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Sorption enhanced coal gasification for hydrogen production using a synthesized CaO–MgOmolecular sieve sorbent



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ABSTRACT

This study tends to investigate sorption enhanced hydrogen production process using MgO-molecular sieve modified CaO-based sorbents in a horizontal fixed bed reactor. The synthesized sorbents were prepared using a wet mixing method for enhancing H₂ yields and concentration as well as capturing CO_2 . The sorbents were characterized by means of X-ray diffraction (XRD), nitrogen adsorption and desorption isotherms test, and scanning electron microscopy (SEM)/energy dispersive spectrometer (EDS). The ash content of coal and the calcined mixture were analyzed by the method of energy dispersive X-ray fluorescence (EDXRF). The CaO-MgO-molecular sieve sorbents were investigated during 20 adsorption and calcination cycles using thermogravimetric analyzer (TGA). The effects of different kinds of CaO-based sorbents, the molar ratio of Ca/C, and diverse coal species on gas yields and concentration were investigated. The experimental results verified that the presence of modified sorbents in the steam coal gasification process enhanced the concentration of hydrogen to more than 80%, with lower concentration of CO₂ emission. The highest hydrogen concentration were obtained using the modified CaO-MgO-5A molecular sieve at the condition that the temperature is 650 $^{\circ}$ C, the N₂ flow rate is 0.5 L/min, and the water injection rate is 0.3 L/min.

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Introduction

Hydrogen is considered to be a promising energy in the future [1,2]. The demand for hydrogen energy is expected to increase rapidly [3,4]. Currently, nearly 20 percent of hydrogen is mainly generated from steam methane reforming and coal gasification [5–9]. Coal is a relatively inexpensive and abundant fossil fuel. Coal gasification is one of the most important efficient technologies for converting coal into fuel gas and

varieties of chemical products [10–15]. The conventional coal gasification process includes the procedure of syngas formation at a high temperature, purification, water-gas shift reaction, CO_2 removal process, and PSA Pressure swing Absorption [16]. Therefore, efforts to develop advanced and less complicated technologies for clean coal gasification with higher efficiency and carbon dioxide capture simultaneously must be intensified [17–19].

In recent years, a new gasification method named sorption enhanced hydrogen production (SEHP) was proposed which

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accomplishes the above processes in a single step [20-25]. CaO is used as CO₂ sorbent to enhance hydrogen production due to its large abundant availability in nature, cheap price, and moderate sorption capacity [26,27]. The typical reactions are described as follows:

Steam methane reforming reaction:

$$CH_4 (g) + H_2O (g) \rightarrow CO (g) + H_2 (g) \Delta H_{298K} = 206 \text{ kJ/mol}$$
 (1)

Water gas shift reaction:

$$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g) \Delta H_{298K} = -41 \text{ kJ/mol}$$
 (2)

CO₂ absorption reaction:

$$\label{eq:CaO} \mbox{(s)} + \mbox{CO}_2 \end{tabular} \rightarrow \mbox{CaCO}_3 \mbox{(s)} \end{tabular} \Delta \mbox{H}_{298K} = -178 \mbox{ kJ/mol} \end{tabular} \mbox{(3)}$$

Overall:

$$\begin{array}{l} {\rm CH}_4 \left(g \right) + {\rm H}_2 {\rm O} \left(g \right) + {\rm CaO} \left(s \right) \to {\rm H}_2 \left(g \right) + {\rm CaCO}_3 \left(s \right) \Delta {\rm H}_{298K} \\ = -13 \ {\rm kJ/mol} \end{array} \tag{4}$$

It can be seen from Eqs. (1)-(4) that the addition of CaObased sorbent shifts the thermodynamic equilibrium of coal gasification toward the hydrogen formation side. A high purity of hydrogen can be obtained from the sorption enhanced coal gasification process. No heat is required in the sorption enhanced coal gasification process because the carbonation of CaO is strongly exothermic. But the sorption enhanced coal gasification process requires energy for the regeneration of the CaO-based sorbents, seen in Eq. (5).



Fig. 1 – Schematic presentation of strategies using the molecular sieve for anti-sintering and anti-agglomeration.

Table 1 – Proximate analysis and ultimate analysis of Yangquan coal (YQ), Shuozhou coal (SZ), Kailuan coal (KL), and Zhundong coal (ZD).

	Proximate analysis			Ultimate analysis					
	Aar	Var	Fcar	Mar	Car	Har	Oar	Nar	Sar
YQ	10.34	10.24	73.82	5.60	76.74	3.32	2.11	0.94	0.95
SZ	17.34	28.30	48.57	5.80	62.05	3.56	9.04	1.00	1.13
KL	31.39	24.26	34.55	9.8	47.42	3.09	7.35	0.47	0.48
ZD	5.41	28.54	53.90	12.15	65.69	4.98	16.33	0.85	1.78



Fig. 2 – The schematic diagram of coal gasification experimental device for hydrogen production.

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