# II.B.3 Novel Sorption Enhanced Reaction Process for Simultaneous Production of $CO_2$ & $H_2$ from Synthesis Gas Produced by Coal Gasification

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## Objectives

Test the feasibility of using a novel concept called thermal swing sorption enhanced reaction (TSSER) process to simultaneously carry out the water-gas-shift (WGS) reaction for the production of a pure stream of $H_2$ (dry basis) and the separation of $CO_2$ as a single unit operation in a sorber-reactor.

## Introduction

The objective of this project is to test the feasibility of using a novel concept called thermal swing sorption enhanced reaction (TSSER) process to simultaneously carry out the WGS reaction for the production of a pure stream of $H_2$ (dry basis) and the separation of $CO_2$ as a single unit operation in a sorber-reactor. If successful, this project would (i) produce two pure products ($H_2$ and $CO_2$) from the gasifier effluent at feed gas pressure, (ii) circumvent the equilibrium limitations of the WGS reaction, (iii) lower the $H_2O$/CO molar ratio in the feed gas, (iv) reduce or eliminate the excess by-product steam generation, (v) eliminate the elaborate separation equipments needed by the conventional approach, and (vi) reduce plant foot-print and cost. This would result in several anticipated benefits including a potential reduction in the cost of production of hydrogen by coal gasification as well as providing a carbon dioxide by-product at gasification pressure for sequestration without large recompression costs, or for its sale as a chemical agent.

## Approach

The end result of this project is limited to the experimental demonstration of the feasibility of the proposed TSSER process and evaluation of the appropriate chemisorbents to be used in the process. The approach will include (i) measurement of $CO_2$ sorption equilibria, kinetics, and ad(de)sorption column dynamics on the chemisorbents under various conditions of operations, (ii) measurement of the column dynamics of the thermal desorption characteristics of $CO_2$ from the chemisorbents, (iii) individual testing of each step of the process, and (iv) use of a mathematical model for data correlation, process design and optimization. The project culminates in an experimental demonstration of the feasibility of the proposed TSSER process and evaluation of the appropriate chemisorbents to be used in the process, but does not include continuous process testing using a bench or pilot scale unit.

## Accomplishments

- Experimentally evaluated isobaric thermal desorption characteristics of $CO_2$ from the chosen chemisorbent under various conditions.
- Ascertained thermal stability of the chemisorbent.

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 by-product at gasification pressure for sequestration without large recompression costs, or for its sale as a chemical agent.

## Future Directions

- Determine chemisorption isotherms and kinetics for $CO_2$ sorption from $N_2$ (proxy for unadsorbed $H_2O$) under various conditions of temperature, pressure and composition using the flow through apparatus.
- Determine isobaric and isothermal adsorption column dynamics for $CO_2 + N_2$ mixtures as well as isothermal and isobaric desorption of $CO_2$ by $N_2$ purge under various conditions. Evaluate the effect of the presence of steam on above properties and select the most attractive chemisorbent for the TSSER process.
- Evaluate the performance of each individual step of the process (separately) in the same apparatus by packing it with an admixture of a WGS reaction catalyst and the chosen chemisorbent.

- Develop a process model for data correlation and process design.
- Ascertain the practical feasibility of the proposed TSSER process using the measured data and the process model.