# **IV.B.3** Novel Sorption-Enhanced Reaction Process for Simultaneous Production of Carbon Dioxide and Hydrogen from Synthesis Gas Produced by Coal Gasification

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# Objectives

- Construct, test and evaluate the feasibility of a novel concept, Thermal Swing Sorption Enhanced Reaction (TSSER), to simultaneously carry out the water-gas-shift (WGS) reaction for the production of pure hydrogen (dry basis) and the separation of carbon dioxide as a single unit operation in a sorber-reactor.
- Characterize the CO<sub>2</sub> chemisorbents under various conditions of temperature, pressure and composition using the flow-through apparatus, and select the most attractive chemisorbent for the TSSER process.
- Evaluate isobaric thermal desorption characteristics of CO<sub>2</sub> from the chosen chemisorbent under various conditions, and determine the thermal stability of the chemisorbent.
- Assess the performance of each individual step of the process under various conditions of operation to develop a process model for data correlation and process design and to ascertain the practical feasibility of the proposed TSSER process.

## **Technical Barriers**

This project addresses the following technical barriers from the Hydrogen Production section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- L. Durability
- O. Selectivity
- Q. Flux
- S. Cost

The project also addresses Section 5.1.5.1., Technical Barriers – Central Production Pathway in the Hydrogen from Coal – Research, Development, and Demonstration Plan of the DOE Office of Fossil Energy. This includes WGS reaction barriers and hydrogen separation barriers.

#### **Technical Targets**

This project consists of four steps for the improvement of hydrogen production. The first is to construct a sorber-reactor and evaluate the Thermal Swing Sorption Enhanced Reaction (TSSER) to simultaneously carry out the WGS reaction for the production of pure hydrogen and the separation of  $CO_2$ . The second is to characterize the  $CO_2$  chemisorbents under various conditions to select the most attractive chemisorbent for the TSSER process. The third is to determine the thermal stability of the chemisorbent. The fourth is to develop a mathematical process design model for scale-up, optimization, and guiding future work.

The objectives of these studies for the production of two pure products ( $H_2$  and  $CO_2$ ) from the gasifier effluent at feed gas pressure include circumventing the equilibrium limitations of the WGS reaction, lowering the  $H_2O/CO$  molar ratio in the feed gas, reducing or eliminating the excess by-product steam generation, eliminating the elaborate separation equipment needed by the conventional approach, and reducing the plant footprint and cost to meet DOE's 2010 and 2015 hydrogen production and separation targets, particularly with respect to cost, durability, operating pressure, hydrogen recovery, and hydrogen quality.

#### Approach

The concept will carry out the WGS reaction and  $CO_2$  separation from the product gas in a single unit, thereby circumventing the thermodynamic limit. Chemisorption and thermal stability studies will be conducted to select the most attractive sorbent for the TSSER process. The results from these studies will be used to develop a mathematical process design model for scale-up, optimization, and guiding future work. The anticipated benefits to be derived from this investigation include potential reduction in the cost of production of hydrogen by coal gasification as well as providing a carbon dioxide byproduct at gasification pressure for sequestration without large recompression costs, or for its sale as a chemical. This project will also open up the possible use of a new genre of chemisorbents as separation agents at elevated temperatures without predrying the feed gas. Industrial participation will be solicited for future scale-up of this concept after successful completion of the proposed phase of the project.

## Accomplishments

This project is newly initiated and no there are no accomplishments to report to date.