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ACCEPTED MANUSCRIPT

Thermodynamic and Kinetic Behaviors of Coal Gasification

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Highlights

- With increasing CO_2 content, the gas utilization rate gradually increases.
- With increasing $H_2O_{(g)}$ content, the gas utilization rate gradually decreases.
- The *E*a of internal diffusion and interface reaction are calculated respectively.
- The controlling step changes from the interfacial reaction to internal diffusion.
- At 1173-1473K, the controlling step is primarily the interfacial reaction.

Abstract:

The thermodynamic and kinetic behaviors of coal gasification were studied via thermodynamic calculations and high-temperature simulation experiments. The results show that, at temperatures greater than 1173 K, the equilibrium concentrations of $H_2O_{(g)}$ and CO_2 are low and decrease with increasing temperature. With increasing CO_2 volume fraction in the gas, the gas utilization rate gradually increases, and with increasing $H_2O_{(g)}$ volume fraction, the rate gradually decreases. As the gasification temperature increases, the time required for completion of coal gasification is shortened, and the rate of coal gasification increases. The activation energies of internal diffusion and the interface reaction are 84.205 kJ/mol and 81.935 kJ/mol, respectively. In the early stage, the controlling factor of coal gasification is the interface reaction. As the reaction ratio increases, the controlling factor gradually changes from the interfacial reaction to internal diffusion. At 1173-1473 K, the controlling step of coal gasification is primarily the interfacial reaction.

Keywords: Coal, gasification, thermodynamic, kinetic, controlling step

1 Introduction

China is a country with "more coal, less oil and less gas". Currently, in the energy consumption structure in China, coal accounts for approximately 70%, whereas oil and natural gas account for 19% and 5%, respectively[1]. These energy resource characteristics demonstrate that China's energy structure is still dominated by coal. In the face of environmental pollution and a shortage of oil and natural gas resources,

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