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# Sorption-enhanced water gas shift reaction using multi-section column for high-purity hydrogen production

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### ABSTRACT

Simultaneous execution of the water gas shift (WGS) reaction and  $CO_2$  separation in the sorption-enhanced water gas shift (SE-WGS) reaction has emerged as a method of enhancing hydrogen production. Herein, a multi-section column was proposed and applied as a new concept for enhancing the efficiency of the SE-WGS reaction. Conventional SE-WGS utilizes a single-section column in which the catalyst and sorbent are packed throughout the column at the same ratio, whereas in the proposed system, the column is divided into multiple sections, and the ratio of catalyst and sorbent are varied in each section. CO conversion and H<sub>2</sub> productivity in the two-section column SE-WGS reaction were investigated based on numerical simulations employing various ratios of catalyst and sorbent in each section of the column. The CO conversion and H<sub>2</sub> productivity could be maximized in the novel two-section SE-WGS reaction by increasing the catalyst content of the first section and the sorbent content of the second section.

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## 1. Introduction

The interest in new clean energy sources has been prompted by heightening concerns about declining conventional energy resources, environmental pollution, and global warming. Research on hydrogen energy, in particular, continues to gather momentum, with the production, transportation, and storage of hydrogen energy being areas of active focus [1,2]. Hydrogen is a highly efficient energy carrier in that the energy content per unit mass is 4 times higher than conventional gasoline, with the added benefit of being environmentally benign. Conversion of stored energy in hydrogen to utilizable energy is attendant with the production of only water as a byproduct. In the proposed hydrogen economy, hydrogen can be used as a potential alternative for conventional fossil fuels which are associated with pollution problems [2,3]. Ultimately, it is desirable that hydrogen for energy is produced from renewable sources such as solar energy, wind power and biomass [4]. However, due to current technical and economical limitations, the steam reforming of methane or natural gas as a hydrogen source has been most widely used. Recently, coal has been highlighted as a promising hydrogen source for bulk hydrogen production because it is cheap, abundant, and world-widely distributed. Coal is converted into synthesis gas by gasification, and hydrogen is subsequently produced by the water gas shift (WGS) reaction of the synthesis gas (Fig. 1(a)) [5–7].

$$CO + H_2O \leftrightarrow H_2 + CO_2 \quad \Delta H = -41.1 \text{ kJ/mol}$$
 (1)

However, the gas produced from the WGS reaction contains a considerable amount of impurities. Remaining steam is relatively easily removed by water condensation, and other

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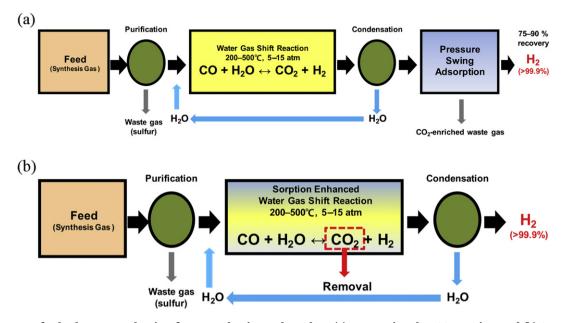


Fig. 1 – Process for hydrogen production from synthesis gas based on (a) conventional WGS reaction and (b) SE-WGS reaction.

gases are removed through purification processes such as pressure swing adsorption (PSA) to produce high purity hydrogen. Following the purification processes, H<sub>2</sub> of purity higher than 99.9% is obtained; however 10-25% of the produced H<sub>2</sub> is consumed, and waste gas containing a significant amount of CO2 is produced in the PSA process [8]. The sorption-enhanced WGS (SE-WGS) reaction has been developed as a means of negating these issues [9,10]. In the SE-WGS reaction, the WGS reaction proceeds with simultaneous separation of byproduct  $CO_2$  by  $CO_2$  adsorption in a single unit operation, which simplifies the overall hydrogen production process. Furthermore, this technique circumvents the thermodynamic limitation of the WGS reaction based on Le Chatelier's principle, and fuel-cell grade high-purity hydrogen (with less than 10 ppm CO) can be directly produced (Fig. 1(b)) [8,11].

There have been several research projects worldwide for commercialization of the SE-WGS reaction process. Air Products Inc. developed the SE-WGS reaction using hydrotalcite as a CO<sub>2</sub> sorbent, and recently, the Energy Research Centre of the Netherlands (ECN) initiated a project in cooperation with 5 countries in Europe [12,13]. Sircar and coworkers at Lehigh University studied the SE-WGS reaction using K<sub>2</sub>CO<sub>3</sub>-promoted hydrotalcite and Na2O-promoted alumina and also developed a novel thermal swing sorption-enhanced reaction process for continuous operation [14,15]. Recently, high temperature CO<sub>2</sub> sorbents based on CaO and Na<sub>2</sub>ZrO<sub>3</sub> have been studied for prospective application to the SE-WGS reaction [16,17]. However, most previous studies targeted toward the SE-WGS reaction have focused on the application of high temperature CO<sub>2</sub> sorbents. Few studies have been centered on the development of alternate efficient reaction processes. In this study, a multi-section column is proposed as a new concept for application to the SE-WGS reaction in order to enhance the process efficiency.

As shown in Fig. 2(a), the original SE-WGS reaction uses a column that is homogeneously packed with catalyst and sorbent. In this manner, the column can be considered as a single section. However, the proposed multi-section column concept, shown in Fig. 2(b), utilizes a column that is divided into more than two sections, and the catalyst and sorbent are packed into each section at different ratios. Based on this column design, additional degree of freedom such as catalyst and sorbent ratio in each section and section length ratio can be obtained for flexible operation.

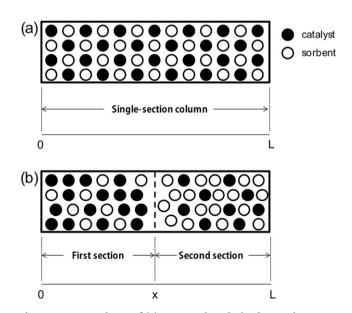


Fig. 2 – Comparison of (a) conventional single-section column and (b) novel multi-section column for SE-WGS reaction.

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