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Research Progress on Combustion and Explosion Risks of Syngas Produced by Pyrolysis of High-Sulfur Coal

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ABSTRACT
In The context of global low-carbon energy transformation, the clean and efficient utilisation of high-sulfur coal is a key issue, and pyrolysis technology can convert it into syngas to achieve added value, but the flammable and explosive characteristics of syngas and the safety hazards of sulphur-containing impurities restrict the industrialisation of this technology. This paper systematically sorts out the gas production characteristics and influencing factors of high-sulfur coal pyrolysis, the risk mechanism and prediction and assessment methods of syngas explosion, and reviews the three mainstream methods of traditional empirical method, experimental test method and numerical simulation method. At the same time, it is pointed out that the current research faces challenges such as the interference of raw coal quality fluctuations, the difference in scenario simulation accuracy, and the insufficient reliability of data and models under sulphur-containing components.

KEYWORDS
High-sulfur coal; Coal pyrolysis; Synthesis gas; Combustion and explosion risk

1 Introduction

At the critical stage of the global energy structure transition to low-carbon, the clean and efficient conversion and utilisation of coal resources is still a key issue [1]. As an important part of coal resources, high-sulfur coal has a low utilisation rate for a long time, and the core reason is its high sulfur content [2]. When burned directly, the sulphur fraction in coal will be converted into acid pollutants, which can easily cause environmental pollution problems such as acid rain [3]. However, with the development of coal chemical technology, high-sulfur coal pyrolysis has become a potential technology to achieve its value-added transformation [4], this process produces syngas with carbon monoxide and hydrogen as the main components by heating and decomposing high-sulfur coal in an air-isolated or inert atmosphere [5], which can be used as a chemical raw material, synthetic fuel or clean power generation fuel, thereby increasing the value of high-sulfur coal.

As a new way of clean utilisation of coal, the industrial application of coal pyrolysis technology faces the core challenge of explosion risk [6]. This risk mainly stems from the inherent flammable and explosive characteristics of pyrolysis product syngas [7]. Syngas has significant flammable properties, and its core is derived from the high-risk combustion and explosion properties of carbon monoxide and hydrogen [8], both of which exhibit extremely low minimum ignition energy (H_2 about 0.017 mJ, CO about 0.045 mJ) and a very wide explosion limit range (H_2 explosion limit in air is 4.0%–75.6%, CO explosion limit is 12.5%–74.2%) [9]. This feature makes it possible to break through the ignition threshold of syngas even if there are micro-energy ignition sources such as electrostatic discharge and local overheating in closed and confined spaces such as pyrolysis reactors and syngas pipelines [10], inducing combustion and even explosion accidents, which pose a serious threat to the safety of system operation. In addition, the sulphur in the raw material high-sulphur coal will be converted into toxic sulphur-containing compounds such as H_2S and SO_2 during pyrolysis [11]. This type of acid gas can corrode the metal material of the equipment and increase the risk of syngas leakage.

In recent years, with the gradual advancement of high-sulfur coal pyrolysis technology towards industrialisation, the need for systematic research on the risk of syngas combustion explosion has become increasingly urgent [12]. Existing research focuses on the combustion characteristics of conventional syngas and the explosion-proof technology of single-component gases, while the research on the pyrolysis of high-sulfur coal to syngas is still relatively fragmented [13]. In this context, this paper systematically sorts out the gas production characteristics and influencing factors of high-sulfur coal pyrolysis, the risk mechanism of syngas explosion, and the risk prediction and assessment methods of syngas explosion. It aims to provide theoretical support for the explosion risk of syngas from pyrolysis of high-sulfur coal and help the resource utilisation of high-sulfur coal.

2 Gas production characteristics of high-sulfur coal pyrolysis

The gas production characteristics of high-sulfur coal pyrolysis need to be comprehensively evaluated, including a comprehensive analysis of gas production composition, yield distribution, calorific value and sulfur-containing compound morphology, which directly determine the risk level of combustion and explosion of syngas [14]. From the perspective of composition, syngas is mainly composed of combustible components such as hydrogen (H_2), carbon monoxide (CO, accounting for 60%~85% of the total volume), methane (CH_4, accounting for 5%~15% of the total volume), and inert components such as carbon dioxide (CO_2) and nitrogen (N_2). Among them, H_2 and CO are the core sources of flammability of syngas, while CH_4 further enhances combustion intensity due to its high calorific value (about 35.8 MJ/m^3). Compared with the gas produced by low-sulfur coal pyrolysis, high-sulfur coal pyrolysis will also produce hydrogen sulfide (H_2S, accounting for 70%~90% of the total volume of sulfur-containing gas), carbonyl sulfur (COS, accounting for 5%~20% of the total volume of sulfur-containing gas) and a small amount of sulfur dioxide (SO_2) [15]. When the H_2S volume fraction exceeds 0.5%, the minimum ignition energy of syngas decreases from 0.017~0.045 mJ to 0.012~ 0.038 mJ, and its explosion sensitivity is significantly increased. From the perspective of yield and calorific value, the yield of syngas produced by pyrolysis of high-sulfur coal is 200~400 m^3/t coal (dry basis), and its low calorific value is 10~15 MJ/ m^3, which belongs to the category of medium calorific value gas.

The gas production characteristics of high-sulfur coal pyrolysis are jointly regulated by the internal coal quality attributes and external process conditions [16]. Among the internal factors, the coal grade determines the volatile content and sulphur content [17]. The volatile content of low-grade high-sulfur coal is higher (volatile content accounts for 30%~ 50%), and the yield of hydrogen (H_2) and methane (CH_4) in the pyrolysis product is high, but the production of hydrogen sulfide (H_2S) is low (<10 g/m^3). The volatile content of high-grade high-sulfur coal was lower (10%~25%), the proportion of carbon monoxide (CO) in pyrolysis gas production was higher (35%~45%), and the H_2S generation was significantly higher (15~30 g/m^3). When the sulphur content of the feedstock coal is increased from 3% to 6%, the volume fraction of H_2S in the pyrolysis syngas increases from 0.8% to 2.1%. In terms of sulphur conversion law, pyrite in coal can decompose to form H_2S at 400~600°C, while organic sulphur needs to be easily converted to H_2S at high temperatures above 600°C [18]. In addition, ferric oxide (Fe_2O_3) in coal ash can catalyse the conversion of sulphur to H_2S and regulate the ratio of H_2 to CO in gas production, while silica (SiO_2) and aluminium trioxide (Al_2O_3) only show weak adsorption effects on sulphur-containing impurities.

In external conditions, temperature is the core regulatory factor [19]. At 300~500° C, pyrolysis gas production is dominated by methane (CH_4) and carbon dioxide (CO_2). In the range of 500~800°C, hydrogen (H_2), carbon monoxide (CO) and sulfur-containing impurities are released in large quantities. At 800~1100°C, the proportion of H_2 in gas production can reach 45%~55%. The effects of stress are characterised by phases [20]. Increasing pressure can promote total gas production but inhibit the yield of H_2 and CO at normal pressure to 0.5 megapascal (MPa). When the pressure exceeds 0.5 MPa, the effect is the opposite – not only inhibiting total gas production, but also reducing the hydrogen sulfide (H_2S) content. The effect of residence time on gas production characteristics is also significant. The appropriate residence time (10–30 seconds) can increase the gas production rate and increase the proportion of H_2 and CO in gas production. If the residence time is too short or too long, it will lead to an imbalance in the gas production composition and change the shape and content of sulphur-containing impurities. The type of atmosphere also changes the pattern of gas production. In an inert atmosphere, the gas-producing components are more stable; the oxidising atmosphere can increase the ratio of H_2 to CO, and at the same time oxidise part of H_2S to sulphur dioxide (SO_2). The reducing atmosphere inhibits the formation of H_2S and increases the content of CH_4.

The gas production characteristics of high-sulfur coal pyrolysis affect the risk of syngas explosion through three dimensions: the proportion of combustible components, the content of sulfur-containing impurities, and the proportion of inert components. When the pyrolysis conditions were high temperature, medium pressure and suitable residence time, the total proportion of H_2 and CO exceeded 80%, and the H_2S content was between 0.8% and 2.1%, resulting in extremely strong ignition sensitivity of syngas and the highest explosion risk. When the pyrolysis conditions were low temperature, high pressure and short residence time, the proportion of CH_4 and inert components was high, the total proportion of H_2 and CO was less than 60%, and the release of H_2S was insufficient. This results in a narrowing of the explosion limit range (e.g. the explosion limit of the H_2/CO mixture is narrowed from 4.0%–75.6% to 8.0%–65.0%), so the risk is relatively low. The presence of sulphur-containing impurities also has an indirect effect, and H_2S increases the risk by reducing the minimum ignition energy. Although SO_2 can slightly dilute the concentration of combustible gases (increasing the lower explosion limit by 1%–2%), its toxicity and corrosiveness can increase the risk of equipment leakage. In summary, gas production characteristics are the "source variables" of explosion risk, and clarifying its regulatory laws is the key to accurately identifying risk triggers and supporting subsequent mechanism analysis and model construction.

3 Syngas explosion risk mechanism

The core mechanism of syngas explosion risk revolves around three stages: chain reaction initiation -intensified flame propagation - rapid energy release, and the intervention of sulfur-containing impurities further alters this reaction pathway [21]. From the perspective of chain reaction, the combustion explosion of H_2 and CO in syngas is essentially a radical chain reaction: H_2 reacts with O_2 to form hydrogen radicals (H・), and CO continues to form H・ by combining with hydroxyl radicals (HO・), forming a cyclic chain reaction that eventually triggers violent combustion. The H_2S produced by the pyrolysis of high-sulfur coal will participate in the radical reaction, and the sulfur radicals (S・) produced by its decomposition will promote the formation of H・ and accelerate the chain reaction rate, thereby reducing the ignition threshold of syngas. From the perspective of flame propagation and energy release, the diffusion coefficient of H_2 in syngas is much higher than that of air, resulting in faster flame propagation. At the same time, H_2 and CO release a large amount of heat when burning, which provides conditions for the continuous propagation of flame and the accumulation of explosive energy, further exacerbating the risk of explosion.

Syngas explosion risk is affected by both internal component characteristics and external environmental conditions, which together determine the intensity of explosion risk [22]. In terms of intrinsic components, the proportion of combustible components is the basis: the higher the proportion of H_2, the wider the explosion limit range, and the lower the ignition energy; H_2S in sulfur-containing impurities can reduce the minimum ignition energy of syngas, while SO_2, as an inert component, can increase the lower limit of explosion limit and mitigate risks. If the proportion of inert components (CO_2 and N_2) is too high, the concentration of combustible gas will be diluted, the flame propagation speed will be reduced, and the explosion will be suppressed. Under external conditions, the increase in temperature will shorten the ignition delay time and improve the explosion reactivity. The increase of pressure will increase the frequency of molecular collisions and increase the peak explosion pressure. The smaller the volume of the confined space, the more difficult it is for heat and pressure to diffuse, and the stronger the explosive destructive force. An ignition source with a certain energy threshold, such as an electrostatic spark, can trigger a high H_2 syngas explosion.

The essence of the relationship between the risk mechanism of syngas explosion and the influencing factors is that "the internal components determine the risk base, and the external conditions amplify or weaken the risk" [23]. When the total proportion of H_2 and CO in syngas is high and contains a certain amount of H_2S (intrinsically high-risk substrate), superimposed on high temperature, high pressure, and confined small space (external strengthening conditions), the chain reaction rate is significantly increased, the flame propagation speed is accelerated, the peak explosion pressure is high, and the risk is at a very high level. If the proportion of inert components in syngas is high and contains a certain amount of SO_2 (intrinsic low-risk base), even in the presence of a high-temperature environment, it is difficult to trigger a violent explosion under external conditions. In addition, dynamic changes in external conditions will change the mechanism effect, such as the sudden increase in pressure will enhance the promotion effect of H_2S on free radicals, causing the syngas, which was originally in a "critical explosion state", to quickly enter a "violent explosion state". In summary, clarifying the correlation between mechanism and influencing factors is the core basis for accurately judging the risk level of syngas explosion and formulating targeted prevention and control measures.

4 Syngas explosion risk prediction and assessment method

Syngas explosion risk prediction and assessment methods can be divided into three categories: traditional empirical methods, experimental testing methods and numerical simulation methods, and various methods can achieve quantitative or qualitative judgment of risks from different dimensions [24]. The traditional empirical method is based on the "simplified model empirical formula", the most typical being the gas explosion triangle method, which quickly determines whether it is in the explosion hazard zone by defining the safety threshold of three key parameters of combustible component concentration, ignition source energy and oxygen concentration in syngas, which is easy to operate and does not require complex equipment, and is suitable for preliminary risk screening. In addition, the risk index method sorts out the risk factors such as syngas leakage, ignition source, and spatial structure in the pyrolysis system, assigns weights to each factor and calculates the risk index cumulatively, in order to divide the overall risk level. The experimental test method relies on physical experiments to obtain real risk data, and commonly used explosive characteristics testing devices (such as 20L spherical explosive tanks) directly measure key parameters such as maximum explosion pressure and pressure rise rate by simulating the explosion process of syngas under different working conditions, providing a measured basis for risk assessment. At the same time, the ignition sensitivity experiment can determine the minimum ignition energy and ignition delay time of syngas, and clarify the critical conditions for triggering explosions. Based on the theory of fluid mechanics and chemical reaction kinetics, the numerical simulation method simulates the diffusion, mixing and explosion propagation process of syngas under different temperatures, pressures and spatial structures by establishing a mathematical model of syngas explosion (such as computational fluid dynamics CFD model), which can dynamically present the spatio-temporal distribution law of explosion shock waves, and can also predict the risk change trend under different prevention and control measures through iterative optimisation of parameters, which is suitable for refined risk assessment of complex industrial systems.

The applicability of different prediction and evaluation methods is significantly different, and their limitations also determine the need to be selected or combined in practical applications[25]. Although the traditional empirical method is simple and quick, it overlooks the dynamic changes of syngas components (such as the influence of sulfur-containing impurities) and the interference of complex flow fields, and can only provide rough risk judgement, failing to accurately reflect the actual explosion intensity and hazard range. The experimental test method is constrained by the scale and working condition control ability of the experimental device, making it difficult to simulate the gas flow characteristics of the industrial-grade pyrolysis reactor in high temperature and high pressure environments and large spaces. At the same time, most of the experimental samples were single or fixed proportions of syngas, which made it difficult to fully reproduce the real-time fluctuations of syngas components in high-sulfur coal pyrolysis. Although the numerical simulation method can overcome the limitations of experimental conditions and realise the simulation of multiple working conditions and large-scale scenarios, it is heavily dependent on model parameters (such as reaction kinetics parameters and turbulence model coefficients), and if the parameter settings deviate significantly from the actual situation, the simulation results will be distorted. In addition, complex models require a large amount of computation, necessitating the support of high-performance computing equipment, and the modelling process requires high professional expertise and is difficult to popularise.

The selection of syngas explosion risk prediction and assessment methods should closely follow the actual scenario of high-sulfur coal pyrolysis systems, combine the comprehensive judgment of "risk assessment objectives, scenario complexity, and data requirements", and pay attention to the complementary integration of multiple methods. For the daily inspection and preliminary risk investigation of the pyrolysis system, the gas explosion triangle method can be used to quickly determine whether the syngas concentration is within the safe range, and the regional risk level can be divided with the risk index method to achieve efficient preliminary control. For the special risk assessment of key equipment (such as syngas pipelines and reactors), the basic explosion parameters of sulfur-containing syngas (such as maximum explosion pressure and minimum ignition energy) can be obtained through experimental tests, and then the measured data can be substituted into the numerical simulation model to calibrate the parameters to improve the accuracy of the simulation results, and then accurately predict the explosion diffusion path and hazard range after the syngas leakage in the equipment. For new or renovated high-sulfur coal pyrolysis projects, the combination of "empirical method preliminary screening, experimental testing to obtain basic data, and numerical simulation and refined evaluation" can be used to ensure not only the evaluation efficiency, but also the accuracy and comprehensiveness of the results. In addition, in view of the particularity of sulfur-containing impurities in syngas in high-sulfur coal pyrolysis, it is necessary to supplement the correction coefficient of sulfur-containing components on explosion parameters in the application of the method, or develop a special model suitable for sulfur-containing syngas to reduce the evaluation bias caused by the influence of impurities and ensure that the method can truly reflect the risk of syngas explosion in the pyrolysis scenario of high-sulfur coal.

5 Conclusions and outlook

The core conclusions are as follows: the risk of syngas explosion is determined by the proportion of combustible components (the highest risk when the total proportion of H_2/CO is over 80%), the form of sulfur-containing impurities (H_2S reduces the minimum ignition energy to 0.012–0.038 mJ) and the content of inert components (greater than 40% can inhibit the explosion), and the explosion sensitivity is the strongest at high temperature (800–1100°C), medium pressure (0.5 MPa), and suitable residence time (10–30 s). The sulfur-containing impurities have a dual effect: H_2S releases S・which accelerates the chain reaction, and SO_2 is prone to cause equipment leakage due to corrosion although the lower explosion limit is slightly increased. The traditional empirical method is suitable for rapid risk screening but overlooks the dynamic changes of sulfur-containing gases, while the experimental test can accurately obtain explosion parameters but is limited by working condition simulation, and the numerical simulation can reproduce large-scale explosion propagation but relies on high-precision parameters.

Based on the current shortcomings, the following research can be focused on in the future: first, to deepen the kinetic mechanism of sulfur-containing impurities, quantify the quantitative contribution of H_2S/SO_2 in the free radical chain reaction, and establish a mapping model of sulfur morphological transformation and explosive susceptibility; The second is to develop adaptive risk assessment technology under working conditions, build a dynamic explosion parameter database covering coal quality fluctuations (sulfur content 3%–6%) and pressure jumps (0.1–2.0 MPa), and develop a CFD explosion model for sulfur-containing syngas embedded in the H_2S reaction module to reduce the empirical hypothesis bias of parameters. The third is to promote the integration and innovation of multidisciplinary methods, and combine machine learning algorithms (such as LSTM) and experimental data to predict the evolution trend of explosion risk under complex working conditions, so as to provide support for the intrinsically safe design of high-sulfur coal pyrolysis systems.

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