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A cost assessment study for a large-scale water gas shift catalytic membrane reactor module in the presence of uncertainty

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ABSTRACT

A comprehensive economic performance evaluation framework for an actual large-scale water-gas-shift Pd-based catalytic membrane reactor (CMR) module for hydrogen production is presented. Since a detailed assessment of the technical performance of the CMR built at WPI has been reported previously (Catalano et al., 2013), the present research study focuses on an assessment of the module's economic performance characteristics, and thus, can be viewed as complementary. The proposed evaluation framework encompasses comprehensive baseline models for both Fixed Capital Investment (FCI) and Total Capital Investment (TCI) while various sources of uncertainty are identified whose effect on CMR's economic performance is explicitly taken into account using Monte Carlo techniques. As a result, insightful distribution profiles of FCI and TCI are derived rather than single-point value estimates and more realistic distributions of CMR economic performance outcomes are generated and statistically characterized. The latter could potentially inform development efforts of this new technology option for hydrogen production purposes.

1. Introduction

Palladium membranes separate H_2 from gas mixtures such as syngas (CO_2, CO, H_2O, N_2), commonly derived from coal gasification units in power generation with high efficiency through the solution-diffusion mechanism. First, molecular hydrogen undergoes a dissociative adsorption process, leading to the dissolution and diffusion of atomic hydrogen through the metallic layer which is driven by a transmembrane hydrogen partial pressure difference. Then, atomic hydrogen associates on the permeate side surface allowing molecular H_2 to desorb from the surface [2]. Consequently, a theoretically infinite selectivity can be achieved at high fluxes as well as good chemical and physical stability [3]. Furthermore, it has been shown that alloying Pd with other metals such as Cu, Au, Pt and Ag enhances the H_2 permeance of the membrane and its resistance to H_2 embrittlement [4].

Palladium-based catalytic membrane reactors (CMRs) represent an efficient technology option that increases the conversion of chemical reactions and accordingly improves product recovery levels [5,6]. Subsequently, the production of hydrogen in CMRs via natural gas steam reforming (MSR) and water–gas shift (WGS) of the coal-derived syngas generates strong interest as an alternative clean process system. In particular, the application of membrane technology to the water-gas shift (WGS) reaction has been shown to be efficient technically and economically [7]. In a WGS CMR module, the catalyst is confined within the reactor (retentate) along with a tubular palladium membrane situated throughout the reaction zone (Fig. 1). The membrane continuously removes "in-situ" the H_2 generated which, in accordance to Le-Chatelier's principle, allows higher CO conversions to be attained and potentially supported by process intensification strategies [1,8]. Notice that this approach yields conversions that exceed the ones commonly attained in conventional packed bed reactors. Additionally, the higher retentate pressure facilitates the acquisition of clean pressurized CO_2 and water, thus enabling the process of carbon capture. For all the aforementioned technical features, Pd-based CMRs have shown to represent an important technology option for the development of H_2 economy [8].

In CMRs, the reaction and separation processes are conducted simultaneously, and therefore, the high- and low-temperature shift reactors along with a hydrogen separation unit, such as pressure swing adsorption (PSA) in the traditional hydrogen production system [9,10] can be eliminated from the structure of the overall process system. Additionally, the simultaneous separation of H_2

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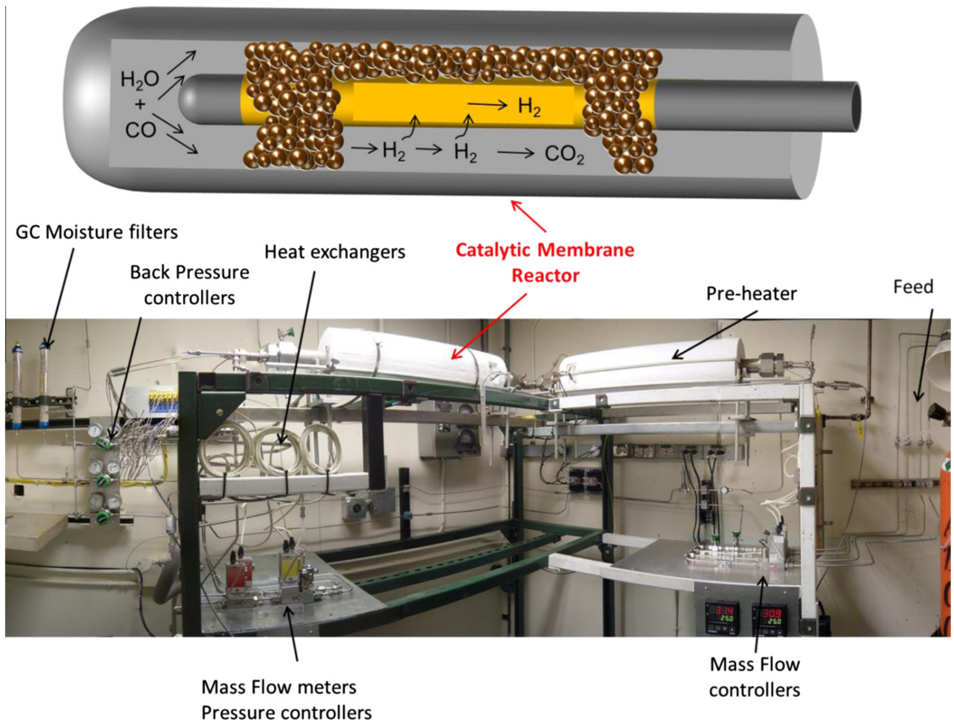

Fig. 1. Schematic of a CMR module for water gas shift reaction and picture of the actual CMR rig built at WPI.

and CO_2 is particularly appealing due to increasing efforts focusing on the reduction of carbon dioxide emissions [11,12]. When compared to the conventional hydrogen production process, a CMR allows lower temperatures of operation, while still reaching higher conversion levels; this enables prolonged catalyst lifetime, lower production costs, reduced material costs for the reactor and a facilitated route for carbon capture. Moreover, process intensification in CMR technology provides compactness, modularity, reduced equipment size to production capacity ratio, practical assembly/disassembly capabilities and operational flexibility [13]. Additional advantageous features include the good allocation of material and energy resources, waste management and superior environmental performance [14].

Many studies have been reported regarding the potential industrial applications of Pd-based CMR technology, but their results rely on a proof-of-concept-centered approach [15,16], giving rise to significant challenges for techno-economic performance evaluation in the absence of any accumulated operating experience at the commercial scale and reliable data. Furthermore, the few large-scale tests of CMRs under actual industrial conditions that have been published do not offer comprehensive sets of pertinent techno-economic data. The study by Catalano et al. [1] showed that H_2 production of 1.2 lb/day with purity higher than 99% can be reached through a WGS-CMR using a gas mixture similar to an actual syngas composition. The surface area of the membrane used in this work was 200 cm^2 with operating conditions corresponding to a temperature range of 420–440 °C and a retentate pressure of 20 bar. In Fig. 1, a photograph of the CMR rig shows its different components, including the mass flow and pressure controllers, the preheater, the heat exchangers, and back pressure regulators. Furthermore, Patrascu et al. [17] reported the use of a large-scale CMR for methane steam reforming (MSR) capable of achieving a H_2 permeate flow rate of 1.6 NL/min while utilizing a membrane with a surface area of 175 cm^2 and being operated at temperatures within the 440–525 °C range and at a pressure of 10 bar. Moreover, Ma et al. [18,19] demonstrated the satisfactory performance characteristics of different Pd and Pd/alloy membranes under actual coal-derived syngas and industrial scenarios but solely for H_2 purification purposes.

Over the years, our group [14,20–24] has developed a comprehensive economic performance assessment framework to evaluate Pd-based CMR technology integrated into power and hydrogen production plants with the purpose of identifying market and regulatory conditions that allow this new technology option to generate superior economic performance outcomes when compared to the traditional ones. In particular, Monte Carlo simulation methods were integrated into the above framework in order to explicitly take into account various sources of irreducible uncertainty in the fuel market and regulatory environments. Such a methodological context enables a comprehensive evaluation of economic performance characteristics of CMRs while overcoming the limitations of conventional valuation/assessment methods that rely on single-point value estimates. The present research study focuses on building upon the promising results reported in [14,20,21] in order to evaluate the profile of economic performance outcomes generated by the large-scale WGS CMR module reported by Catalano et al. [1] under the aforementioned uncertainties. The objective of the present study is to obtain realistic profiles of economic outcomes and other valuable information by explicitly acknowledging uncertainty sources, and therefore, inform potential demonstration and deployment efforts of CMR technology in an industrial setting. In particular, the contribution of this study can be traced in the following directions:

(i) In the presence of new knowledge and available data, the present research work offers a systematic and comprehensive framework to reliably assess and characterize the cost profile of a new technology option realized by an actual large-scale membrane reactor module.
(ii) In the absence of any significant accumulated operating experience regarding this new membrane reactor module, the present research work provides preliminary insights