



Conceptual designs of hydrogen production, purification, compression and carbon dioxide capture



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ABSTRACT

The design of hydrogen production, purification, compression and carbon dioxide capture is developed as two types of heat-integrated processes. The SWP (SMR + WGS + PCC) is mainly composed of the steam methane reforming (SMR) reactor, the low temperature water–gas-shift (WGS) reactor and the process of hydrogen purification, compression and carbon dioxide capture (PCC), and the SCWP (SMR + CO₂R + WGS + PCC) primarily consists of the SMR reactor, the carbon dioxide reforming of methane (CO₂R) reactor, the WGS reactor and the PCC. From economic aspects, it is expectable that the SWP process is superior to the SCWP process due to lower energy demand and less equipment. From aspects of energy utilization and CO₂ capture, it is verified that the SCWP process is superior to the SWP process.

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1. Introduction

Cost-effective hydrogen production and CO₂ capture are required for a hydrogen economy [1]. About 95% of the hydrogen produced in the U.S. is obtained using a thermal process with natural gas as the feedstock. The conventional hydrogen production process primarily consists of a steam methane reforming (SMR) and a water gas shift (WGS) reaction [2]. Since the use of hydrogen in fuel cell applications requires a high purity by 99.99 + %, the pressure swing adsorption (PSA) process is widely used for hydrogen purification and separation [3]. In addition, a small amount of carbon monoxide may poison fuel cell electrodes. The WGS reactor can effectively reduce CO amount in the hydrogen stream [4]. However, the most hydrogen production processes would accompany with a large CO₂ emissions due to the WGS reactions.

The CO₂ capture is a well-developed technique to reduce their emissions of CO₂ [5]. Some schemes such as a monoethanolamine (MEA) CO₂ scrubbing process and cardo polyimide hollow fiber membrane capture [6,7] are applied to reduce the emissions of greenhouse gases including methane and carbon dioxide. Koumpouras et al. [8] introduced a low-temperature hydrogen production with in situ CO₂ capture. CO₂ adsorbent particles are passed through a stationary SMR catalyst monolith, but adsorbent regeneration was carried out in an external unit. Nord et al. [9] proposed pre-combustion CO₂ capture to reduce greenhouse gas emissions but the complexity of the plant increases. The advantage for a

post-combustion capture system could deal with separating out CO₂ from flue gases at a low pressure. To consume or suppress the CO₂ emissions of hydrogen production processes, Song and Pan [10] presented a configuration for tri-reforming methane, which involved a carbon dioxide reforming of methane (CO₂R), steam reforming and the partial oxidation of methane, to enhance CO₂ conversion and utilization. Farniaei et al. [11] proposed a new system configuration in which the steam reforming reaction was preceded by excess generated heat from tri-reforming reaction instead of huge fired-furnace in conventional steam reformer. Fan et al. [12] utilized greenhouse gases as the feed of the catalytic carbon dioxide reforming process to improve hourly space velocity and hydrogen production. Fan et al. [13] also studied the optimization of hydrogen production from the CO₂ reforming of methane. Wang and Cao [14] studied the simulation of the hydrogen production by the ethanol steam reforming process and the carbon dioxide reforming unit. Recently, Wu et al. [15] developed the design for a combination of the SMR and CO₂R reactors to achieve the stand-alone syngas production process. Although CO₂ emissions can be effectively suppressed, the syngas yield is low due to the internal combustion to recovering the energy demands. Many steam reforming processes in refineries are usually connected to the process for hydrogen purification and compression in order to store the pure hydrogen [16]. The heat integration using pinch analysis is a feasible method to utilize the waste heat, such as industrial chemical plants [17,18]. Synthesis of heat exchanger networks (HENs) was successfully implemented to the steam reforming process for producing high-pressure hydrogen [19,20].

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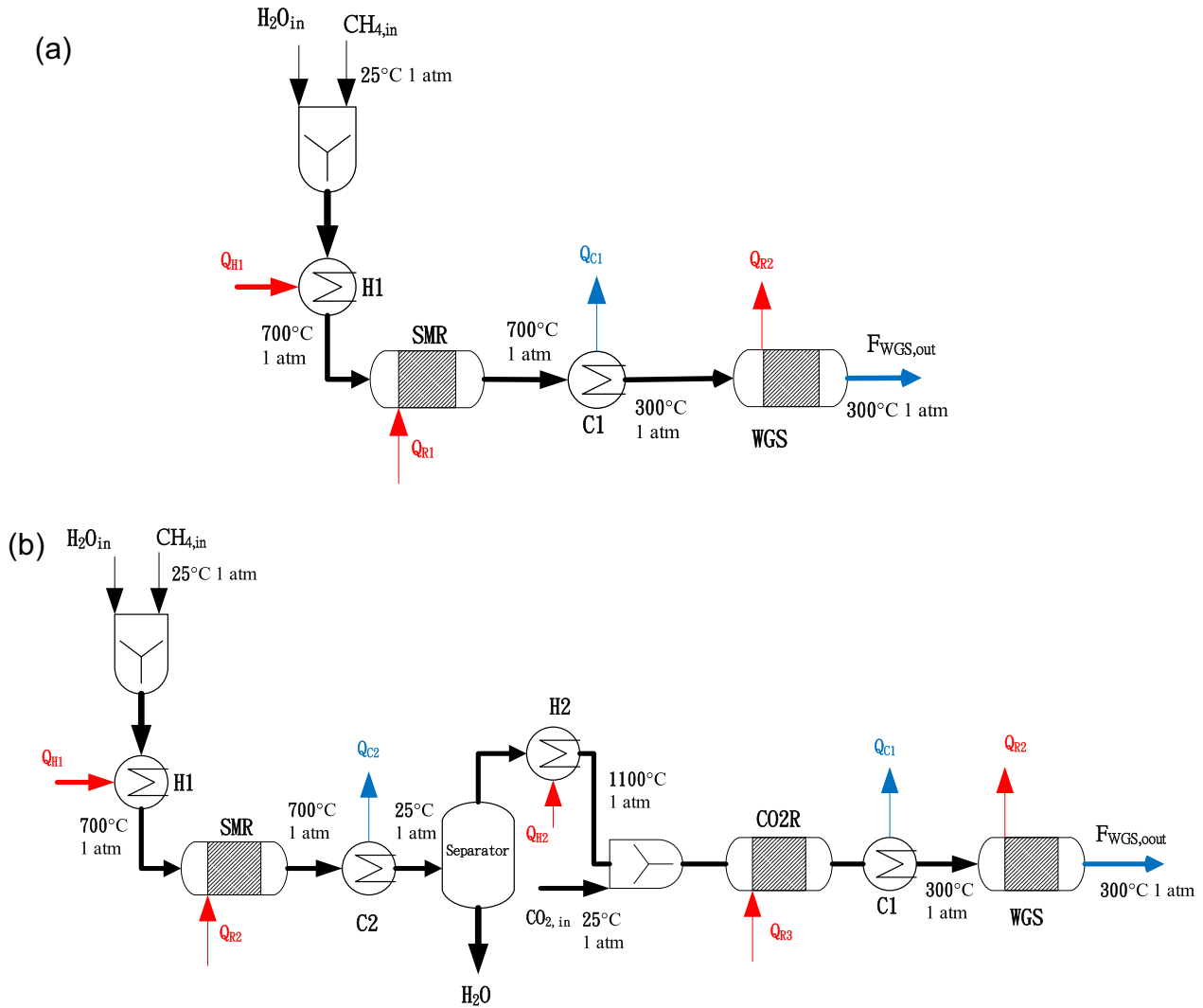


Fig. 1. Hydrogen production system configurations: (a) SMR + WGS; (b) SMR + CO₂R + WGS.

To develop the process of hydrogen production, purification and compression, the heat and power integration is necessary. The synthesis of HENs is an effective approach for waste heat recovery, but CO₂ emissions of the processes cannot be suppressed. In our approach, an extension of the steam reforming process is presented to pursue the hydrogen production process with near-zero carbon emissions. A carbon dioxide reforming of methane (CO₂R) reactor is added into the SMR process to produce the hydrogen by consuming greenhouse gases with methane and carbon dioxide. Since the process of hydrogen purification and compression would release heat and waste gas, the oxy combustion technique, which was successfully implemented to the clean coal-fired power plant [21], is added to increase the CO₂ concentration of exhausted flue gas such that the energy penalty of the CO₂ capture is dramatically reduced. To address near-zero carbon emissions of high-pressure hydrogen process, the performance of CO₂ reduction and energy efficiency improvements are verified by the Aspen Plus simulator.

2. Hydrogen production processes

2.1. Kinetics and process design

In general, the conventional hydrogen production process is a combination of SMR and WGS reactors. The SMR reactor is

considered as a plug-flow reactor where three exothermic/endothermic reactions are shown as follows:

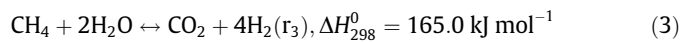
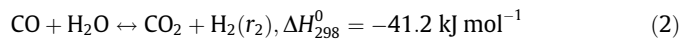
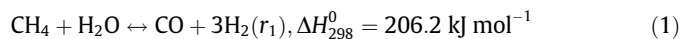


Table 1
Specifications of major process units.

Equipment	Aspen model	Specification/configuration
SMR	RPLUG	Heat duty required, reactor length = 5 m, reactor diameter = 1.5 m, pressure drop = 50 kPa, and void fraction = 0.6
CO ₂ R	RPLUG, REquil	Heat duty required, reactor length = 5 m, reactor diameter = 1.5 m, pressure drop = 60 kPa, and void fraction = 0.6
WGS	RPLUG	No heat duty, reactor length = 3 m, reactor diameter = 0.15 m, pressure drop = 50 kPa, and void fraction = 1
PSA	Component splitter	No heat duty and 99.95% purity of H ₂
Combustor	RStoic	Stoichiometry reactor
Separator	Flash2	Two phase flash drum

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