as changes in intensity at several of these wavenumbers with variations in time or temperature. The wavenumbers that were monitored during these trials were: 2960 and 2875 cm^{-1} (corresponding to the

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