

## II.C.1 Single Membrane Reactor Configuration for Separation of Hydrogen, Carbon Dioxide and Hydrogen Sulfide

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overall footprint than can be achieved by utilizing separate components for each required unit process/unit operation. Specifically, research is sought to perform a combination of theoretical and experimental research to provide a scientific basis needed to develop a novel “one-box” process to combine synthesis gas cleanup, water-gas shift reaction, hydrogen separation and carbon dioxide separation. A successful strategy will have the potential to selectively remove pure hydrogen, carbon dioxide and synthesis gas impurities in a single reactor configuration that can operate simultaneously at high temperature and high conversion, possibly without the requirement of excess steam.

### Approach

The objective of this research is to develop a “one-box” approach that can consolidate two or more downstream reaction/separation units of a coal gasification system in a single module for production of a pure stream of hydrogen. The project will evaluate the technical feasibility of using two or three types of membranes to selectively separate pure hydrogen, carbon dioxide and hydrogen sulfide in a single reactor configuration that can operate simultaneously at high temperatures (e.g., 700-900°C). The project team will synthesize nanosized CaCO<sub>3</sub> and CaO powders, analyze the powders for chemical and physical characteristics, fabricate membranes, test membranes in permeation units, and demonstrate the feasibility of CO<sub>2</sub> separation and H<sub>2</sub>S removal using the high temperature Ca-based membranes. Additionally, perovskite-type of ceramic membranes will be tested for their chemical stability under H<sub>2</sub>S and CO<sub>2</sub> environments. Theoretical models for CO<sub>2</sub> permeation through the Ca-based membranes and H<sub>2</sub> permeation through the perovskite membranes will be developed. Simulation will be performed to evaluate the performance of hydrogen production from coal gasification systems based on the complementary membrane water-gas-shift reactor process.

### Objectives

- Develop a novel membrane process concept that would combine hydrogen sulfide removal, water-gas shift reaction, hydrogen separation and carbon dioxide separation in a single membrane configuration.
- Develop a new class of microporous membranes for hydrogen sulfide removal and carbon dioxide separation, characterized and tested for high-temperature application feasibility.
- Test proton conducting membranes for chemical stability under hydrogen sulfide and carbon dioxide atmospheres.
- Develop theoretical models for permeation and simulation to evaluate the performance of hydrogen production from gasification systems based on the complementary membrane water-gas-shift reactor process.

### Introduction

This project seeks to develop advanced technologies that offer the potential to consolidate two or more unit processes/unit operations such as gas separation processes in one module (process intensification) that would be integrated downstream of a coal gasification system designed to produce a pure stream of hydrogen. The motivation for process intensification is to achieve higher efficiencies, lower capital costs and a smaller

### Accomplishments

- Initiated task to develop a membrane based on nanosized particles for increased permeation rate of CO<sub>2</sub>.
- Initiated task to prepare and test a CaO membrane.
- Completed construction of a permeation unit capable of operations up to 10 atm with the capability to handle H<sub>2</sub>S-containing gas streams.
- Conducted CO<sub>2</sub> permeation testing on selected Ca-based membranes.

**Future Directions**

- Conduct hydrogen permeation testing with proton-conducting membranes under CO<sub>2</sub>/H<sub>2</sub>S-containing gas streams.
- Conduct hydrogen permeation testing with hydrogen-selective membranes under H<sub>2</sub>S-containing gas streams.
- Conduct hydrogen sulfide permeation testing on selected Ca-based membranes.
- Make go/no-go decision for proceeding to Phase II.
- Complete Phase I final report and make go/no-go decision on a Phase II effort.
- Assuming a “go” decision is made to proceed to Phase II, expand on prior work with binary gas mixtures by initiating membrane permeation and durability testing using gas mixtures representative of a real syngas stream.