Thermal simulation experiment and research on the system of coal/coal and water/coal and water and MgSO$_4$/coal and water and CaSO$_4$

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**ABSTRACT**

The role of thermochemical sulfate reduction (TSR) is one of the main causes of high contents of hydrogen sulfide (H$_2$S) in coal and rock formations. Sulfurous gas coal was selected from the Jurassic Xishanyao Formation in the Xishan coal mine of the Urumqi Anomaly Accumulation Area, using high-temperature and high-pressure reactors to simulate eight temperature-level experiments at 250°C–600°C. Four reaction systems of coal, coal + water, coal + water + sulfate, and coal + water + calcium sulfate and the evolution characteristics of gaseous products were analyzed. The TSR reaction has three stages of initial non-autocatalytic reaction, autocatalytic reaction, and late non-autocatalytic reaction. In the initial low temperature stage, physical desorption mainly occurs and TSR is weak. With the progress of the TSR reaction, hydrocarbon gases increase and non-hydrocarbon gases decrease. TSR can greatly promote the formation of hydrocarbon gases, especially methane gas, and methane is difficult to participate in TSR. TSR action occurs with the generation of heavy hydrocarbons. The TSR reaction leads to the drying of gaseous components, that is, the TSR reaction is more likely to occur in gaseous hydrocarbons with more carbon numbers. The change of CO$_2$ yield from down to rising can be better characterized as the characteristics of TSR. The yield of H$_2$, the change is wavy, which may be related to the supply and consumption of sulfur radicals and hydrogen in the coal and the formation of H$_2$S. In the coal and coal + water reaction systems, H$_2$S production is less; it is a low degree of response to the TSR reaction, mainly the hydrocarbon thermal cracking; the water in the process of the pyrolysis of coal into a gas cracking process plays an enormous role. The addition of calcium sulfate and magnesium sulfate promotes the TSR reaction and accelerates the cracking of heavy hydrocarbon gases. MgSO$_4$ initiates the TSR reaction more easily than CaSO$_4$.

**Keywords:** Coal-bearing water; Thermochemical sulfate reduction (TSR); Simulation experiment; Hydrogen sulfide; Evolution characteristic