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Simulation of solid oxide fuel cell systems integrated with sequential CaO–CO_2 capture unit

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ABSTRACT

This paper presents preliminary simulation results from the performance analysis of the integrated systems of calcium oxide (CaO)–carbon dioxide (CO_2) capture unit and solid oxide fuel cell (SOFC). The CO_2 was extracted for further sequestration in the CaO–CO_2 capture unit. Three configurations of the integrated systems (CaO-Before-SOFC: CBS, CaO-After-SOFC: CAS and CaO-After-Burner: CAB) were considered. It was found that the CO_2 capture efficiency (E_c) is dependent on CaO fresh feed rate (F_0) and CaO recycle rate (F_R). The improvement of SOFC performance was only realized for the CBS system. The SOFC performance increases with increasing CO_2 E_c. The preliminary economic analysis was carried out considering total additional cost per mole of CO_2 captured. At a low percentage of CO_2 capture (<42.5%), the CBS system is the most suitable configuration while the CAS system becomes an attractive choice at higher values. However, only the CAB system could be possible at a very high range of CO_2 capture (>94%).

1. Introduction

Nowadays, global warming is considered to be an important problem of the world. A major cause is arisen from a large emission of carbon dioxide to the environment which has been particularly driven by the growth of economics. Therefore, low-CO_2-emission processes are desired. Fuel cell is one of the novel processes for electrical power generation via an electrochemical reaction of hydrogen. Small amount of CO_2 is emitted from the fuel cell. Among a various type of fuel cell, solid oxide fuel cell (SOFC) is the most promising process. Due to high electrical efficiency of SOFC, lower amount of fuel is consumed, resulting in a lower amount of generated CO_2. At present, a number of efforts have been carried out to improve its efficiency. An integration of an SOFC with a CaO–CO_2 capture unit is one of an attractive choice for electrical power generation. The use of the CaO–CO_2 capture unit for CO_2 sequestration could further reduce the amount of CO_2 emitted to the environment.

The in situ CaO–CO_2 capture for shifting equilibrium of reaction was studied [1–6]. A coal/H_2O/CaO gasification system offers a higher yield of hydrogen production compared to a conventional coal/H_2O gasification system [1]. Methane steam reforming reaction (MSR) combined with CaO-carbonation showed a potential benefit on CO_2 acceptor and hydrogen production at 1023 K [2]. The simulation of in situ carbonation of CaO in MSR was studied [3,4] and the kinetics of the carbonation of CaO were proposed. The addition of CaO in a methane steam reforming system can increase the purity of hydrogen to be higher than 95% in a laboratory-scale operation [5]. The similar result was also reported in an ethanol steam reforming with addition of CaO [6].

Although CaO is a good candidate for CO_2 capture, the main problem of CaO–CO_2 capture is the generation of $CaCO_3$. Therefore, a carbonation–calcination cycle of CaO was considered as reported in many researches [7–10]. Gupta and Fan [7] used the reaction based on the cycle of separated CO_2 with CaO from flue gas. Sintering of CaO sorbent was not observed within 2–3 cycles of carbonation–calcination at 973 K. However, carbonation conversion decreased with increasing the number of cycles [8,9]. Abanades [10] proposed an expression for calculating the maximum CO_2 capture efficiency of CaO.

Some researchers have investigated the combined system of fuel cell and CO_2 capture unit to improve the system efficiency and reduce the global warming gas. Amorelli et al. [11] reported that a 1.6 MW MCFC-gas turbine (MCFC/GT) incorporated with a CO_2 capture unit could reduce the CO_2 emission by 50% from the conventional MCFC/GT system. Moreover, Fredriksson Möller et al. [12] showed that an SOFC/GT system can be operated at an electrical efficiency close to 65% when incorporating with a CO_2 capture unit.

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Nomenclature

a_j	constant in Eq. (11) (Ω m)
b	constant in Eq. (4) (0.174)
b_j	constant in Eq. (11) (K)
d_p	particle diameter (m)
D	diameter of reactor (m)
E	open circuit voltage (OCV) (V)
E_c	CO_2 capture efficiency (%)
E_0	reversible potential (V)
f	constant in Eq. (4) (0.782)
f_g	gas friction factor [14]
f_s	solid friction factor [14]
F	Faraday constant (96,485.34) (C mol^{-1})
F_0	fresh feed rate of CaO (mol s^{-1})
F_{CO_2}	molar flow rate of CO_2 (mol s^{-1})
F_R	recycle rate of CaO (mol s^{-1})
g	gravity acceleration (m s^{-2})
i	current density (A m^{-2})
i_0	exchange current density (A m^{-2})
L	length of reactor (m)
m	exponent parameter in Eq. (15)
n_e	number of electron transfer
P	total pressure (atm)
P_i	partial pressure (atm)
R	universal gas constant (8.31447×10^{-3}) (kJ mol^{-1} K^{-1})
T	absolute temperature (K)
u	velocity (m s^{-1})
U_f	fuel utilization (%)
v_t	gas terminal velocity (m s^{-1})
V	operating voltage (V)

Greeks letters

α	electron transfer coefficient
δ	thickness (m)
ε	bed void fraction
η_i	overpotential (Ω m^2)
μ	viscosity of fluid (Pa s)
ρ	density (kg m^{-3})
ρ_ι	specific ohmic resistance (Ω m)

Subscript

A	anode
C	cathode
f	fluid
p	particle

In this study, performances of various systems of SOFC integrated with carbonation–calcination systems (SOFC–CaO system) were simulated. The effects of location of CaO–CO_2 acceptor in the SOFC system, the CaO fresh feed rate, the CaO recycle rate and the fuel utilization were studied in terms of amount of CO_2 captured and SOFC performance. Finally, preliminary economic analysis was also considered.

2. Theory

2.1. Methane steam reforming

Methane steam reforming is the conventional route for hydrogen production. The major reactions taking place in the reactor are methane steam reforming (MSR, Eq. (1)) and water gas shift reaction (WGSR, Eq. (2)).

$$CH_4 + H_2O \leftrightarrows CO + 3H_2 \tag{1}$$

$$CO + H_2O \leftrightarrows CO_2 + H_2 \tag{2}$$

$$CH_4 + 2H_2O \leftrightarrows CO_2 + 4H_2 \tag{3}$$

In order to avoid a carbon formation problem, the molar ratio of H_2O:CH_4 in the feed stream should be higher than 2.5 [13]. In this work, it was assumed that the gas exiting the reformer is at its equilibrium composition.

2.2. CaO–CO_2 acceptor systems

Carbonation reaction of calcium oxide (CaO) can convert carbon dioxide (CO_2) to calcium carbonate ($CaCO_3$) whereas $CaCO_3$ can reverse to CaO at high temperature calcinations. The carbonation–calcination cycle for CO_2 separation is illustrated in Fig. 1. The maximum efficiency of CO_2 capture can be expressed as follows [10]:

$$E_c = \frac{F_R + F_0}{F_0 + F_{CO_2}} \cdot \left(\frac{f \cdot F_0}{F_0 + F_R(1-f)} + b \right) \tag{4}$$

where $b = 0.174$, $f = 0.782$, F_0 is fresh feed rate of CaO, F_R is feed recycle rate of CaO and F_{CO_2} is feed rate of CO_2.

The circulating fluidized bed was chosen for the CaO carbonation–calcination operation. The constraint of circulating fluidized bed is that gas velocity (v) must be higher than gas terminal velocity (v_t), ($v > v_t$) (Eq. (5)). Pressure drop along the reactor can be calculated by Eq. (6) [14].

$$v_t = \frac{g(\rho_p - \rho_f)d_p^2}{18\mu} \tag{5}$$

$$\frac{\Delta P}{L} = \rho_p(1-\varepsilon)g + \rho_f \varepsilon g + \frac{2f_g \rho_f u_f^2}{D} + \frac{2f_s \rho_p (1-\varepsilon) u_p^2}{D} \tag{6}$$

2.3. SOFC

An SOFC unit consists of two porous ceramic electrodes (i.e., an anode and a cathode) and a solid ceramic electrolyte. In theory, both hydrogen and CO can react electrochemically with oxygen ions at the anode of the SOFC cells. However, it was reported that about 98% of current is produced via H_2 oxidation in common situations [15]. Therefore it was assumed in this study that the CO electro-oxidation is neglected. The theoretical open-circuit voltage of the cell (E), which is the maximum voltage under specific operating conditions, can be calculated from the following equations [16]:

$$E = E_0 + \frac{RT}{2F} \ln \left(\frac{P_{H_2} P_{O_2}^{0.5}}{P_{H_2O}} \right) \tag{7}$$

$$E_0 = 1.253 - 2.4516 \times 10^{-4} T \tag{8}$$

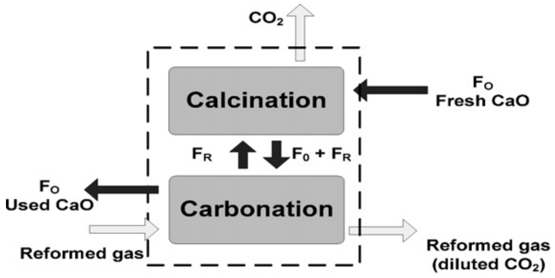

Fig. 1. Schematic diagram of a CaO–CO_2 acceptor system.