A High Efficiency, Ultra-Compact Process For Pre-Combustion CO_2 Capture

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•Professor Theo Tsotsis, University of Southern California, Los Angeles, CA
•Professor Vasilios Manousiouthakis, University of California, Los Angeles, CA
•Dr. Rich Ciora, Media and Process Technology Inc., Pittsburgh, PA

USC VITERBI SCHOOL OF ENGINEERING

UCLA ENGINEERING Chemical and Biomolecular Engineering

U.S. Department of Energy
National Energy Technology Laboratory
Office of Fossil Energy
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Presentation Outline

- **Project Overview**
- **Technology Background**
- **Technical Approach/Project Scope**
- **Progress and Current Status of Project**
- **Plans for Future Testing/Development/Commercialization**

Project Overview

Performance Period: 10-01-2015 – 9-31-2018

Project Budget: Total/$1,909,018; DOE Share/$1,520,546; Cost-Share/$388,472

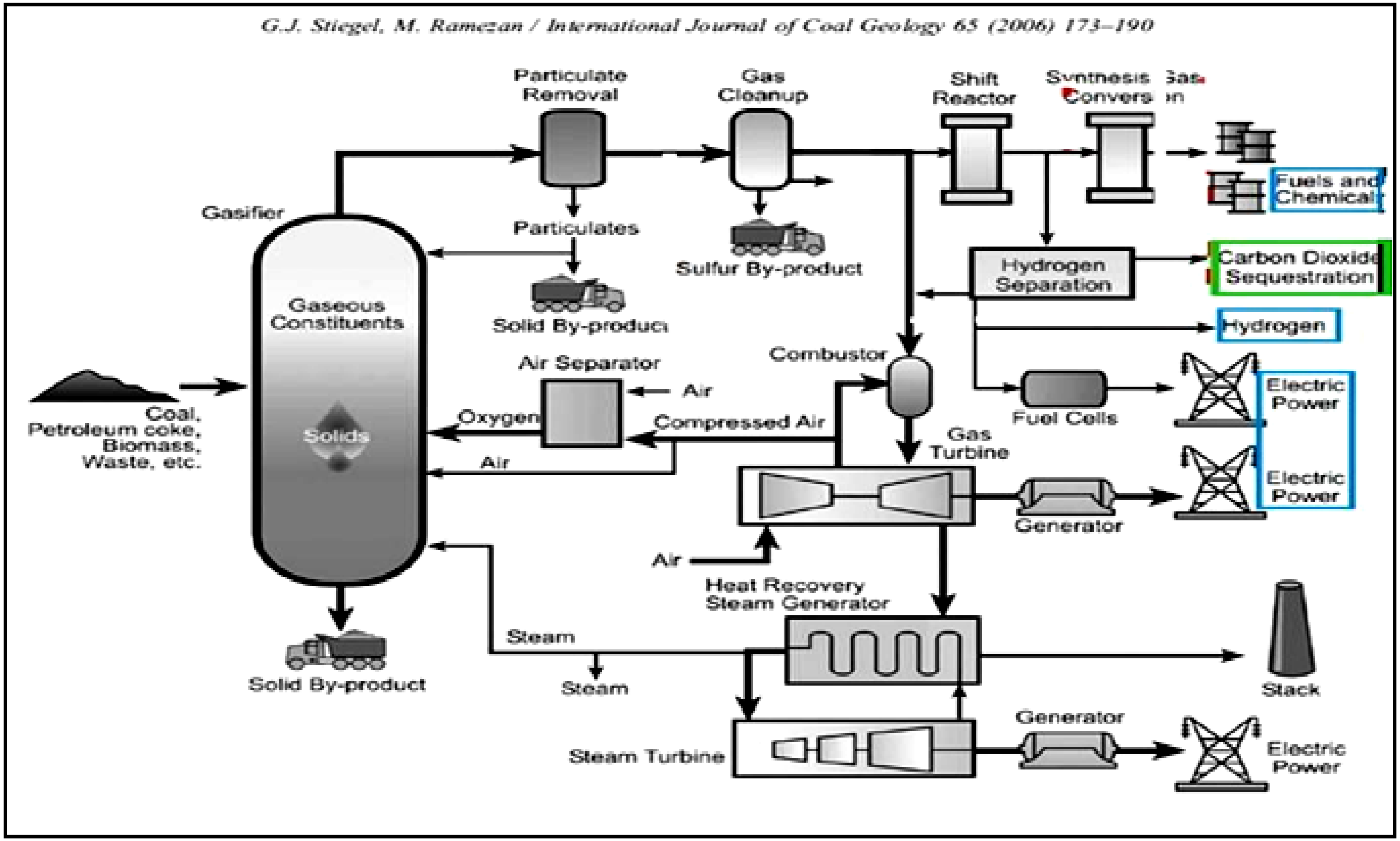
Overall Project Objectives:

1. *Prove the technical feasibility of the membrane- and adsorption-enhanced water gas shift (WGS) process.*
2. *Achieve the overall fossil energy performance goals of 90% CO_2 capture rate with 95% CO_2 purity at a cost of electricity of 30% less than baseline capture approaches.*

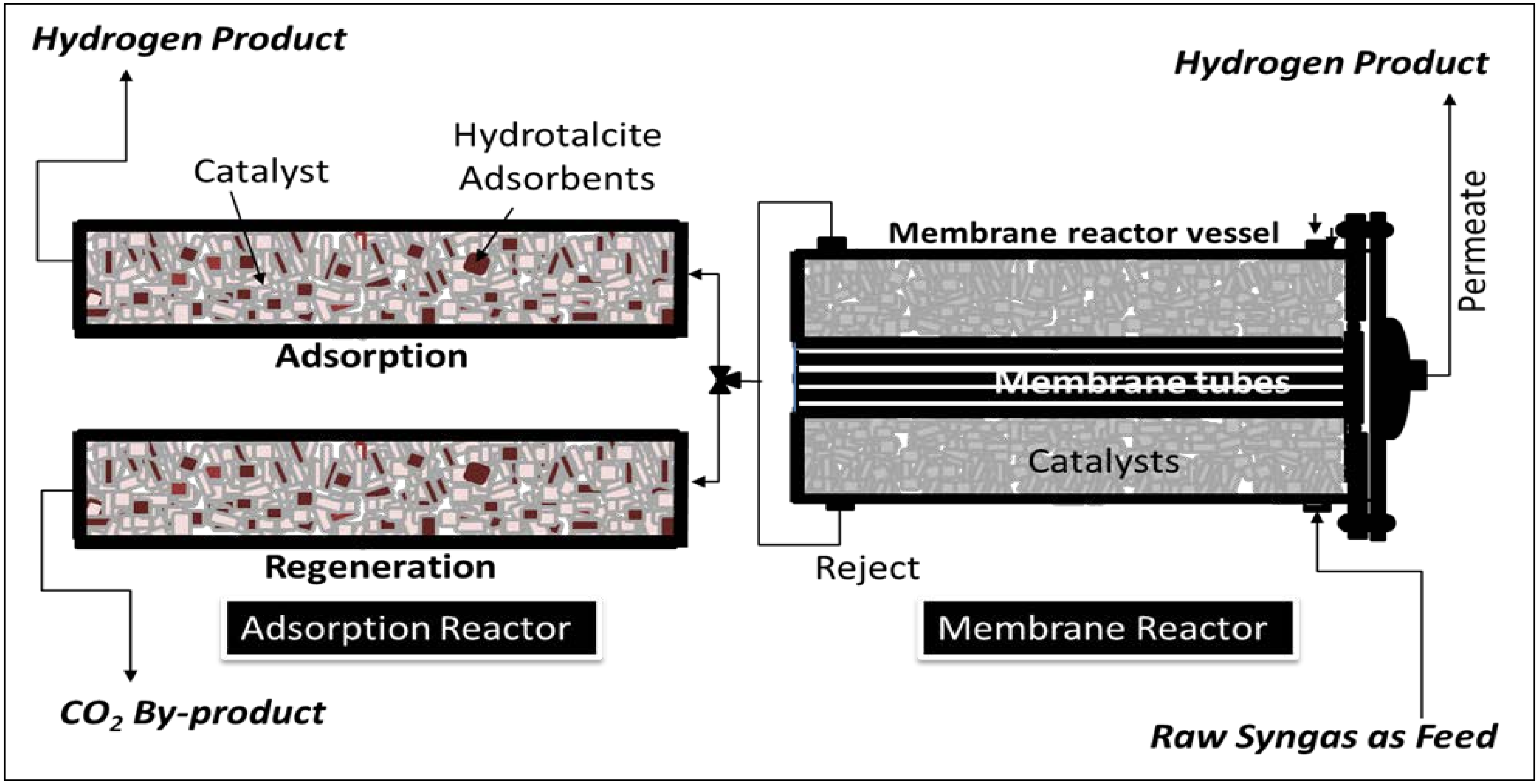
Key Project Tasks/Participants:

1. *Design, construct and test the lab-scale experimental MR-AR system.**-----USC***
2. *Select and characterize appropriate membranes, adsorbents and catalysts.**-----M&PT, USC***
3. *Develop and experimentally validate mathematical model.**-----UCLA, USC***
4. *Experimentally test the proposed novel process in the lab-scale apparatus, and complete the initial technical and economic feasibility study. .**----- M&PT, UCLA, USC***

Conventional IGCC Power Plant



MR-AR Process Scheme



- Potential use of a TSA regeneration scheme allows the recovery of CO_2 at high pressures.
- The MR-AR process overcomes the limitations of competitive singular, stand-alone systems, such as the conventional WGSR, and the more advanced WGS-MR and WGS-AR technologies.

MR-AR Process Scheme – Advantages over SOTA

Key Innovation:

- *Highly efficient, low-temperature reactor process for the WGS reaction of coal-gasifier syngas for pre-combustion CO_2 capture, using a unique adsorption-enhanced WGS membrane reactor (MR-AR) concept.*

Unique Advantages:

- ***No syngas pretreatment required:*** *CMS membranes proven stable in past/ongoing studies to all of the gas contaminants associated with coal-derived syngas.*

- ***Improved WGS Efficiency:*** *Enhanced reactor yield and selectivity via the simultaneous removal of H_2 and CO_2.*

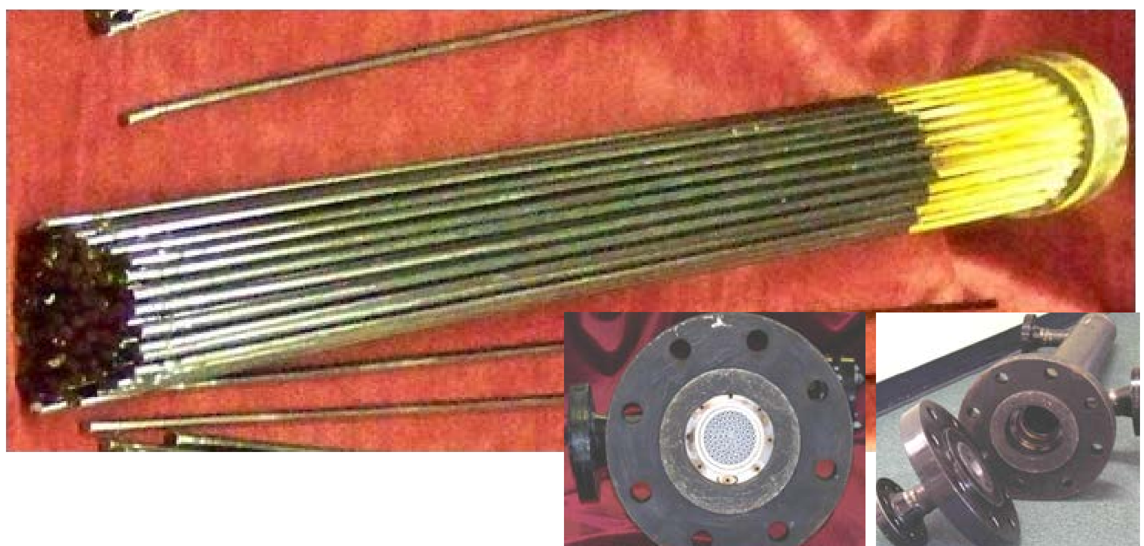
- ***Significantly reduced catalyst weight usage requirements:*** *Reaction rate enhancement (over the conventional WGSR) that results from removing both products, potentially, allows one to operate at much lower W/F_{CO} (K_{gcat}/mol.hr).*

- ***Efficient H_2 production, and superior CO_2 recovery and purity:*** *The synergy created between the MR and AR units makes simultaneously meeting the CO_2 recovery/purity targets together with carbon utilization (CO conversion) and hydrogen recovery/purity goals a potential reality.*

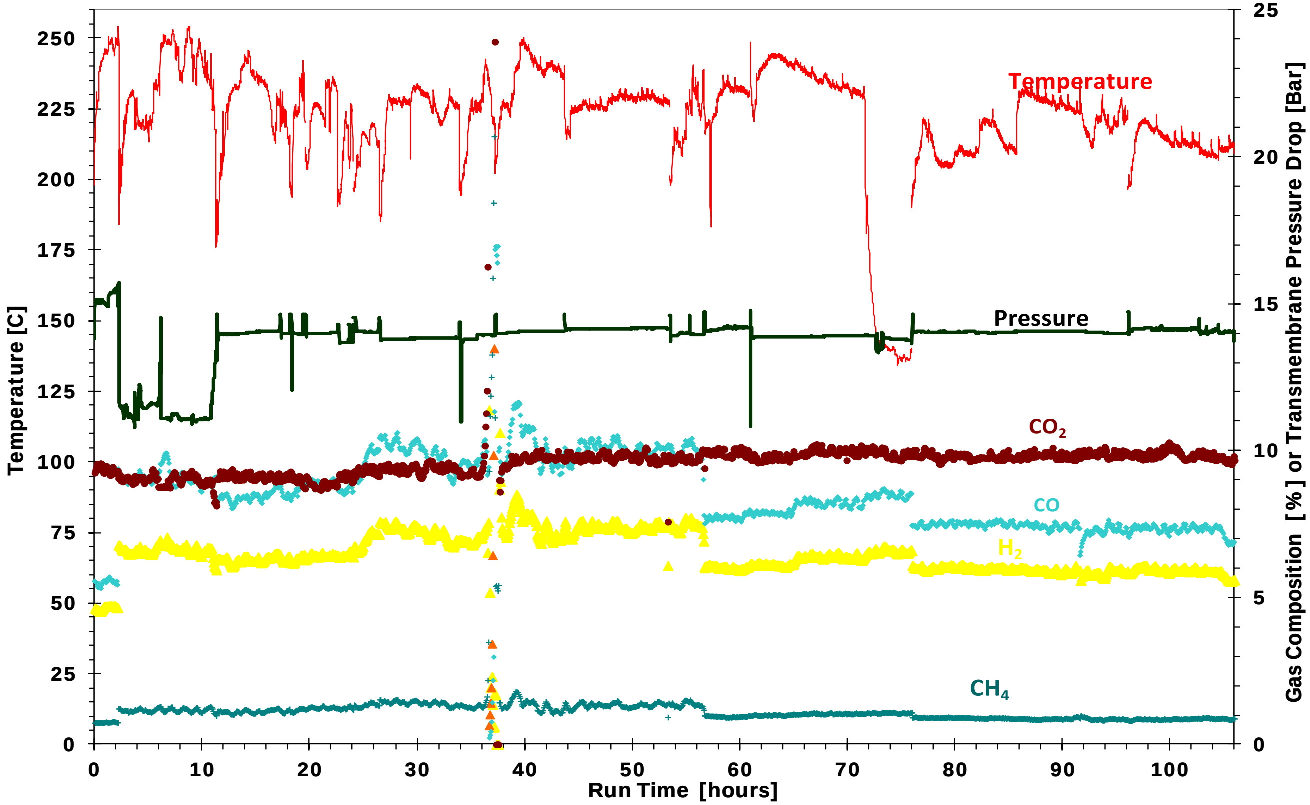
Field-Testing of CMS Membranes

M&PT test-unit at NCCC for hydrogen separation

CMS membranes and modules

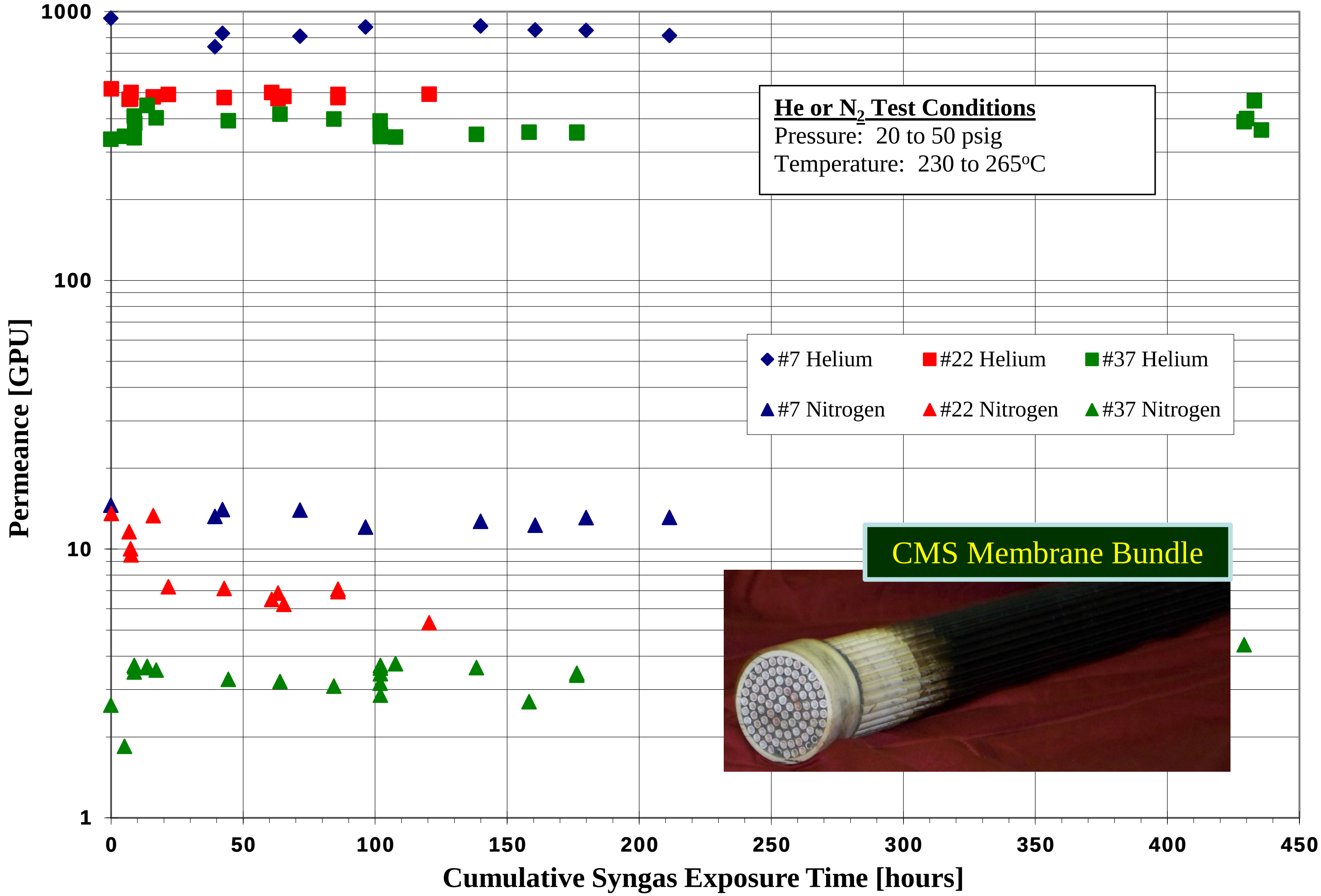


Field Test – Syngas Composition

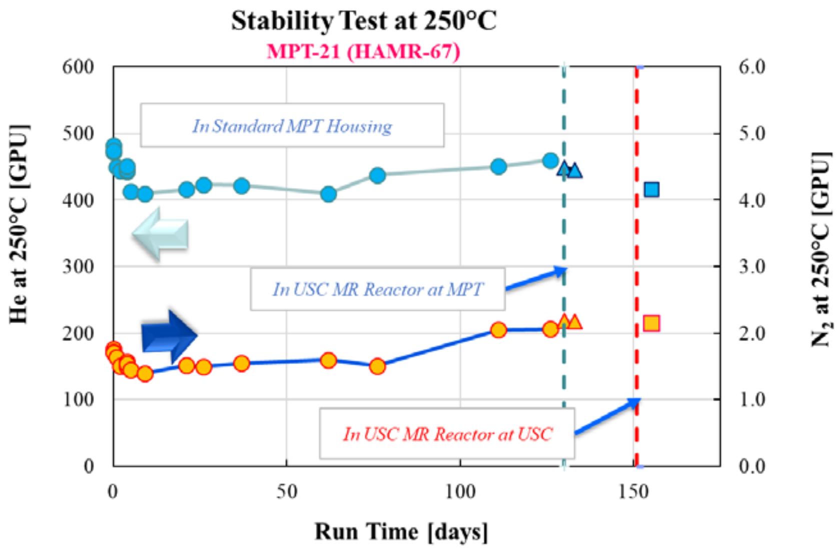


NH_3 ~1000 ppm; S ~1000 ppm; HCl < 5 ppm; HCN ~ 20 ppm; H_2O >10%; high concentrations of napthalenic and other condensable hydrocarbons

Long-Term Stability Testing in Gasifier Off-gas [NCCC]



A New Generation of CMS Membranes

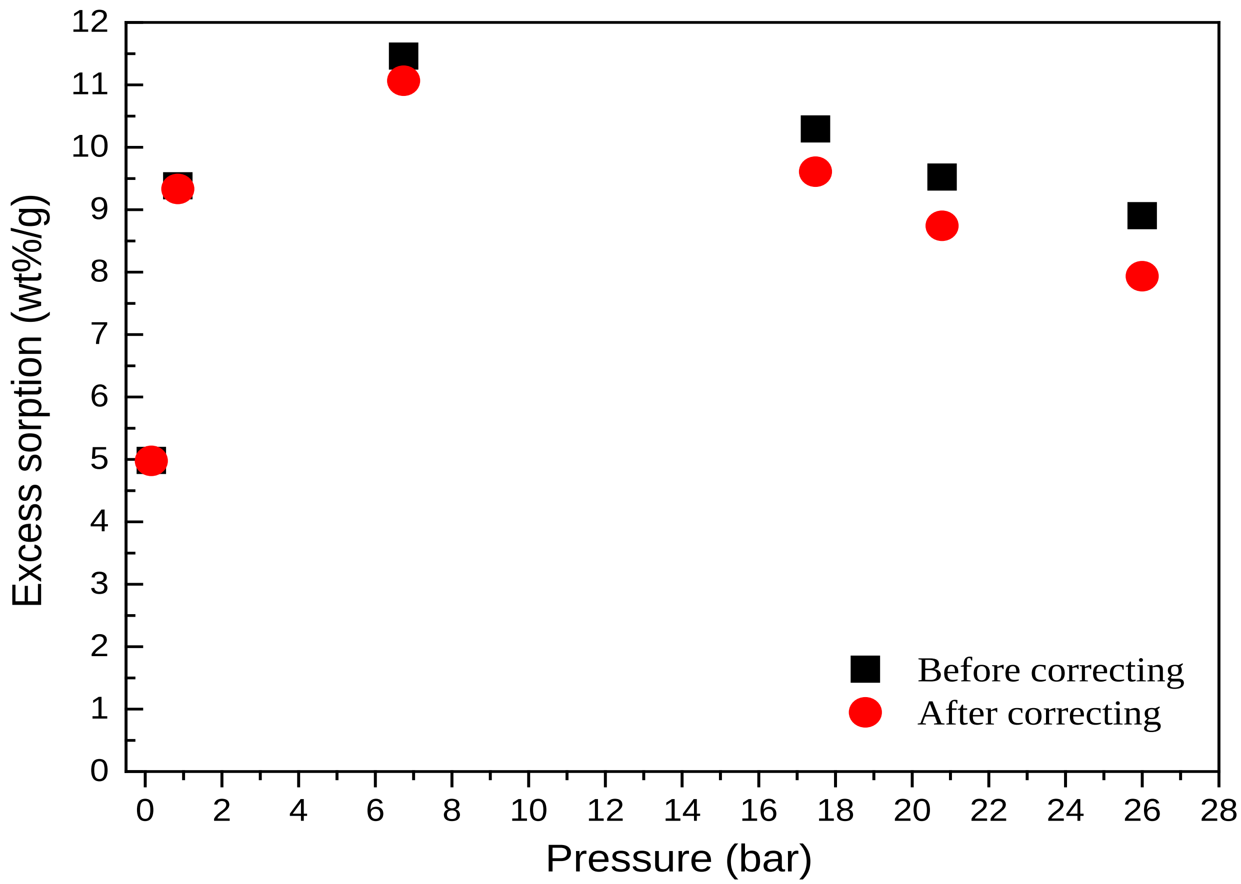


Original Project Targets:
H_2_Permeance (350 – 500 GPU);
$H_2/CO>80$ (Equivalent to $H_2/N_2>100$)

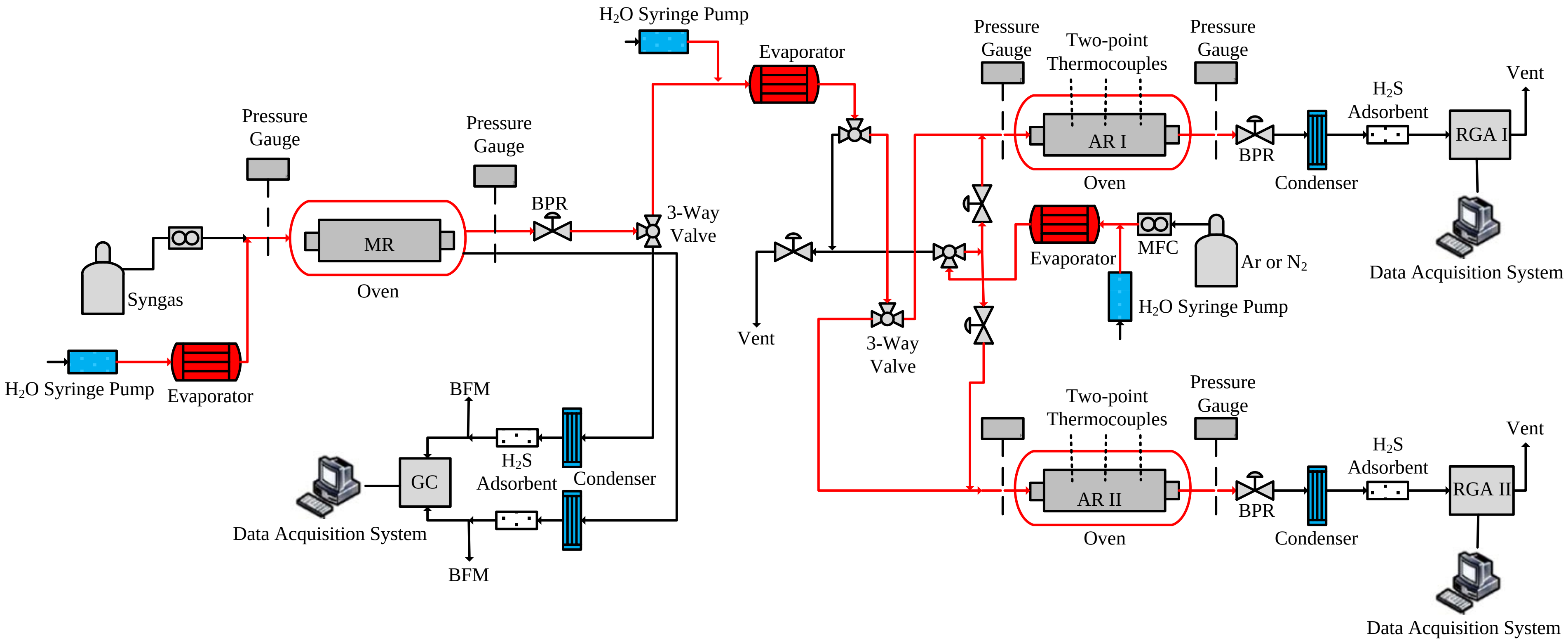
Part ID	*He [GPU]*	*N_2 [GPU]*	*H_2 [GPU]*	*CO_2 [GPU]*	*H_2/N_2 [-]*	*H_2/CO_2 [-]*
HMR-61	578	2.5	550	1.0	219	558
HMR-67	450	1.6	581	2.8	354	211
HMR-68	591	3.0	675	2.7	227	248
MR-70	445	1.5	502	0.7	344	738
HMR-72	500	1.7	602	2.5	359	246
HMR-104	542	1.5	540	2.0	361	270

Adsorbent Preparation and Characterization

High-Pressure Adsorption Isotherm at 250 °C



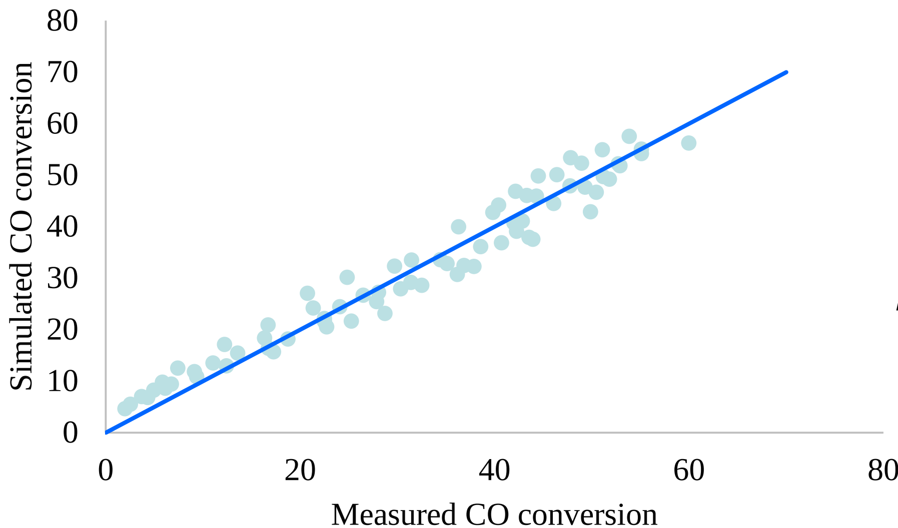
Lab-Scale Experimental Set-Up



Lab-Scale Experimental Results and Analysis

Co-Mo/Al_2O_3 Sour-Shift Catalyst Characterization

Global Reaction Kinetics- Empirical Model and Comparison with Microkinetc Models



$$-r_{co} = A\, e^{\frac{-E}{RT}}\, p_{co}^{a} p_{H_2O}^{b} p_{co_2}^{c} p_{H_2}^{d}\, (1-\beta)$$

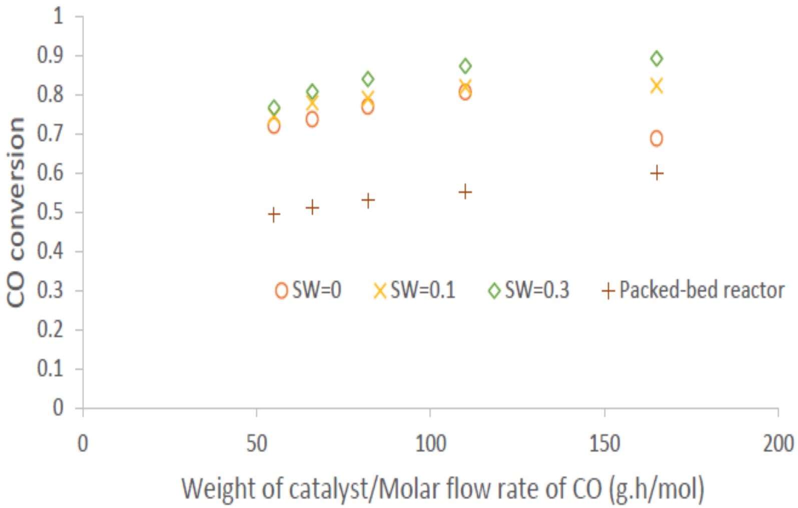
$$\beta = \frac{1}{K_{eq}} \frac{(P_{CO_2} . P_{H_2})}{(P_{CO} . P_{H_2O})} \quad K_{eq} = \exp\left(\frac{4577.8}{T} - 4.33\right)$$

Root-Mean-Square Deviation (RMSD)	
Direct oxidation	3.38
Associative	5.12
Formate intermediate	8.04
Empirical model	3.32

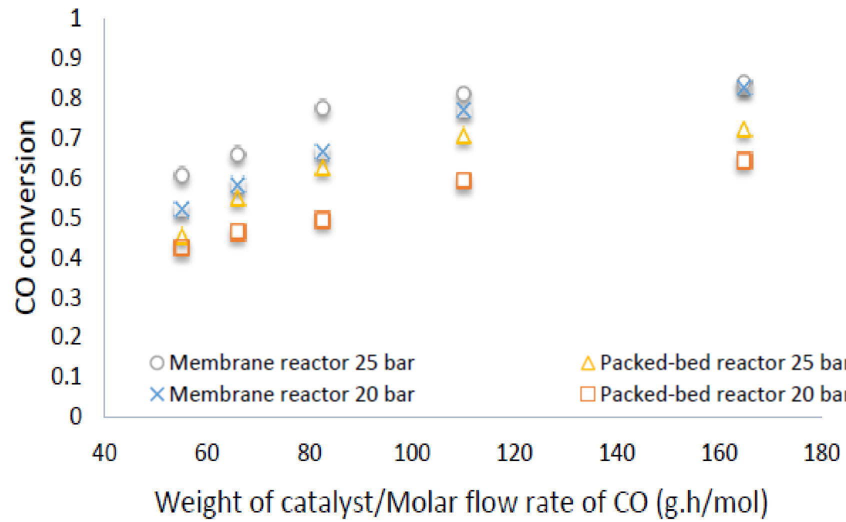
A[mol/(atm$^{(a+b+c+d)}$ · h · g)]	**18957**
E [J/mol]	58074
a	4
b	-1.46
c	0.13
d	-1.44

Lab-Scale Experimental Results and Analysis, Cont.

Experimental Conversion vs. W/F_{CO} for MR and PBR



Conversion of MR and PBR with three different steam sweep ratios (300 ºC, feed pressure of 15 bar, CMS#1)

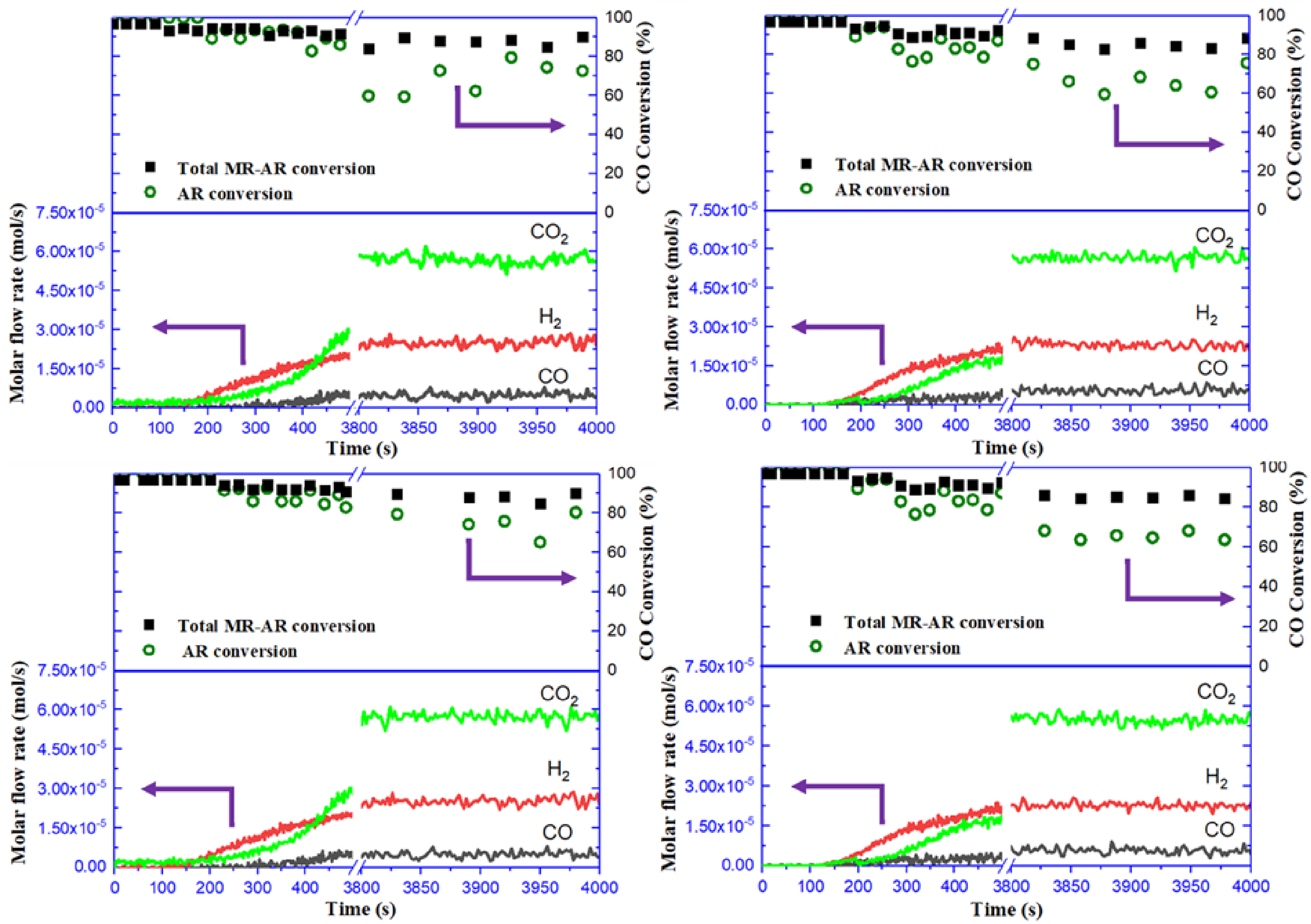


Conversion of MR and PBR with no sweep (250 ºC, feed pressure of 20 and 25 bar, CMS#2)

$$X_{CO} = \frac{n^F_{COo} - (n^F_{CO,exit} + n^P_{CO,exit})}{n^F_{COo}}$$

Lab-Scale Experimental Results and Analysis, Cont.

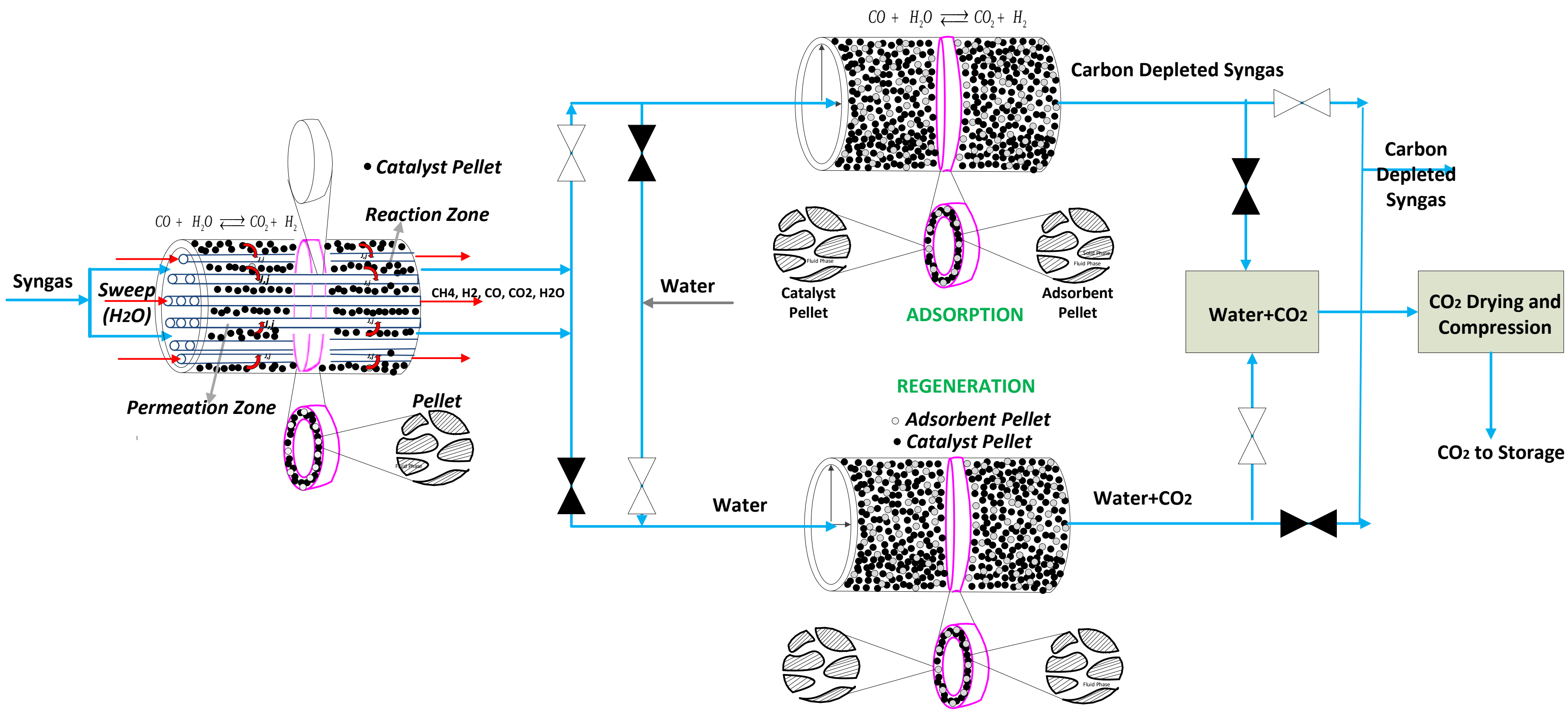
Experimental Results of MR-AR Performance



CO in the AR and total MR-AR conversion, and species molar flow rates. (Left Top) AR I, first cycle, (Right Top) AR II, first cycle, (Left Bottom) AR I, second cycle, (Right Bottom) AR II, second cycle. Temp.=250 °C, pressure=25 bar, H_2O/CO ratio=2.8, W/F_{CO}=55 g·h/mol.

Multi-Scale MR-AR Model for Process Scale-Up

Membrane Reactor (MR)/Adsorptive Reactor (AR) Sequence



Multi-Scale MR-AR Model for Process Scale-Up – MR System

Pellet-scale Model Equations & Boundary Conditions

Constitutive laws

Continuity Equation:

$$\vec{\nabla}\cdot\left(\varepsilon_A^p c_f^p \overrightarrow{v_f^p}\right)=\sum_{j=1}^{n_s}\left(1-\varepsilon_v^p\right)\rho_s^p\sum_{k=1}^{n_R}R_k v_{jk}$$

Component mass conservation:

$$\vec{\nabla}\cdot\left(\varepsilon_A^p x_j^p c_f^p \overrightarrow{v_f^p}\right)+\vec{\nabla}\cdot\left(\varepsilon_A^p \overrightarrow{n_j^p}\right)=\left(1-\varepsilon_v^p\right)\rho_s^p\sum_{k=1}^{n_R}R_k v_{jk}$$

Energy conservation:

$$\left(\sum_{j=1}^{n_s}\varepsilon_A^p x_j^p c_f^p C_j^p\right)\overrightarrow{v_f^p}\cdot\left(\vec{\nabla}T^p\right)=\vec{\nabla}\cdot\left(\lambda\vec{\nabla}T^p\right)+\left(1-\varepsilon_v^p\right)\rho_s^p\left(\sum_{k=1}^{n_R}-\Delta H_{R,k}R_k\right)$$

Initial Conditions:

$$\left.\begin{array}{l} x_j^p=0 \\ \overrightarrow{n_j^p}=0 \\ T^p=T^r=T_{in} \\ p^p=0 \\ Q_r=-\lambda\vec{\nabla}T^p=0 \\ \vec{\nabla}p^p=0 \end{array}\right\} \textit{for } t=0,\ \forall r \quad (30)$$

Boundary Conditions:

$$\left.\begin{array}{l} \overrightarrow{n_j^p}=0 \\ Q_r=-\lambda\vec{\nabla}T^p=0 \\ \vec{\nabla}p^p=0 \end{array}\right\} \textit{for } r=0$$

$$\left.\begin{array}{l} \left(1-\varepsilon_V^r\right)\eta_j\rho_s\sum_{k=1}^{n_s}R_k v_{jk}=\overrightarrow{n_j^p}+x_j^p c_f^p\overrightarrow{v_f^p} \\ -h\left(T^r-T^p\right)=Q_r+\left(\sum_{j=1}^{n_s}x_j^p c_f^p C_j^p\right)\overrightarrow{v_f^p}T^p \\ x_j^p=x_j^r \\ p^p=p^r \end{array}\right\} \textit{for } r=r^p$$

Reactor-scale Reaction Zone Model Equations & Boundary Conditions

Bulk Gas Constitutive laws

Continuity Equation:

$$\vec{\nabla}\cdot\left(\varepsilon_A^r c_f^r \overrightarrow{v_f^r}\right)=\sum_{j=1}^{n_s}\beta_{cat}\left(1-\varepsilon_v^r\right)\eta_j\rho_s^r\sum_{k=1}^{n_R}R_k v_{jk}-\frac{2}{R_{mem}}\sum_{j=1}^{N_s}J_j^{perm}$$

Component mass conservation:

$$\vec{\nabla}\cdot\left(\varepsilon_A^r x_j^r c_f^r \overrightarrow{v_f^r}\right)+\vec{\nabla}\cdot\left(\varepsilon_A^r \overrightarrow{n_j^r}\right)=\beta_{cat}\left(1-\varepsilon_v^r\right)\eta_j\rho_s^r\sum_{k=1}^{n_R}R_k v_{jk}-\frac{2}{R_{mem}}J_j^{perm}$$

Energy conservation:

$$\left\{\begin{array}{l} \left(\varepsilon_A^r\sum_{j=1}^{n_s}x_j^r c_j^r C_j^r\right)\overrightarrow{v_f^r}\cdot\left(\vec{\nabla}T^r\right)-\vec{\nabla}\cdot\left(\lambda'\vec{\nabla}T^r\right)+\frac{A^{SM}}{V^r}J_j^{perm}\left(H_j^r-H_j^{perm}\right)= \\ a_{cat}h_{cat}\left(T^r-\left(T^{cat}\right)^s\right)+a_{qua}h_{qua}\left(T^r-\left(T^{qua}\right)^s\right)-\frac{A^{SM}U'}{V^r}\left(T^r-T^{perm}\right)+\frac{4U}{d_t}\left(T^{fur}-T^r\right) \end{array}\right\}$$

Initial Conditions:

$$\left.\begin{array}{l} x_j^r=0 \\ T^r=T_{in}^r \\ p^r=p_{in}^r \end{array}\right\} \textit{for } t=0,\ \forall z \quad (35)$$

Boundary Conditions:

$$\left.\begin{array}{l} \overrightarrow{v_f^r}=\left(\overrightarrow{v_f^r}\right)_{in} \\ p^r=p_{in}^r \\ \overrightarrow{x_f^r}=\left(\overrightarrow{x_f^r}\right)_{in} \\ T^r=T_{in}^r \end{array}\right\} \textit{for } z=0$$

$$\left.\begin{array}{l} \vec{\nabla}T^r=0 \\ \overrightarrow{n_j^r}=0 \\ \vec{\nabla}p^r=0 \end{array}\right\} \textit{for } z=L$$

Multi-Scale MR-AR Model for Process Scale-Up – MR System

MR Reactor-scale Permeation Zone Model Equations

Bulk Gas Constitutive laws

Continuity Equation:

$$\vec{\nabla}\cdot\left(c_f^{perm}\overrightarrow{v_f^{perm}}\right)=\frac{2}{R_{mem}}\sum_{j=1}^{N_s}J_j^{perm}$$

Component mass conservation:

$$\vec{\nabla}\cdot\left(x_j^{perm}c_f^{perm}\overrightarrow{v_f^{perm}}\right)=\frac{2}{R_{mem}}J_j^{perm}$$

Energy conservation:

$$\left\{\begin{aligned}&\left(\sum_{j=1}^{n_s}x_j^{perm}c_f^{perm}C_j^{perm}\right)\overrightarrow{v_f^{perm}}\cdot\left(\vec{\nabla}T^{perm}\right)=\\&=\vec{\nabla}\cdot\left(\lambda''\vec{\nabla}T^{perm}\right)+\frac{A^{SM}U'}{V^{perm}}\left(T^r-T^{perm}\right)+\frac{A^{SM}}{V^{perm}}J_j^{perm}\left(H_j^r-H_j^{perm}\right)\end{aligned}\right\}$$

Initial Conditions:

$$\left.\begin{aligned}x_j^{perm}&=0\\T^{perm}&=T_{in}^{perm}\\p^{perm}&=p_{in}^{perm}\end{aligned}\right\}\ for\ t=0,\ \forall z\quad(47)$$

Boundary Conditions:

$$\left.\begin{aligned}\overrightarrow{v_f^{perm}}&=\left(\overrightarrow{v_f^{perm}}\right)_{in}\\p^{perm}&=p_{in}^{perm}\\\overrightarrow{x_f^r}&=\left(\overrightarrow{x_f^r}\right)_{in}\\T^r&=T_{in}^{perm}\end{aligned}\right\}\ for\ z=0$$

$$\left.\begin{aligned}\vec{\nabla}T^{perm}&=0\\\vec{\nabla}p^{perm}&=0\end{aligned}\right\}\ for\ z=L$$

Dusty Gas Model

$$-\frac{1}{\sum_{j=1}^{N_s}c_j}\sum_{\substack{j=1\\j\neq i,p}}^{N_s}\left(\frac{c_j}{D_{ij}^{eff}}\overrightarrow{N_i}-\frac{c_j}{D_{ij}^{eff}}\overrightarrow{N_j}\right)-\frac{\overrightarrow{N_i}}{D_{iK}^{eff}}=\vec{\nabla}c_i+\frac{c_i}{\sum_{i=1}^{N_s}c_i\,RT}\left(1+\frac{p}{D_{iK}^{eff}}\frac{B_O}{\mu_f}\right)\vec{\nabla}p$$

The Stefan-Maxwell Equation

$$\vec{\nabla}x_i=\sum_{j=1}^{N_s}\frac{x_i\,x_j}{D_{ij}^{eff}}\left(\frac{1}{\rho_j}\overrightarrow{J_j}-\frac{1}{\rho_i}\overrightarrow{J_i}\right)+\left(w_i-x_i\right)\left(\frac{\vec{\nabla}p}{p}\right)+\sum_{j=1}^{N_s}\frac{x_i\,x_j}{\rho_f D_{ij}^{eff}}\left(\frac{D_j^T}{w_j}-\frac{D_i^T}{w_i}\right)\left(\frac{\vec{\nabla}T}{T}\right)$$

Momentum Equation

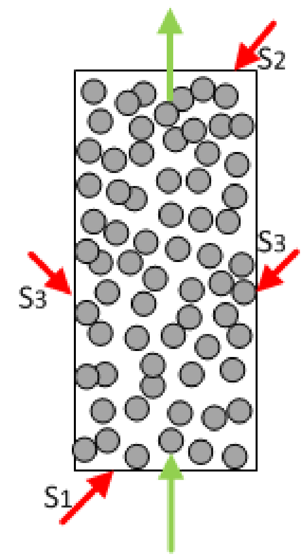
$$\vec{\nabla}P^r=-K_D\overrightarrow{v_f^r}-K_v\overrightarrow{v_f^r}^2=\vec{\nabla}p^r=\left(-150\frac{\left(1-\varepsilon_V^r\right)^2}{\left(\varepsilon_V^r\right)^3 d_p^{\,2}}-\mu_f^r 1.75\frac{\left(1-\varepsilon_V^r\right)}{\left(\varepsilon_V^r\right)^3 d_p}\rho_f^r\left|\overrightarrow{v_f^r}\right|\right)\overrightarrow{v_f^r}$$

Multi-Scale MR-AR Model for Process Scale-Up – AR System

Component Mass Balances

$$\frac{\partial}{\partial t}\left(\varepsilon^{r}_{tot.gas} c^{r}_{j}\right) + \vec{\nabla}\cdot\left(\vec{v}^{r}_{f} c^{r}_{j}\right) = \varepsilon_{gas\cdot bed}\vec{\nabla} D_{z,i}\left(\vec{\nabla} c^{r}_{j}\right) + \left(1-\varepsilon_{gas\cdot bed}\right)\eta_{j}\beta_{cat}\rho_{cat}R_{j} - \left(1-\varepsilon_{gas\cdot bed}\right)\phi_{ad}\rho_{ad}R_{ad}$$

$$\beta_{cat} + \phi_{ad} + \varphi_{qua} = 1$$



Energy balance:

$$\left\{\begin{aligned}
&\left\{\begin{aligned}
&\left(\left(1-\varepsilon_{gas\cdot bed}\right)\beta_{cat}\rho^{r}_{c}C^{r}_{c} + \left(1-\varepsilon_{gas\cdot bed}\right)\phi_{ad}\rho^{r}_{ad}C^{r}_{ad} + \left(1-\varepsilon_{gas\cdot bed}\right)\varphi_{qua}\rho^{r}_{qua}C^{r}_{qua} + \sum_{j=1}^{n_s}\varepsilon^{r}_{tot.gas}c^{r}_{j}C^{r}_{j}\right)\frac{\partial T^{r}}{\partial t} + \\
&\left(\varepsilon^{r}_{A}\sum_{j=1}^{n_s}c^{r}_{j}C^{r}_{j}\right)\vec{v}^{r}_{f}\cdot\left(\vec{\nabla}T^{r}\right)
\end{aligned}\right\} = \\
&= \vec{\nabla}\cdot\left(\lambda^{r}\vec{\nabla}T^{r}\right) + \left(1-\varepsilon_{gas\cdot bed}\right)\eta_{j}\beta_{cat}\rho_{cat}\sum_{j=1}^{n_s}H_{j}R_{j} - \left(1-\varepsilon_{gas\cdot bed}\right)\phi_{ad}\rho_{ad}\Delta H_{ad}R_{ad} + \frac{4h_{w}}{d_{t}}\left(T_{w}-T^{r}\right)
\end{aligned}\right\}$$

$$\left\{\begin{aligned}
&\rho_{w}C_{w}\frac{\partial T_{w}}{\partial t} = \frac{d_{t}}{\left(w_{thick}\left(d_{t}+w_{thick}\right)\right)}h_{w}\left(T_{w}-T^{r}\right) - \frac{U\left(T_{w}-T_{fur}\right)}{\left(d_{t}+w_{thick}\right)\cdot\ln\left(\dfrac{\left(d_{t}+w_{thick}\right)}{d_{t}}\right)} \\
&\frac{\lambda_{z}}{\lambda_{g}} = \frac{\lambda^{0}_{z}}{\lambda_{g}} + 0.75\cdot Pr\cdot Re_{p} \\
&\frac{\lambda^{0}_{z}}{\lambda_{g}} = \varepsilon^{r}_{tot.gas} + \frac{1-\varepsilon^{r}_{tot.gas}}{0.139\varepsilon_{gas\cdot bed} - 0.0339 + 2/3\left(\lambda_{g}/\lambda_{p}\right)} \\
&\frac{h_{w}d_{t}}{\lambda_{g}} = 2.03\cdot Re_{p}exp\left(-\frac{d_{p}}{d_{t}}\right)
\end{aligned}\right.$$

Momentum balance:

$$\vec{\nabla}P^{r} = -K_{D}\vec{v}^{r}_{f} - K_{v}\vec{v}^{r\,2}_{f} = \vec{\nabla}P^{r} = \left(-150\frac{\left(1-\varepsilon_{gas\cdot bed}\right)^{2}}{\left(\varepsilon_{gas\cdot bed}\right)^{3}d_{p}^{\,2}} - \mu^{r}_{f}1.75\frac{\left(1-\varepsilon_{gas\cdot bed}\right)}{\left(\varepsilon_{gas\cdot bed}\right)^{3}d_{p}}\rho^{r}_{f}\left|\vec{v}^{r}_{f}\right|\right)\vec{v}^{r}_{f}$$

Multi-Scale MR-AR Model for Process Scale-Up – AR System

Initial and boundary conditions for the AR model.

Initial Conditions:	*Boundary Conditions:*
$$\left.\begin{aligned} c_j^r &= 0 \\ T^r &= T_{in}^r \\ P^r &= P_{in}^r \end{aligned}\right\} \text{for } t=0,\ \forall z$$	$$\left.\begin{aligned} \vec{v}_f^r &= \left(\vec{v}_f^r\right)_{in} \\ P^r &= P_{in}^r \\ \vec{c}_j^r &= \left(\vec{c}_j^r\right)_{in} \\ T^r &= T_{in}^r \end{aligned}\right\} \text{for } z=0$$ $$\left.\begin{aligned} \vec{\nabla} T^r &= 0 \\ \vec{n}_j^r &= 0 \\ \vec{\nabla} P^r &= 0 \end{aligned}\right\} \text{for } z=L$$

Constitutive laws and other property equations.

Gas Law:

$$c_{TOT}^r = \frac{P}{ZRT}$$

Definitions:

$$\sum_{j=1}^{n_s} x_j = 1,\ c_{tot}^p = \sum_{j=1}^{n_s} c_j^r,\ P = \sum_{j=1}^{n_s} P_i,\ \beta_{cat} + \phi_{ad} + \varphi_{qua} = 1$$

Heat Flux (Fourier's Law):

$$Q = -\lambda \nabla T$$

Dimensionless Groups :

$$Nu = \frac{hd_p}{\lambda_g},\ Re_p = \frac{\vec{v}_f \rho_g d_p}{\mu_g},\ Pr = \frac{C_{p,g}\mu_g}{\lambda_g}$$

Viscosity of Gas Mixture :

$$\mu_g = \sum_{i=1}^{N_s} \frac{x_i \mu_i}{\sum_{j=1}^{N_s} x_i \phi_{ij}}, \qquad \phi_{ij} = \frac{\left[1 + \left(\mu_i/\mu_j\right)^{1/2}\left(M_j/M_i\right)^{1/4}\right]^2}{8\left(1 + \left(M_i/M_j\right)\right)^{1/2}}$$

Thermal Conductivity:

$$\lambda^r = \left(1-\varepsilon_v^r\right)\beta_{cat}\lambda_{cat} + \left(1-\varepsilon_v^r\right)\varphi_{qua}\lambda_{qua} + \left(1-\varepsilon_v^r\right)\phi_{ad}\lambda_{qua} + \varepsilon_v^r \lambda_g$$

Thermal Conductivity of Pure Gases:

$$\lambda_i = A_i + B_i T + C_i T^2 + D_i T^3$$

Thermal Conductivity of Gas Mixture:

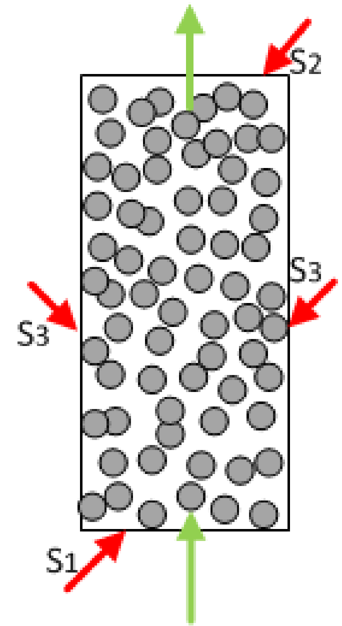
$$\lambda_g = \sum_{i=1}^{N_s} \frac{x_i \lambda_i}{\sum_{j=1}^{N_s} x_i \phi_{ij}}, \qquad \phi_{ij} = \frac{\left[1 + \left(\mu_i/\mu_j\right)^{1/2}\left(M_j/M_i\right)^{1/4}\right]^2}{8\left(1 + \left(M_i/M_j\right)\right)^{1/2}}$$

Specific Heat Capacity of Pure Gases:

$$C_i = a_{0,i} + a_{1,i}t + a_{2,i}t^2 + a_{3,i}t^3 + a_{4,i}/t^2,\quad t = \left(T/1000\right)$$

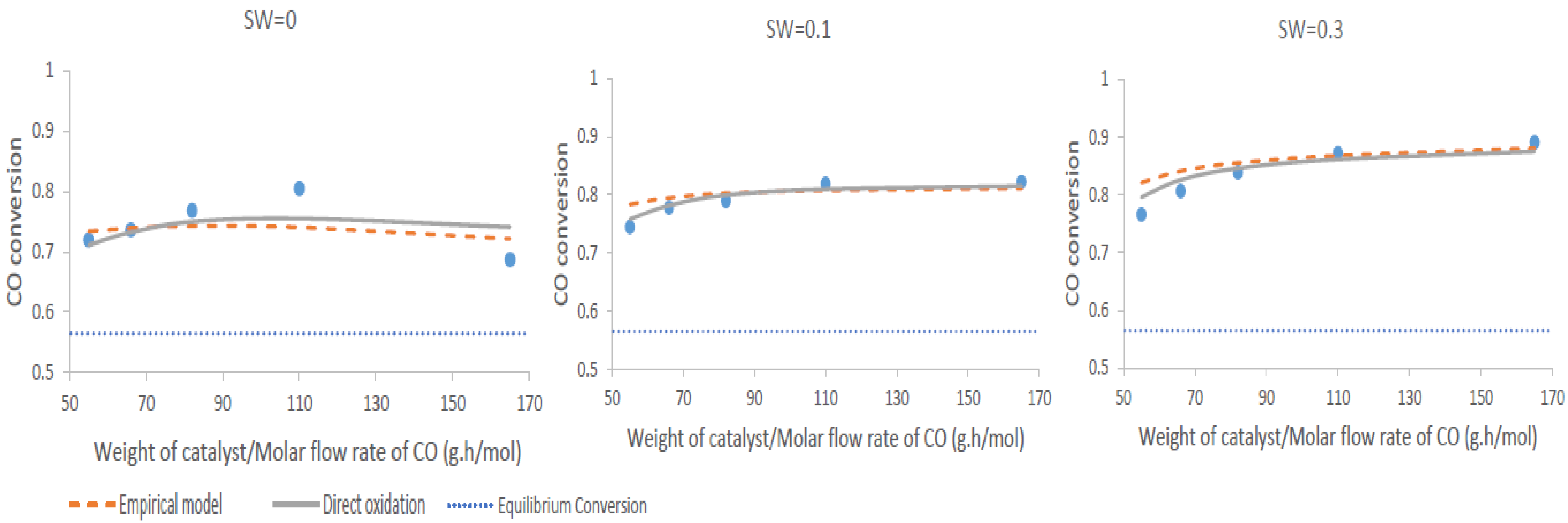
Specific Heat Capacity of Gas Mixture:

$$C_{p,g} = \sum_{i=1}^{N_s} \frac{x_i M_i C_{p,i}}{\sum_{j=1}^{N_s} x_i M_i}$$



Lab-Scale Experimental Results and Model Fits - MR

Experimental Conversion for Various Sweep Ratios and Model Predictions

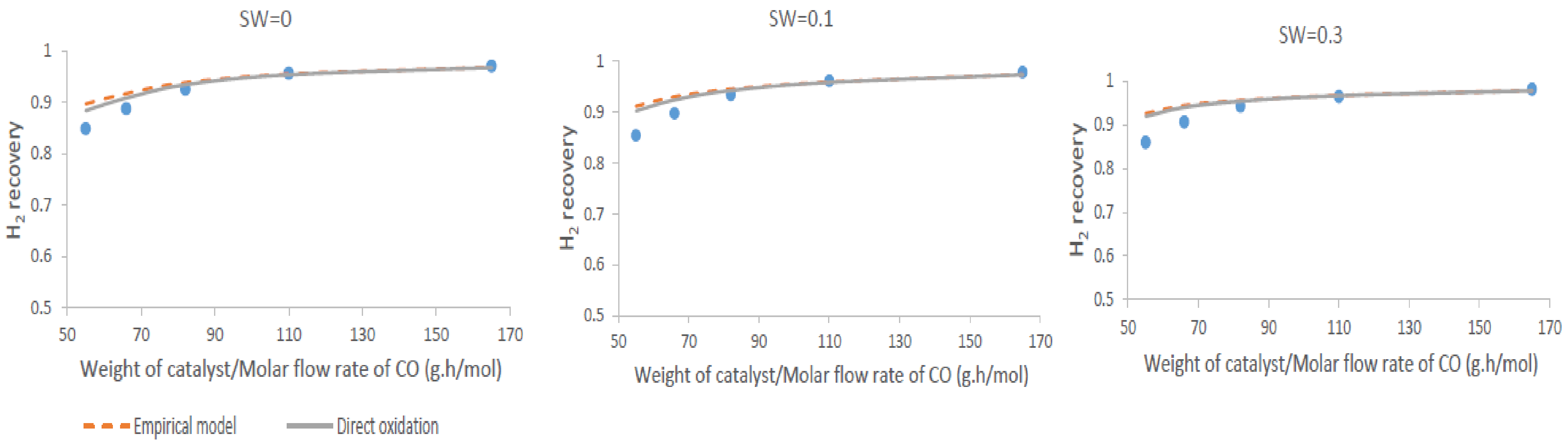


Experimental conversion for the MR with different sweep ratios and the corresponding MR model fits using both the empirical and microkinetic models. (300 ºC, feed pressure of 15 bar, CMS#1)

$$X_{CO} = \frac{n^{F}_{COo} - (n^{F}_{CO,exit} + n^{P}_{CO,exit})}{n^{F}_{COo}}$$

Lab-Scale Experimental Results and Model Fits - MR

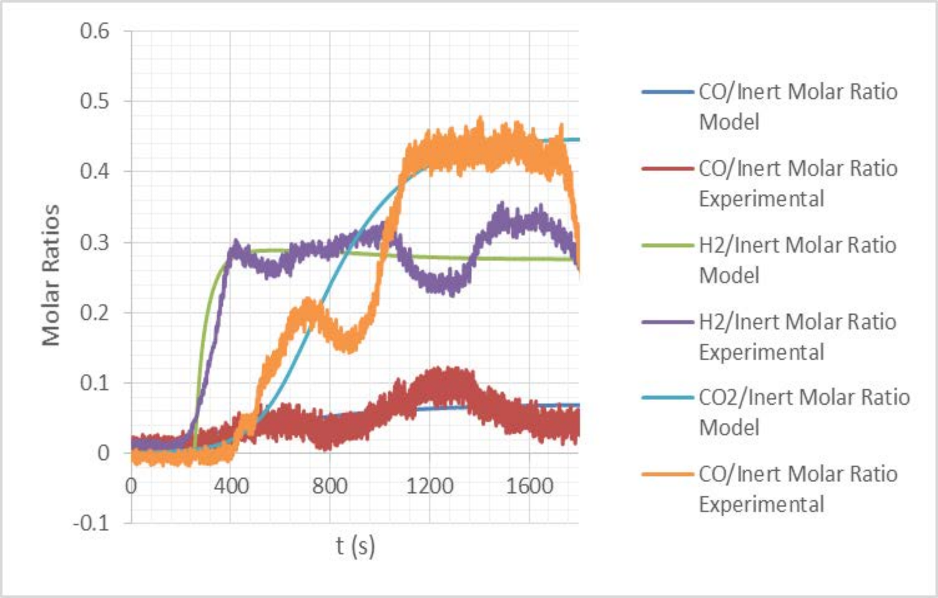
Experimental Hydrogen Recovery for Various Sweep Ratios and Model Predictions



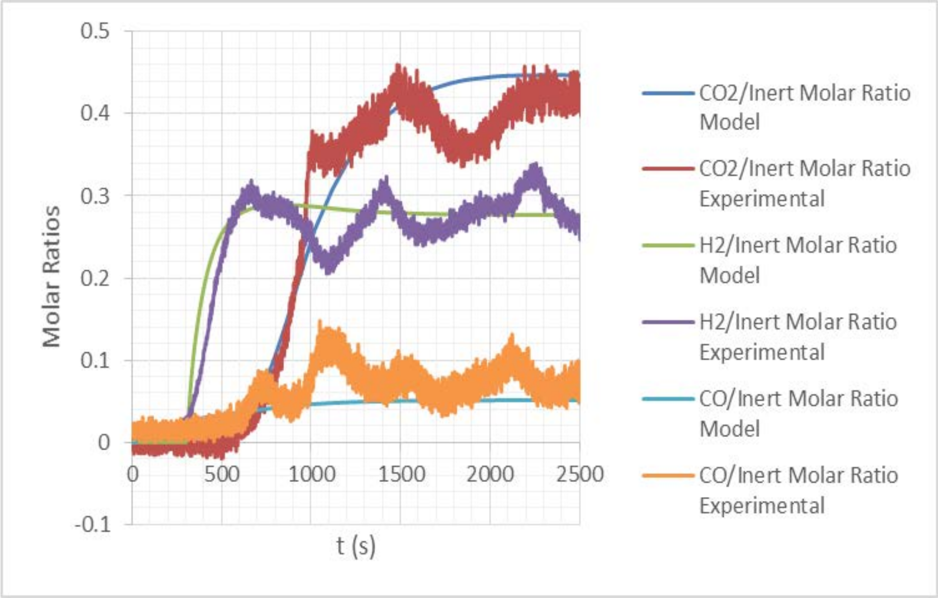
Experimental hydrogen recovery and the corresponding MR model fits using both the empirical and microkinetic models. (300 ⁰C, feed pressure of 15 bar, CMS#1)

$$Re_{H_2} = \frac{n^{P}_{H_2,exit}}{(n^{F}_{H_2,exit} + n^{P}_{H_2,exit})}$$

Lab-Scale Experimental Results and Model Fits - AR



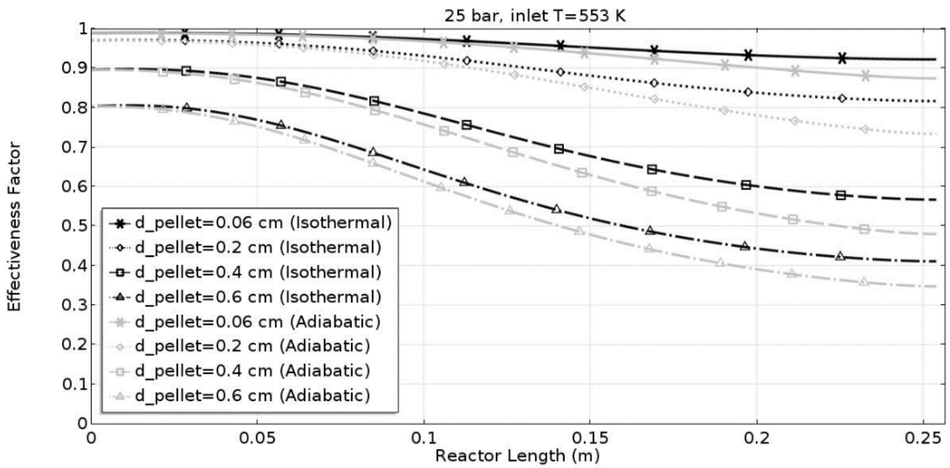
Temperature = 250 °C, Pressure = 15 bar.
(W_{cat}/F_{CO}=55 on MR)

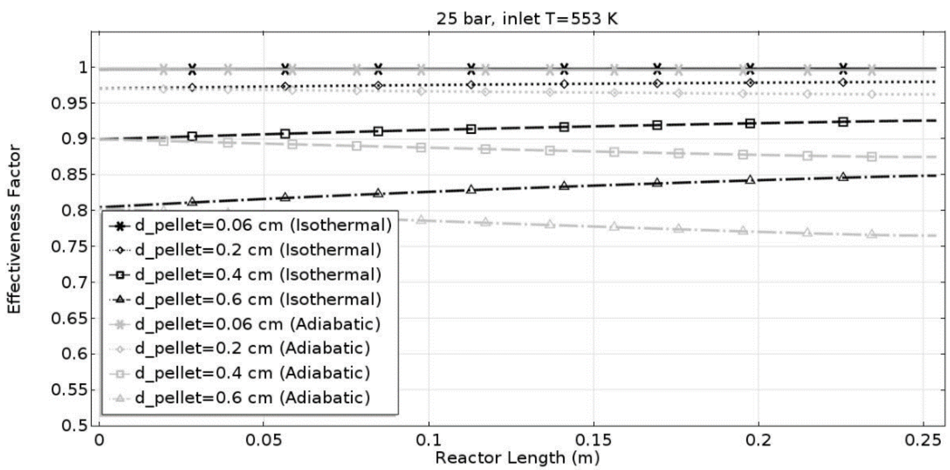


Temperature = 250 °C, Pressure = 15 bar.
(W_{cat}/F_{CO}=66 on MR)

Model Predictions for Industrial-Scale Systems

Axial Profiles of Catalyst Effectiveness Factors in MR (Top) and PBR (Bottom)



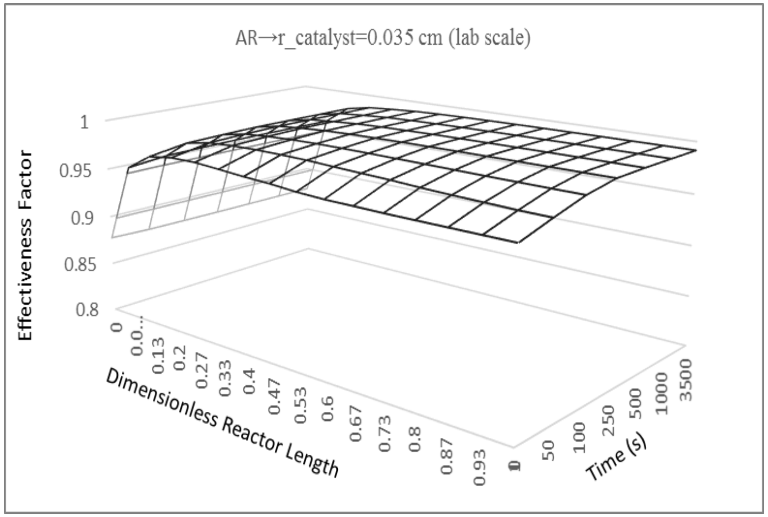


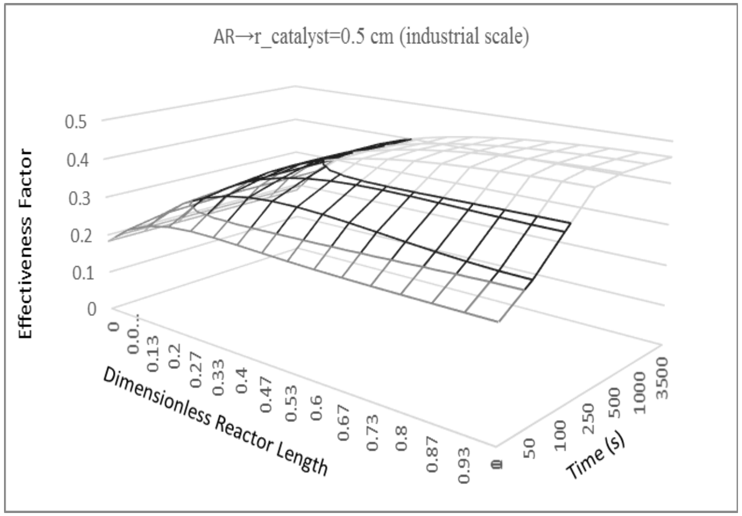
Key Results

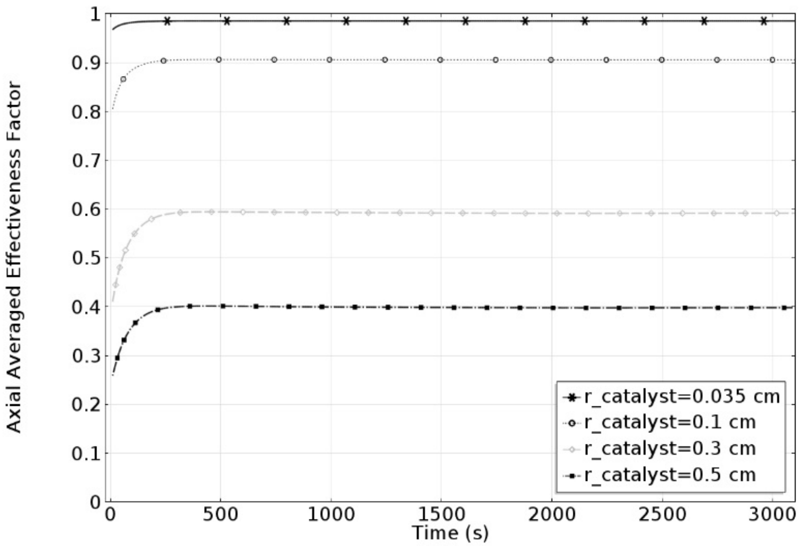
- Catalyst effectiveness factors in PBR and MR vary significantly along reactor length
- Catalyst pellets of same diameter exhibit different effectiveness factors
- Sweep gas pressure/temperature and membrane area have a significant impact on MR behavior
- The adiabatic MR gives higher conversion values as compared to the wall-isothermal MR for the same operating conditions.

Model Predictions for Industrial-Scale Systems

Catalyst Effectiveness Factor Profiles in AR

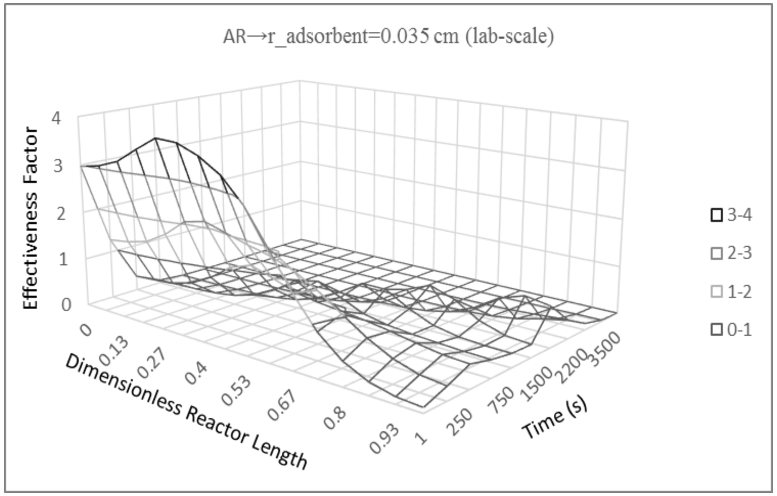


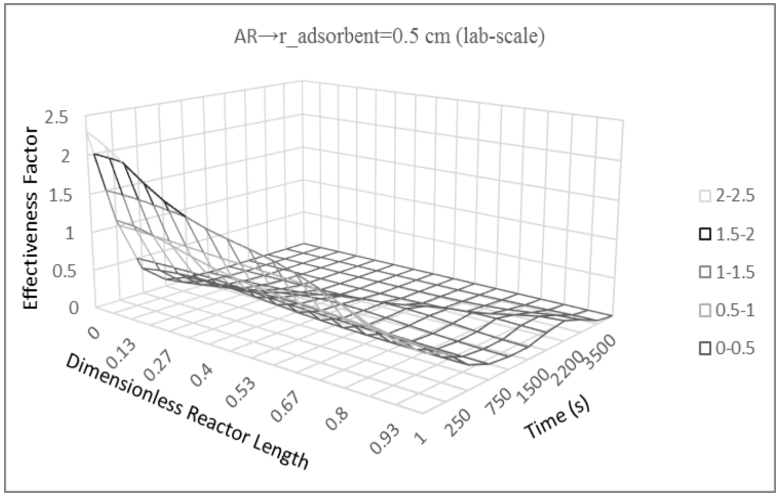


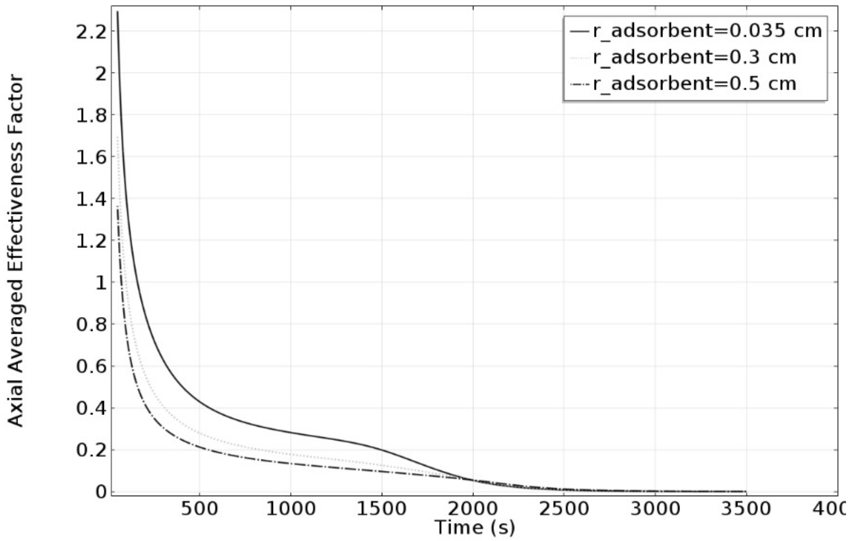


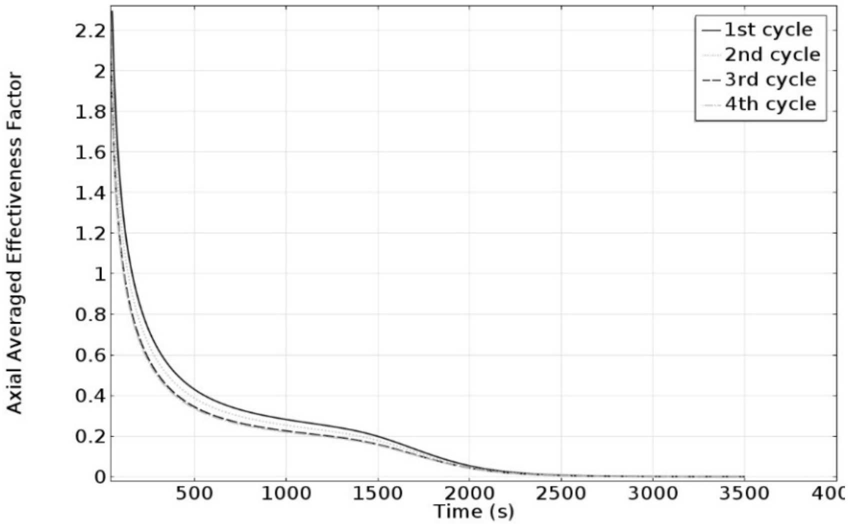
Model Predictions for Industrial-Scale Systems

Adsorbent Effectiveness Factor Profiles in AR

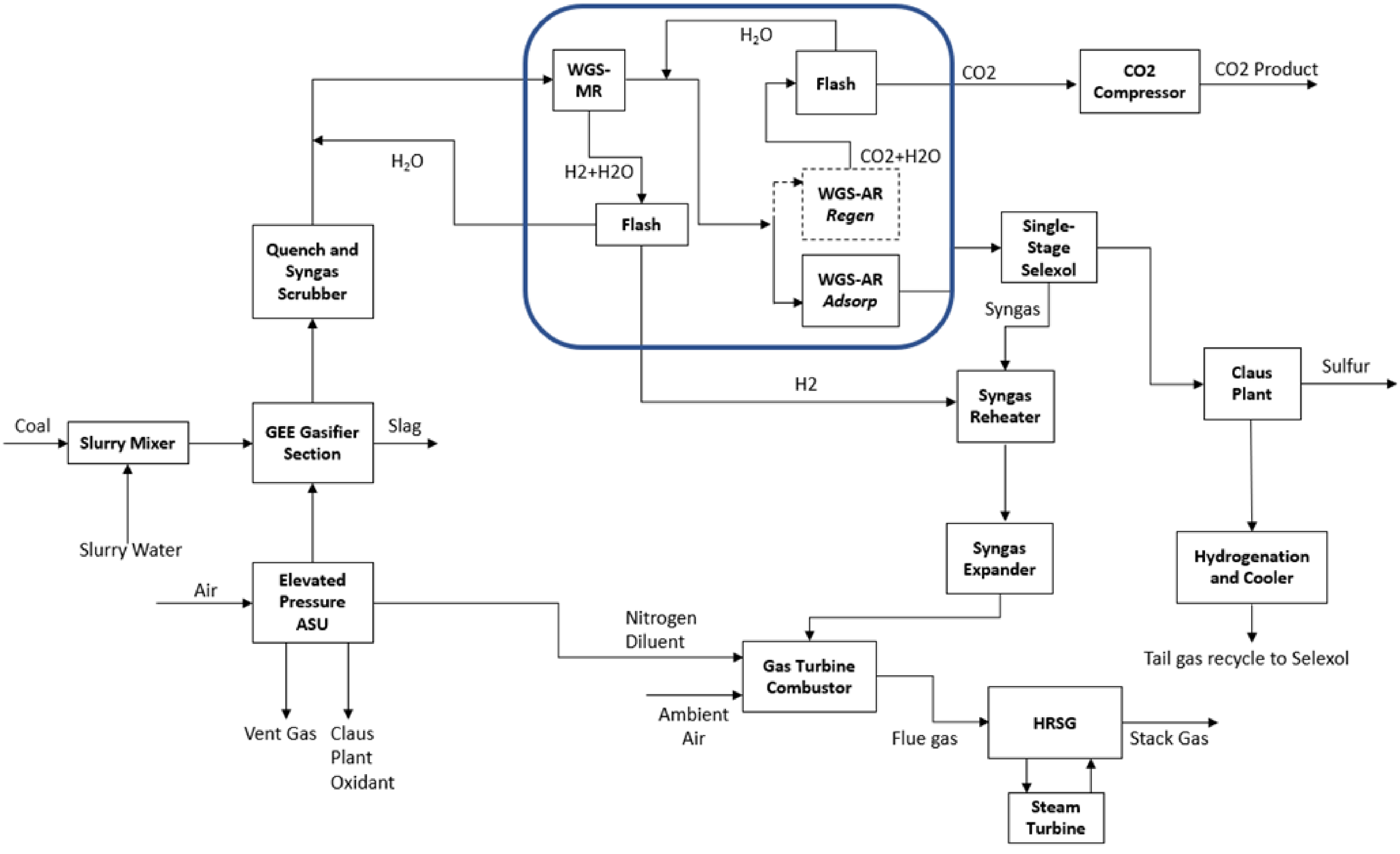








Preliminary TEA - MR-AR IGCC Process Scheme



Preliminary TEA - CAPEX/OPEX of the MR-AR Process

Capital Cost Analysis of the MR-AR IGCC Process

Item No.	Description	Equipment Cost	Material Cost	Labor Direct	Labor Indirect	Bare Erected Cost	Eng'g CM H.O.& Fee	Contingencies Process	Contingencies Project	Total Plant Cost $/1,000	Total Plant Cost $/kW
	5A	Gas Cleanup & Piping									
5A.1	Single Stage Selexol	$27,889	$0	$23,502	0	$51,391	$5139	$0	$11,306	$67,836	$117
5A.2	Elemental Sulfur Plant	$12,451	$2,427	$15,954	$0	$30,833	$3,083	$0	$6,783	$40,699	$70
5A.3	Mercury Removal	$1,973	$0	$1,491	$0	$3,464	$346	$173	$797	$4,780	$8
5A.4	Reactor Vessels (MR+AR)	$2,415	$0	$966	$0	$3,381	$338	$0	$744	$4,463	$8
5A.5	Membrane Pack	$20,241	$0	w/equip	$0	$20,241	$2,024	$0	$4,452	$26,717	$46
5A.6	Flash Separators	$690	$0	$276	$0	$966	$97	$0	$212	$1,275	$2
5A.7	Fuel Gas Piping	$0	$812	$531	$0	$1,344	$134	$0	$296	$1,774	$3
5A.9	HGCU Foundations	$0	$735	$495	$0	$1,231	$123	$0	$406	$1,760	$3
	Subtotal	**$65,659**	**$3,974**	**$43,215**	**$0**	**$112,851**	**$11,284**	**$173**	**$24,996**	**$149,304**	**$258**
	5B	CO_2 Compression									
5B.2	CO_2 Compression & Drying	$5,126	$769	$2220	0	$8,115	$811	0	$1,785	$10,711	$18
	Subtotal	**$5,126**	**$769**	**$2220**	**0**	**$8,115**	**$811**	**0**	**$1,785**	**$10,711**	**$18**
	Capital Cost Total	**$819,238**	**$93,474**	**$302,270**	**$0**	**$1,214,986**	**$121,497**	**$45,482**	**$212,551**	**$1,594,515**	**$2,754**

Operating Cost Analysis of the MR-AR IGCC Process

Variable Operating Costs					
	Consumption				**Cost ($)**
	Initial	**Daily**	**Per Unit**	**Initial Fill**	
Water (/1000 gallons):	0	4,201	$1.67	$0	$2,053,253
Makeup and Waste Water Treatment Chemicals (lbs)	0	25,026	$0.27	$0	$1,957,230
Carbon (Mercury Removal) (lb):	135,182	231	$5.50	$743,501	$371,751
Shift Catalyst (ft^3):	5,452	3.39	$610.9	$3,816,105	$763,221
Adsorbent (lb)	910,368	0.81	$145.7	$910,368	$182,074
Selexol Solution (gal):	242,554	36	$36.79	$8,923,873	$386,554
Claus Catalyst (ft^3):	w/equip	2.01	$203.15	$0	$119,487
Subtotal:				**$14,393,847**	**$5,833,570**

Preliminary TEA - MR-AR IGCC Process

Differences in Performance between MR-AR and Baseline IGCC Plants

Performance Summary	Baseline IGCC with CCS (Case B5B)	MR-AR IGCC
Combustion Turbine Power, MWe	464	464
Sweet Gas Expander Power, MWe	7	4
Steam Turbine Power, MWe	264	264
Total Gross Power, MWe	**734**	**731**
CO_2 Compression, kWe	31,160	2,997
Hydrogen Compression, kWe	0	5,692
Water Pump, kWe	0	150
Acid Gas Removal, kWe	19,230	2,590
Total Auxiliaries, MWe	**191**	**152**
Net Power, MWe	**543**	**579**

COE Breakdown for the MR-AR and Baseline IGCC Plants

Baseline IGCC with CCS (Case B5B)		MR-AR IGCC	
COE Component	**Value, $/MWh**	**COE Component**	**Value, $/MWh**
Capital Cost	74.2	Capital Cost	60.3/(56.1)
Fixed Operating Cost	18.2	Fixed Operating Cost	17.1/(15.9)
Variable Operating Cost	12.2	Variable Operating Cost	9.8/(9.1)
Fuel Cost	30.7	Fuel Cost	28.8/(26.8)
Total COE	135.4	Total COE (N_2 sale)	51.4/(43.3)

Comparison in Performance between MR-AR and Baseline IGCC Plants

Designs	Net Power Production (MWe)	CO2 Capture (%)	CO2 Purity	COE ($/MWh)
IGCC w/o CCS (Case B5A)	622	0	n/a	102.6
IGCC w/ CCS–Dual Stage Selexol (Case B5B)	543	90	99	135.4
MR-AR IGCC Plant	588	90.6	99	51.4/(43.3)

Milestone Log – BP2

Budget Period	ID	Task	Description	Planned Completion Date	Actual Completion Date	Verification Method
2	i	5	Parametric testing of the integrated, lab-scale MR-AR system and identification of optimal operating conditions for long-term testing completed	9/30/2017	9/30/2017	Results reported in the quarterly report
2	j	5	Short-term (24 hr for initial screening) and long-term (>100 hr) hydrothermal and chemical stability (e.g., NH_3, H_2S, H_2O, etc.) materials evaluations at the anticipated process conditions completed	3/31/2018	3/31/2018	Results reported in the quarterly report
2	k	5	Integrated system modeling and data analysis completed	3/31/2018	3/31/2018	Results reported in the quarterly report
2	l	5	Materials optimization with respect to membrane permeance/selectivity and adsorbent working capacity at the anticipated process conditions (up to 300ºC for membranes and 300-450ºC for adsorbents, and up to 25 bar total pressure) completed	12/31/2018		Results reported in the quarterly report
2	m	5	Operation of the integrated lab-scale MR-AR system for at least 500 hr at the optimal operating conditions to evaluate material stability and process operability completed	12/31/2018		Results reported in the quarterly report
2	n	6	Preliminary process design and optimization based on integrated MR-AR experimental results completed	3/31/2019		Results reported in Final Report
2	o	6	Initial technical and economic feasibility study and sensitivity analysis completed	3/31/2019		Results reported in Final Report
1,2	QR	1	Quarterly report	Each quarter		Quarterly Report files
2	FR	1	Draft Final report	4/30/2019		Draft Final Report file

Success Criteria - BP2

Decision Point	Basis for Decision/Success Criteria
Completion of **Budget Period 2**	Successful completion of all work proposed in Budget Period 2.
	Completion of short-term (24 hr) and long-term (>100 hr) hydrothermal/chemical stability evaluations. Membranes/adsorbents are stable towards fuel gas constituents (e.g., NH_3, H_2S, H_2O) at the anticipated process operating conditions. Target <10% decline in performance over 100 hr of testing.
	Completion of integrated testing and system operated for >500 hr at optimal process conditions.
	Results of the initial technical and economic feasibility study show significant progress toward achievement of the overall fossil energy performance goals of 90% CO_2 capture rate with 95% CO_2 purity at a cost of electricity 30% less than baseline capture approaches
	Submission of updated membrane and adsorbent state-point data tables based on the results of integrated lab-scale MR-AR testing
	Submission of a Final Report

Acknowledgements

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