BENCH-SCALE TESTING OF A HIGH EFFICIENCY, ULTRA-COMPACT PROCESS FOR PRE-COMBUSTION CO_2 CAPTURE

DE-FE 0031737

Professor Theo Tsotsis, University of Southern California, Los Angeles, CA

Professor Vasilios Manousiouthakis, University of California, Los Angeles, CA

Dr. Rich Ciora, Mr. Doug Parsley, Media and Process Technology Inc., Pittsburgh, PA

PRESENTER: Vasilios Manousiouthakis

U.S. Department of Energy

National Energy Technology Laboratory

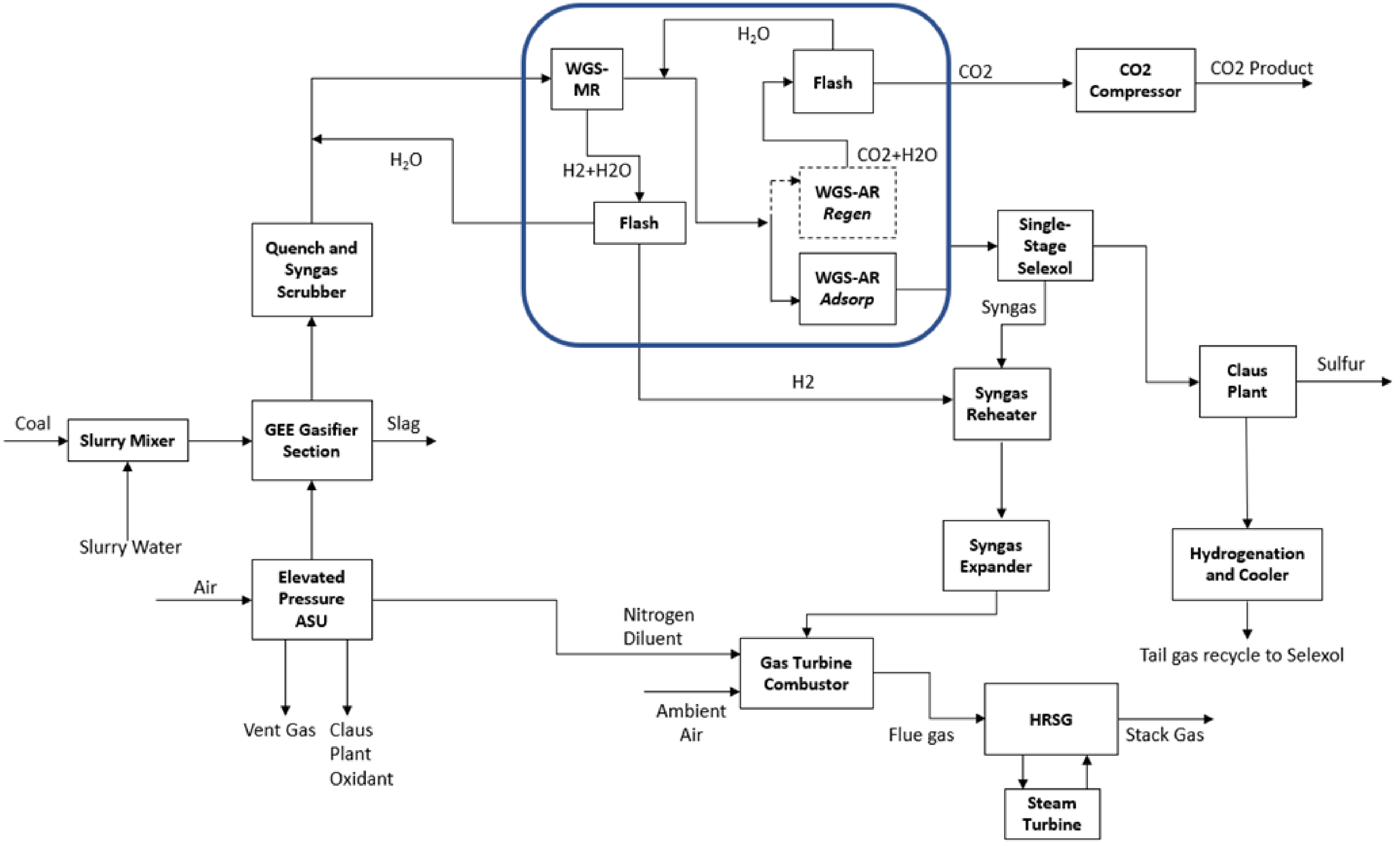
Office of Fossil Energy

2022 Carbon Management Project Review Meeting

August 19, 2022

Overview

Process Scheme: MR-AR IGCC

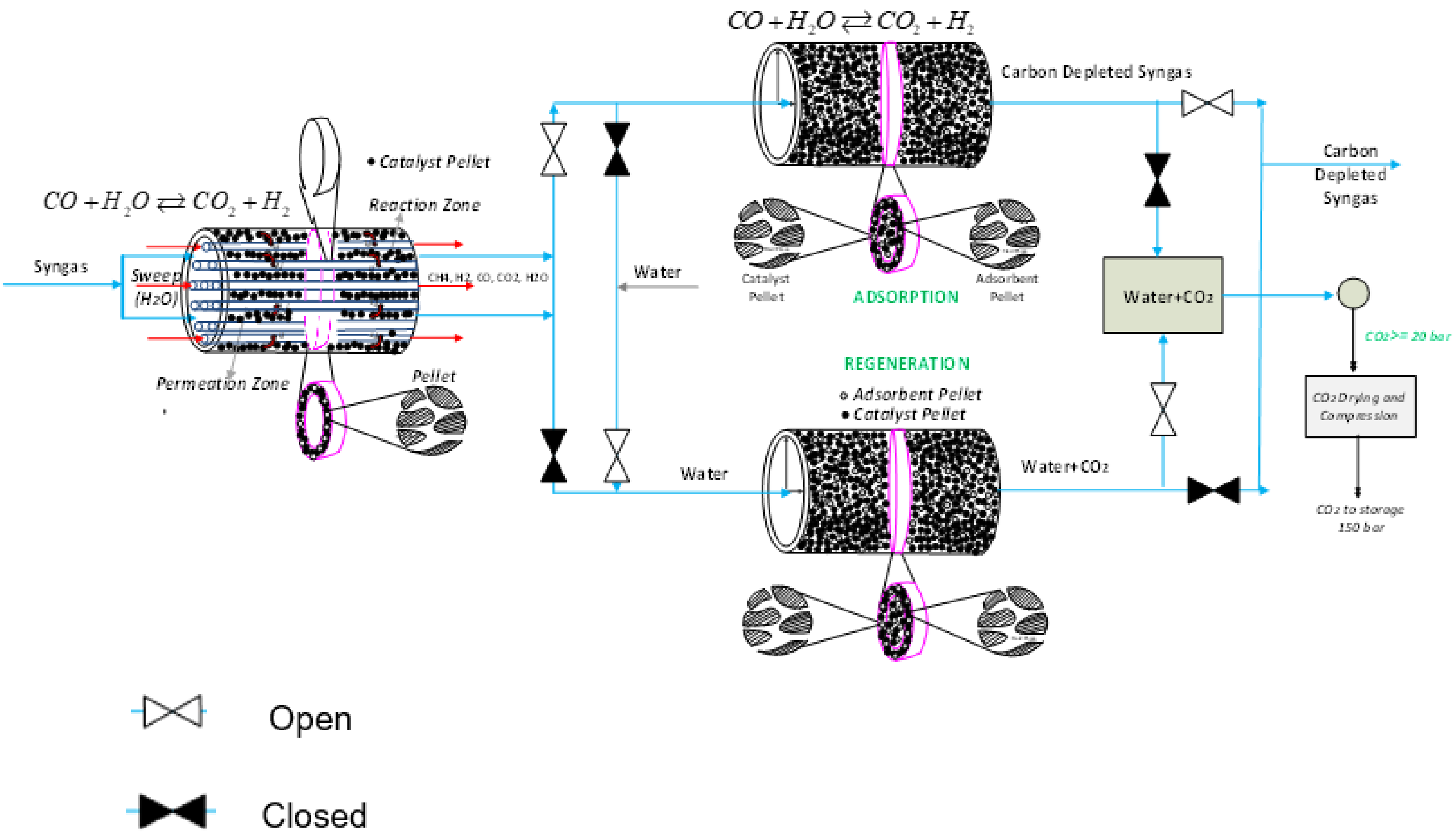


MR-AR Technology: Key departures from baseline

- WGS occurs in MR and AR with simultaneous H_2 and CO_2 removal respectively
- Steam is used as a sweep medium for product evacuation
- Single stage Selexol for H_2S removal only.
- Steam is used as diluent in the combustion turbine.
- Potential N_2, Ar sales to further boost plant economics

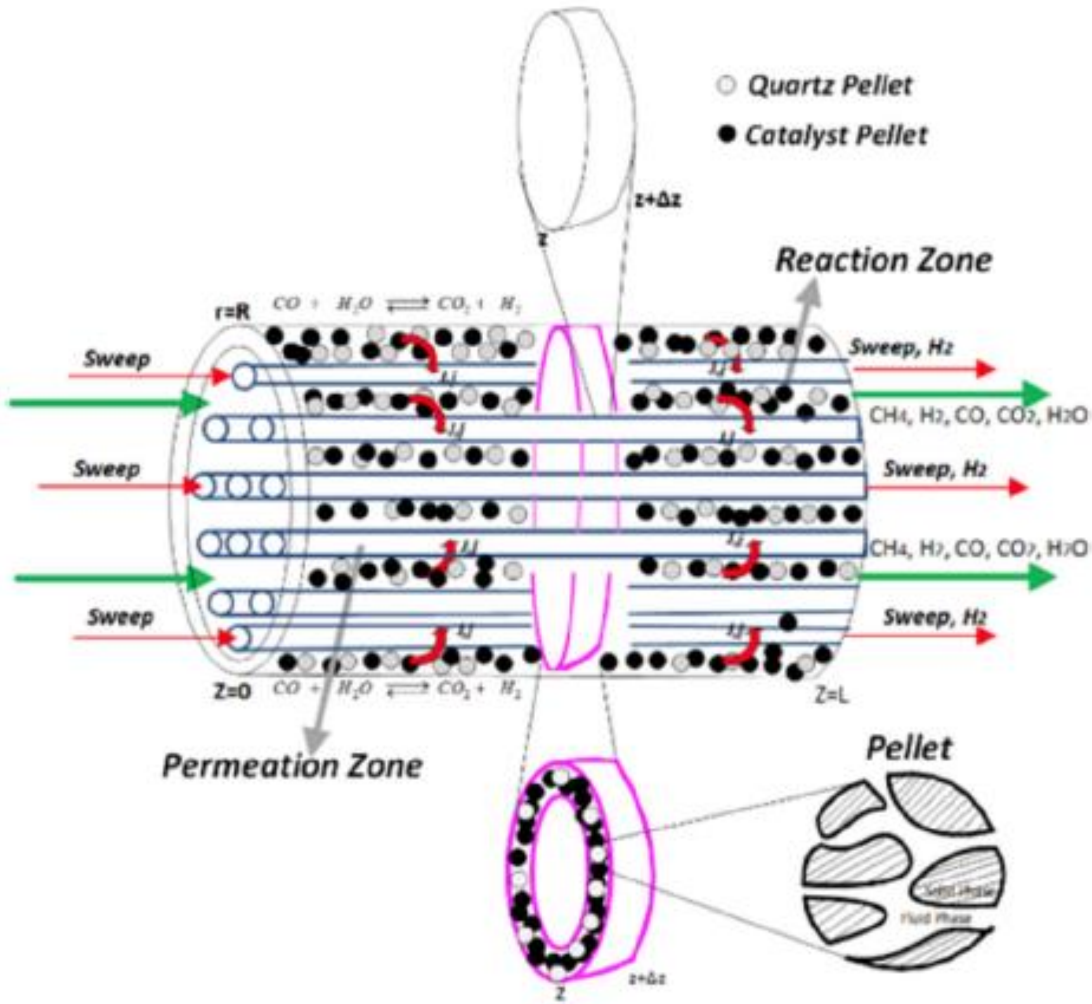
Baseline reference case is Case B5B of the reference document "Cost and Performance Baseline for Fossil Energy Plants – Volume 1: Bituminous Coal and Natural Gas to Electricity. September 24, 2019)"

MR-AR Process Schematic



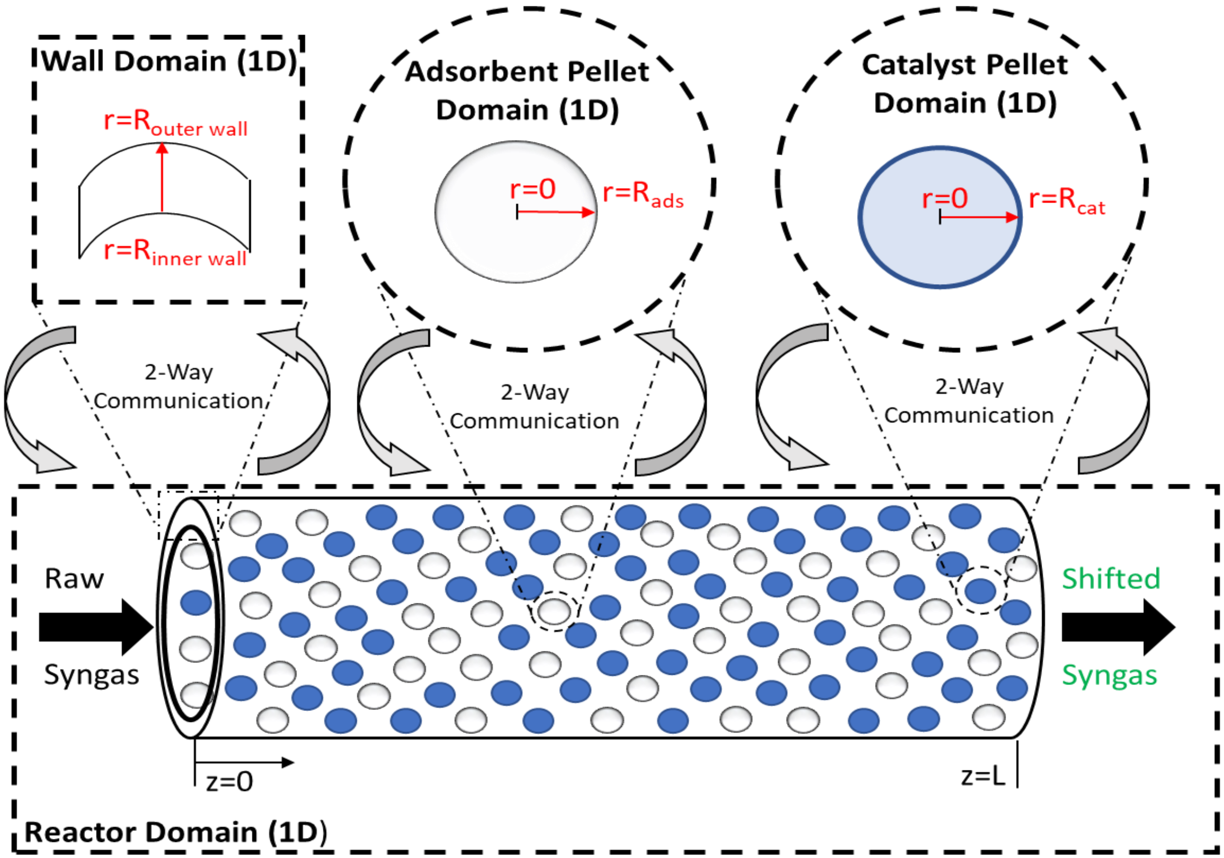
MR-AR multidomain multiscale model

MR Model



MR Multidomain Modeling Concept

AR Model



AR Multidomain Modeling Concept

MR Multiscale Equations (Reactor fluid domain)

Species Mass Balance:

$$R_{i,f}^{r} - N_T \frac{A^{per}}{V^r} \overrightarrow{N_{i,f}^{per}}\Big|_{surface}^{mem} = \frac{\partial}{\partial t}\left(w_{i,f}^{r}\phi_V \rho_f^r\right) + \vec{\nabla}\cdot\left(\phi_A \overrightarrow{N_{i,f}^{r}}\right) \qquad i = 1, n$$

Momentum conservation:

$$-\vec{\nabla}\left(\phi_A p_f^r\right) = \phi_A \left(150 \frac{(1-\phi_V)^2 \mu_f^r}{d_{pellet}^2 \phi_V^3} \overrightarrow{v_f^r} + \frac{1.75(1-\phi_V)\rho_f^r}{d_{pellet}\phi_V^3} \overrightarrow{v_f^r}\,\overrightarrow{v_f^r}\right) + \frac{\partial}{\partial t}\left(\phi_V \overrightarrow{v_f^r} \rho_f^r\right)$$
$$+\vec{\nabla}\cdot\left(\phi_A \rho_f^r \overrightarrow{v_f^r}\,\overrightarrow{v_f^r}\right)$$

Energy Balance:

$$\phi_V \rho_f^r C_{v,f}^r \frac{\partial T_f^r}{\partial t} - \phi_V \frac{p_f^r}{\rho_f^r}\frac{\partial \rho_f^r}{\partial t} + \phi_A \rho_f^r \overrightarrow{v_f^r} C_{p,f}^r \vec{\nabla} T_f^r$$
$$= \vec{\nabla}\cdot\left(\phi_A k_f^r \vec{\nabla} T_f^r\right) - \sum_{i=1}^{n} \frac{1}{M_i}\overline{h_{f,i}}\cdot R_{i,f}^r - \phi_I \psi_{A,c} h_c^r (T_f^r - T^c\Big|_{Surface}^{Cat.})$$
$$+ N_T \frac{A^{per}}{V^r}\left[H_f^r \sum_{i=1}^{n} \overrightarrow{N_{i,f}^{per}}\Big|_{surface}^{mem} - \sum_{i=1}^{n}\frac{1}{M_i}\overline{h_{f,i}}\cdot \overrightarrow{N_{i,f}^{per}}\Big|_{surface}^{mem}\right] - \frac{A^{per}}{V^r} h_{per}^r (T_f^r - T^{per}\Big|_{Surface}^{Membrane}) - \frac{A_{Surface}^{Reactor}}{V^{Reactor}} U (T_f^r - T_w)$$

MR Multiscale Equations (Catalyst pellet domain)

Species Mass Balance:

$$\boxed{R_{i,f}^{c} = \frac{\partial}{\partial t}\left(w_{i,f}^{c}\varepsilon_{V}^{c}\rho_{f}^{c}\right) + \frac{1}{r^{2}}\frac{d}{dr}\left(r^{2}\varepsilon_{A}^{c}\overrightarrow{N_{i,f}^{c}}\right) \qquad i = 1, n}$$

Energy Balance:

$$\boxed{\varepsilon_{V}^{c}\rho_{f}^{c}C_{v,f}^{c}\frac{\partial T_{f}^{c}}{\partial t} - \frac{p_{f}^{c}}{\rho_{f}^{c}}\frac{\partial\left(\varepsilon_{V}^{c}\rho_{f}^{c}\right)}{\partial t} = \vec{\nabla}\cdot\left(\varepsilon_{A}^{c}k_{f}^{c}\vec{\nabla}T_{f}^{c}\right) - \sum_{i=1}^{n}\left[\varepsilon_{A}^{c}\overrightarrow{j_{i,f}^{c}}\cdot C_{p,i,f}^{c}\vec{\nabla}T_{f}^{c}\right] - \sum_{i=1}^{n}\frac{1}{M_{i}}\overline{h_{f,i}}\cdot R_{i,f}^{c}}$$

Boundary Conditions:

$$\left.\begin{aligned} w_{f,i}^{c} &= \left(w_{f,i}^{c}\right)_{in} \\ T_{f}^{c} &= T_{s}^{c} = T_{in} \\ p_{f}^{c} &= \left(p_{f}^{c}\right)_{in} \end{aligned}\right\} for\ t = 0,\ \forall r \qquad \left.\begin{aligned} \overrightarrow{N_{f,i}^{c}} &= 0 \\ Q^{c} &= -k^{c}\vec{\nabla}T^{c} = 0 \\ \vec{\nabla}p_{f}^{c} &= 0 \end{aligned}\right\} for\ r = 0 \qquad \left.\begin{aligned} -K_{m,i}\left(w_{f,i}^{r}\rho_{f}^{r} - w_{f,i}^{c}\rho_{f}^{c}\right) &= \overrightarrow{N_{f,i}^{c}} \\ -h_{c}^{r}\left(T_{f}^{r} - T^{c}\right) &= -k^{c}\vec{\nabla}T^{c} \\ p_{f}^{c} &= p_{f}^{r} \end{aligned}\right\} for\ r = R_{cat}$$

MR Multiscale Equations (Permeation domain)

Species Mass Balance:

$$\boxed{N_T \frac{A^{per}}{V^r}\overrightarrow{N_{i,f}^{per}} = \frac{\partial}{\partial t}\left(w_{i,f}^{per}\phi_V \rho_f^{per}\right) + \vec{\nabla}\cdot\left[\phi_A\left(w_{i,f}^{per}\rho_f^{per}\overrightarrow{v_f^{per}}\right)\right] \qquad i = 1, n}$$

Momentum conservation:

$$\boxed{\frac{\partial}{\partial t}\left(\phi_V \overrightarrow{v_f^{per}}\rho_f^{per}\right) + \vec{\nabla}\cdot\left(\phi_A \rho_f^{per}\overrightarrow{v_f^{per}}\,\overrightarrow{v_f^{per}}\right) = -\vec{\nabla}\left(\phi_A p_f^{per}\right) - \vec{\nabla}\cdot\overrightarrow{v_f^{per}}\left(-\mu_f^{per}\vec{\nabla}\overrightarrow{v_f^{per}}\right)}$$

Energy Balance:

$$\phi_V \rho_f^{per} C_{v,f}^{per}\frac{\partial T_f^{per}}{\partial t} - \frac{p_f^{per}}{\rho_f^{per}}\frac{\partial\left(\phi_V \rho_f^{per}\right)}{\partial t} + \phi_A \rho_f^{per}\overrightarrow{v_f^{per}} C_{p,f}^{per}\vec{\nabla}T_f^{per}$$

$$= \vec{\nabla}\cdot\left(\phi_A k_f^{per}\vec{\nabla}T_f^{per}\right) + N_T\frac{A^{per}}{V^r}\left(\sum_{i=1}^{n}\frac{1}{M_i}\overline{h_{f,i}}\cdot\overrightarrow{N_{i,f}^{per}} - H_f^{per}\sum_{i=1}^{n}\overrightarrow{N_{i,f}^{per}}\right)$$

$$+\frac{A^{per}}{V^r}h_{perm}^{per}(T_f^r - T^{per}\Big|_{Surface}^{Membrane})$$

MR Boundary Conditions (Reactor & Permeation Domain)

Reactor Domain:

$$\left.\begin{cases} \overrightarrow{v_f^r} = \overrightarrow{v_f^r}(t) \\ w_{f,i}^r = w_{f,i}^r(t) \\ T_f^r = T_f^r(t) \\ p_f^r = p_{f,in}^r \;\forall t \end{cases}\right\} for\; x = 0 \;\; ; \qquad \left.\begin{matrix} \vec{\nabla} w_{f,i}^r = 0 \\ \vec{\nabla} T_f^r = 0 \end{matrix}\right\} for\; x = L \wedge \;\forall t$$

Permeation Domain:

$$\left.\begin{matrix} \overrightarrow{v_f^{per}} = \left(\overrightarrow{v_f^{per}}\right)_{in} \\ p_f^{per} = \left(p_f^{per}\right)_{in} \\ w_{f,i}^{per} = \left(w_{f,i}^{per}\right)_{in} \\ T_f^{per} = \left(T_f^{per}\right)_{in} \end{matrix}\right\} for\; x = 0 \wedge \forall\, t; \qquad \left.\begin{matrix} \vec{\nabla} w_{i,f}^{per} = 0 \\ \vec{\nabla} T_f^{per} = 0 \end{matrix}\right\} for\; x = L \wedge \forall\, t$$

AR Multiscale Equations (Reactor fluid domain)

Species Mass Balance:

$$\boxed{R_{i,f}^{r} = \frac{\partial}{\partial t}\left(w_{i,f}^{r}\phi_V \rho_f^{r}\right) + \overrightarrow{\nabla}\cdot\left(\phi_A \overrightarrow{N_{i,f}^{r}}\right) \qquad i = 1, n}$$

Where: $\overrightarrow{N_{i,f}^{r}} = w_{i,f}^{r}\rho_f^{r}\overrightarrow{v_f^{r}} + \overrightarrow{j_{i,f}^{r}}$

Newly incorporated Dispersion Model:

$$\boxed{\overrightarrow{j_{i,f}^{r}} = -D^{*}\overrightarrow{\nabla}\left(\rho_f^{r} w_{i,f}^{r}\right)}$$

D^{*} is determined empirically from tracer pulse experiments from which we can infer the degree of dispersion in the reactor

AR Multiscale Equations (Reactor fluid domain) Cont.

Momentum conservation:

$$-\vec{\nabla}\left(\phi_A p_f^r\right)=\phi_A\left(150\frac{\left(1-\phi_V\right)^2\mu_f^r}{d_{pellet}^2\phi_V^{\ 3}}\overrightarrow{v_f^r}+\frac{1.75\left(1-\phi_V\right)\rho_f^r}{d_{pellet}\phi_V^{\ 3}}\overrightarrow{v_f^r}\,\overrightarrow{v_f^r}\right)+\frac{\partial}{\partial t}\left(\phi_V\overrightarrow{v_f^r}\rho_f^r\right)$$
$$+\vec{\nabla}\cdot\left(\phi_A\rho_f^r\overrightarrow{v_f^r}\,\overrightarrow{v_f^r}\right)$$

Energy Balance:

$$\phi_V\rho_f^r C_{v,f}^r\frac{\partial T_f^r}{\partial t}-\phi_V\frac{p_f^r}{\rho_f^r}\frac{\partial\rho_f^r}{\partial t}+\phi_A\rho_f^r\overrightarrow{v_f^r}C_{p,f}^r\vec{\nabla}T_f^r$$
$$=\vec{\nabla}\cdot\left(\phi_A k_f^r\vec{\nabla}T_f^r\right)-\sum_{i=1}^{n}\frac{1}{M_i}\overline{h_{f,i}}\cdot R_{i,f}^r-\phi_I\psi_{A,c}h_c^r(T_f^r-T^c\Big|_{Surface}^{Cat.})$$
$$+N_T\frac{A^{per}}{V^r}\left[H_f^r\sum_{i=1}^{n}\overrightarrow{N_{i,f}^{per}}\Big|_{surface}^{mem}-\sum_{i=1}^{n}\frac{1}{M_i}\overline{h_{f,i}}\cdot\overrightarrow{N_{i,f}^{per}}\Big|_{surface}^{mem}\right]-\frac{A^{per}}{V^r}h_{per}^r(T_f^r-T^{per}\Big|_{Surface}^{Membrane})-\frac{A_{Surface}^{Reactor}}{V^{Reactor}}U(T_f^r-T_w)$$

AR Reactor fluid domain: Boundary conditions

$$\left.\begin{aligned}\vec{\nabla} T_f^r &= 0\\ \vec{\nabla} w_{f,i}^r &= 0\end{aligned}\right\} for\ \ x = L \ \wedge\ \forall t$$

$$\left.\begin{aligned}
&\vec{v_f^r} = \vec{v_f^r}(t) = \left\{\begin{matrix} v_{Ads}^r & for\ \ (k-1)\left(\Delta t_{Ads} + \Delta t_{Reg}\right) \le t < k\Delta t_{Ads} + (k-1)\Delta t_{Reg} \\ v_{Reg}^r & for\ \ k\Delta t_{Ads} + (k-1)\Delta t_{Reg} \le t < k\left(\Delta t_{Ads} + \Delta t_{Reg}\right) \end{matrix}\right\} \\
&w_{f,i}^r = w_{f,i}^r(t) = \left\{\begin{matrix} w_{f,i,\ Ads}^r & for\ \ (k-1)\left(\Delta t_{Ads} + \Delta t_{Reg}\right) \le t < k\Delta t_{Ads} - \Delta t_{Pur} + (k-1)\Delta t_{Reg} \\ w_{f,i,\ Reg}^r & for\ \ k\Delta t_{Ads} - \Delta t_{Pur} + (k-1)\Delta t_{Reg} \le t < k\left(\Delta t_{Ads} + \Delta t_{Reg}\right) \end{matrix}\right\} \\
&T_f^r = T_f^r(t) = \left\{\begin{matrix}
T_{Ads} & for\ \ (k-1)\left(\Delta t_{Ads} + \Delta t_{Reg}\right) \le t < k\Delta t_{Ads} + (k-1)\Delta t_{Reg} \\
T_{Ads} + \dfrac{T_{Reg} - T_{Ads}}{\Delta t_{Hea}}\left(t - \begin{bmatrix} k\Delta t_{Ads} + \\ (k-1)\Delta t_{Reg} \end{bmatrix}\right) & for\ \ \left\{\begin{matrix} k\Delta t_{Ads} + (k-1)\Delta t_{Reg} \le t \\ t < \begin{bmatrix} k\Delta t_{Ads} + \\ (k-1)\Delta t_{Reg} + \Delta t_{Hea} \end{bmatrix} \end{matrix}\right\} \\
T_{Reg} & for\ \ \begin{bmatrix} k\Delta t_{Ads} + \\ (k-1)\Delta t_{Reg} + \Delta t_{Hea} \end{bmatrix} \le t < k\left(\Delta t_{Ads} + \Delta t_{Reg}\right) - \left(\Delta t_{Coo} + \Delta t_{Tra}\right) \\
T_{Reg} - \dfrac{T_{Reg} - T_{Ads}}{\Delta t_{Coo}}\left(t - \begin{bmatrix} k\left(\Delta t_{Ads} + \Delta t_{Reg}\right) - \\ \left(\Delta t_{Coo} + \Delta t_{Tra}\right) \end{bmatrix}\right) & for\ \ \left\{\begin{matrix} k\left(\Delta t_{Ads} + \Delta t_{Reg}\right) - \\ \left(\Delta t_{Coo} + \Delta t_{Tra}\right) \le t \\ < k\left(\Delta t_{Ads} + \Delta t_{Reg}\right) - \Delta t_{Tra} \end{matrix}\right\} \\
T_{Ads} & for\ \ \left\{k\left(\Delta t_{Ads} + \Delta t_{Reg}\right) - \Delta t_{Tra} \le t < k\left(\Delta t_{Ads} + \Delta t_{Reg}\right)\right\}
\end{matrix}\right\} \\
&p_f^r = p_{f\,in}^r \ \forall t
\end{aligned}\right\} for\ \left\{\begin{matrix} x = 0 \\ k \in \{1, \ldots, n\} \end{matrix}\right\}$$

AR Multiscale Equations (Catalyst pellet domain)

Species Mass Balance:

$$\boxed{R_{i,f}^{c} = \frac{\partial}{\partial t}\left(w_{i,f}^{c}\varepsilon_V^{c}\rho_f^{c}\right) + \frac{1}{r^2}\frac{d}{dr}\left(r^2\varepsilon_A^{c}\overrightarrow{N_{i,f}^{c}}\right) \qquad i = 1, n}$$

Energy Balance:

$$\boxed{\varepsilon_V^{c}\rho_f^{c}C_{v,f}^{c}\frac{\partial T_f^{c}}{\partial t} - \frac{p_f^{c}}{\rho_f^{c}}\frac{\partial\left(\varepsilon_V^{c}\rho_f^{c}\right)}{\partial t} = \vec{\nabla}\cdot\left(\varepsilon_A^{c}k_f^{c}\vec{\nabla}T_f^{c}\right) - \sum_{i=1}^{n}\left[\varepsilon_A^{c}\overrightarrow{j_{i,f}^{c}}\cdot C_{p,i,f}^{c}\vec{\nabla}T_f^{c}\right] - \sum_{i=1}^{n}\frac{1}{M_i}\overline{h_{f,i}}\cdot R_{i,f}^{c}}$$

Boundary Conditions:

$$\left.\begin{aligned} w_{f,i}^{c} &= \left(w_{f,i}^{c}\right)_{in} \\ T_f^{c} &= T_s^{c} = T_{in} \\ p_f^{c} &= \left(p_f^{c}\right)_{in} \end{aligned}\right\} for\ t = 0,\ \forall r \qquad \left.\begin{aligned} \overrightarrow{N_{f,i}^{c}} &= 0 \\ Q^{c} &= -k^{c}\vec{\nabla}T^{c} = 0 \\ \vec{\nabla}p_f^{c} &= 0 \end{aligned}\right\} for\ r = 0 \qquad \left.\begin{aligned} -K_{m,i}\left(w_{f,i}^{r}\rho_f^{r} - w_{f,i}^{c}\rho_f^{c}\right) &= \overrightarrow{N_{f,i}^{c}} \\ -h_c^{r}\left(T_f^{r} - T^{c}\right) &= -k^{c}\vec{\nabla}T^{c} \\ p_f^{c} &= p_f^{r} \end{aligned}\right\} for\ r = R_{cat}$$

AR Multiscale Equations (Adsorbent pellet domain)

Species Mass Balance:

$$\boxed{R_{i,f}^{a} = \frac{\partial}{\partial t}\left(w_{i,f}^{a}\varepsilon_{V}^{a}\rho_{f}^{a}\right) + \vec{\nabla}\cdot\left(\varepsilon_{A}^{a}\overrightarrow{N_{i,f}^{a}}\right) \qquad i = 1, n}$$

Energy Balance:

$$\boxed{\varepsilon_{V}^{a}\rho_{f}^{a}C_{v,f}^{a}\frac{\partial T_{f}^{a}}{\partial t} - \frac{p_{f}^{a}}{\rho_{f}^{a}}\frac{\partial\left(\varepsilon_{V}^{a}\rho_{f}^{a}\right)}{\partial t} = \vec{\nabla}\cdot\left(\varepsilon_{A}^{a}k_{f}^{a}\vec{\nabla}T_{f}^{a}\right) - \varepsilon_{A}^{a}\sum_{i=1}^{n}\left[\overrightarrow{j_{i,f}^{a}}\cdot C_{p,i,f}^{a}\vec{\nabla}T_{f}^{a}\right] - \sum_{i=1}^{n}\left[\frac{1}{M_{i}}\overline{h_{f,i}}\cdot R_{i,f}^{a}\right]}$$

Boundary Conditions:

$$\left.\begin{aligned} w_{f,i}^{c} &= \left(w_{f,i}^{c}\right)_{in} \\ T_{f}^{c} &= T_{s}^{c} = T_{in} \\ p_{f}^{c} &= \left(p_{f}^{c}\right)_{in} \end{aligned}\right\} for\ t = 0,\ \forall r$$

$$\left.\begin{aligned} \overrightarrow{N_{f,i}^{a}} &= 0 \\ Q^{a} = -k^{a}\vec{\nabla}T^{a} &= 0 \\ \vec{\nabla}p^{a} &= 0 \end{aligned}\right\} for\ r = 0$$

$$\left.\begin{aligned} -K_{m,i}\left(w_{f,i}^{r}\rho_{f}^{r} - w_{f,i}^{a}\rho_{f}^{a}\right) &= \overrightarrow{N_{f,i}^{a}} \\ -h^{a}\left(T_{f}^{r} - T^{a}\right) &= -k^{a}\vec{\nabla}T^{a} \\ p^{a} &= p_{f}^{r} \end{aligned}\right\} for\ r = R_{ads}$$

Common MR/AR Multiscale Equations

Equation of State (Ideal Gas) :

$$\boxed{p_f^\alpha V_f^\alpha = n_f^\alpha R T_f^\alpha}, \quad \alpha \in \{r, c, a, p\}$$

DGM Diffusion Model (for Catalyst/Adsorbent):

$$\left\{\begin{array}{l}
\displaystyle\sum_{j=1}^{n} \frac{1}{D_{ij}^{eff}} \left[\frac{x_{f,j}^\alpha}{M_i} \left(\varepsilon_A^\alpha \overrightarrow{N_{f,i}^\alpha} \right) - \frac{x_{f,i}^\alpha}{M_j} \left(\varepsilon_A^\alpha \overrightarrow{N_{f,j}^\alpha} \right) \right] + \left(\frac{1}{M_i D_{iK}^{eff}} \right) \left(\varepsilon_A^\alpha \overrightarrow{N_{f,i}^\alpha} \right) = \\
\displaystyle = -\left[c_{f,tot}^\alpha \vec{\nabla} x_{f,i}^\alpha + \left(\frac{1}{p_f^\alpha} + \frac{1}{D_{iK}^{eff}} \frac{B_O}{\mu_f^\alpha} \right) c_{f,i}^\alpha \vec{\nabla} p_f^\alpha \right] \qquad i = 1, n \quad \wedge i \neq j \\
\displaystyle D_{ij}^{eff} = \left(\frac{\varepsilon_A^\alpha}{\tau^\alpha} \right) \frac{\left(8.5872 \cdot 10^{-24} \dfrac{m^3 kg^{\frac{1}{2}}}{s^3 K^{\frac{3}{2}} mol^{\frac{1}{2}}} \right)}{p_f^\alpha} \frac{\sqrt{\dfrac{\left(T^\alpha\right)^3}{M_{ij}}}}{\sigma_{ij}^2 \, \Omega_{ij}} \\
\displaystyle M_{ij} = 2 \left[\frac{1}{M_i} + \frac{1}{M_j} \right]^{-1} \\
\displaystyle D_{iK}^{eff} = \left(\frac{\varepsilon_A^\alpha}{\tau^\alpha} \right) \left(\frac{4 \, d_{pore}^\alpha}{3} \right) \sqrt{\frac{\tilde{R} T^\alpha}{2 \pi M_i}} \\
\displaystyle B_O = \frac{d_{pore,\alpha}^2}{32}
\end{array}\right\}$$

Experimental Design basis

MR-AR Bench-scale Design Basis

MR

- Feed Pressure: ~10 - 25 bar
- Feed temperature: 510 - 535 K
- Syngas feed flowrate: 1-5 scfm
- Feed composition: As delivered from Uky CAER facility.

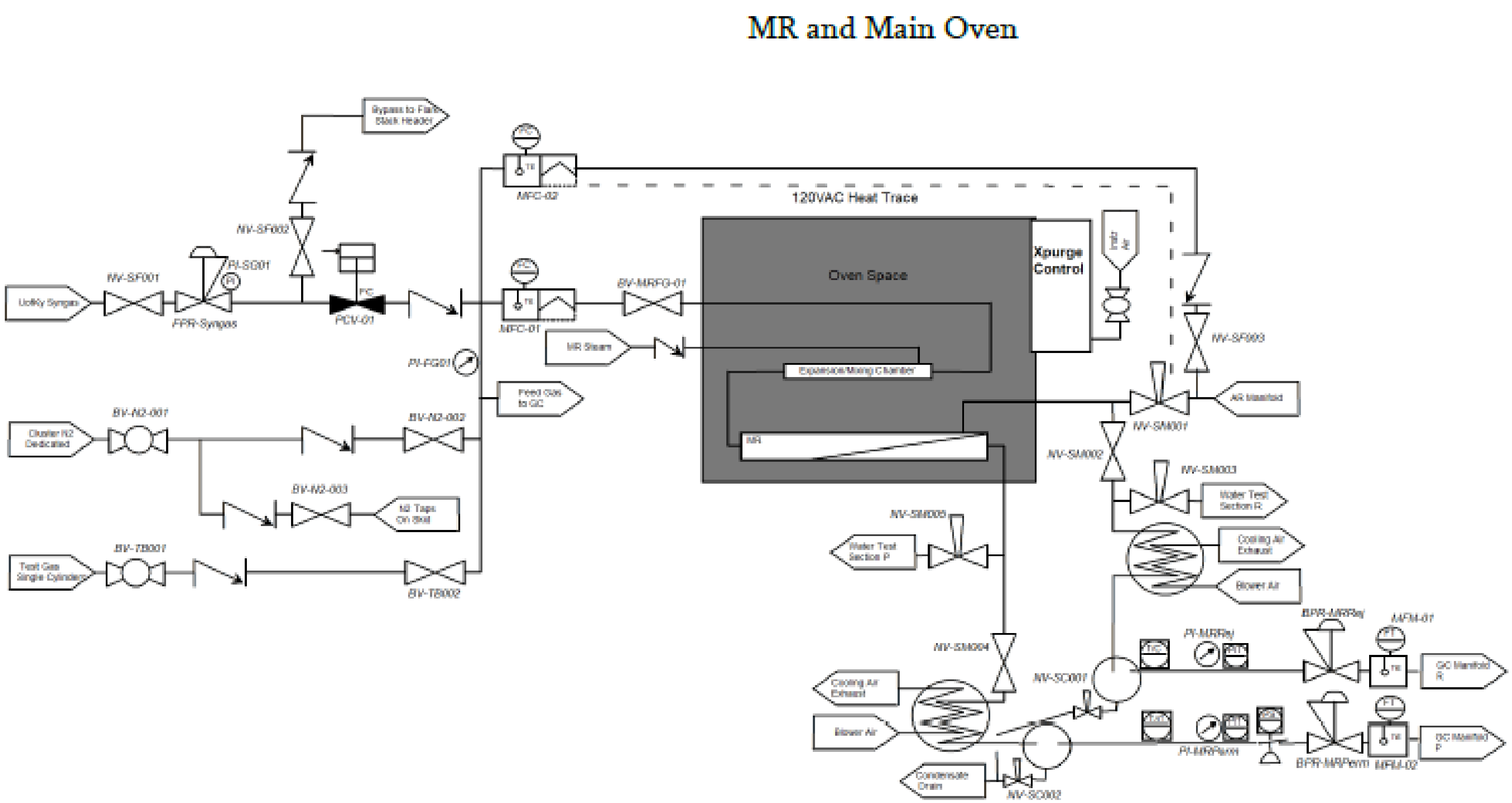
AR

- Temperature: Adsorption @ 523 K & Regeneration @ 523K - 673 K

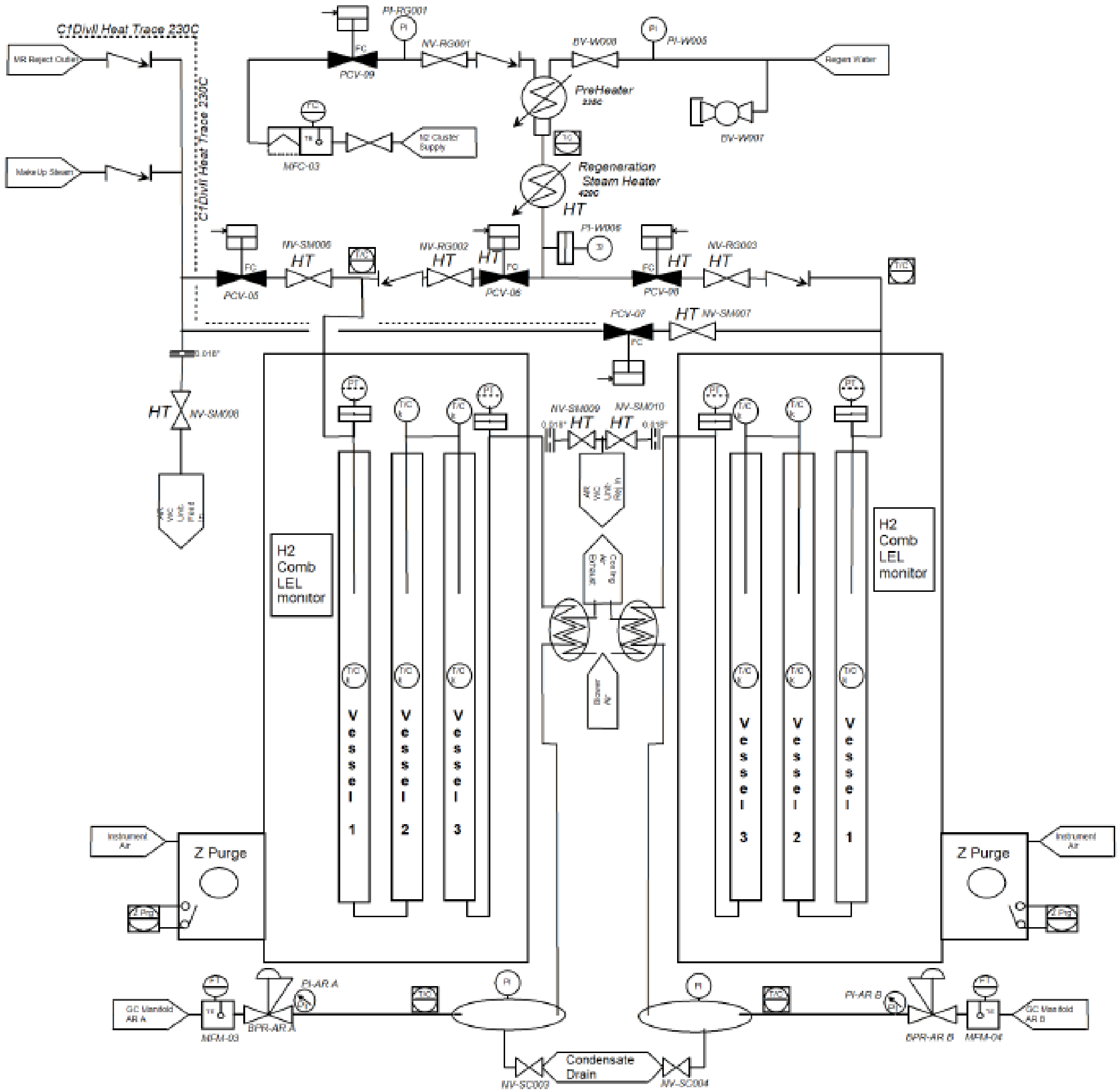
General

- Catalyst (MR and AR): Clariant
- Adsorbent (AR): Hydrotalcite pellets

MR P&ID


MR and Main Oven
120VAC Heat Trace
Oven Space
Xpurge
Control
Expansion/Mixing Chamber
MR
MR Steam
Feed Gas to GC
Air Manifold
Water Test Section R
Water Test Section P
Cooling Air Exhaust
Blower Air
Condensate Drain
GC Manifold R
GC Manifold P
MFC-02
MFC-01
BV-MRFG-01
PCV-01
FPR-Syngas
PI-SG01
NV-SF001
NV-SF002
NV-SF003
PI-FG01
BV-N2-001
BV-N2-002
BV-N2-003
N2 Taps On Skid
BV-TB001
BV-TB002
NV-SM001
NV-SM002
NV-SM003
NV-SM004
NV-SC001
NV-SC002
PI-MRRej
PI-MRPerm
BPR-MRRej
BPR-MRPerm
MFM-01
MFM-02

AR P&ID


C1Divll Heat Trace 230C
MR Reject Outlet
Make Up Steam
PI-RG001
PCV-09
NV-RG001
BV-W008
PI-W005
Regen Water
PreHeater
BV-W007
MFC-03
N2 Cluster Supply
Regeneration Steam Heater
HT
PI-W006
NV-SM006
NV-RG002
NV-RG003
PCV-05
PCV-06
PCV-08
PCV-07
NV-SM007
NV-SM008
NV-SM009
NV-SM010
H2 Comb LEL monitor
Vessel 1
Vessel 2
Vessel 3
Z Purge
Instrument Air
GC Manifold AR A
GC Manifold AR B
MFM-03
MFM-04
BPR-AR A
BPR-AR B
PI-AR A
PI-AR B
Condensate Drain
NV-SC003
NV-SC004

MR-AR bench scale sizing details

MR

- MR tubes ID: 3.5 mm
- MR tubes OD: 5.7 mm
- MR tube length: 482.6 mm
- No of tubes/bundle: 7 – 18

AR (single bed)

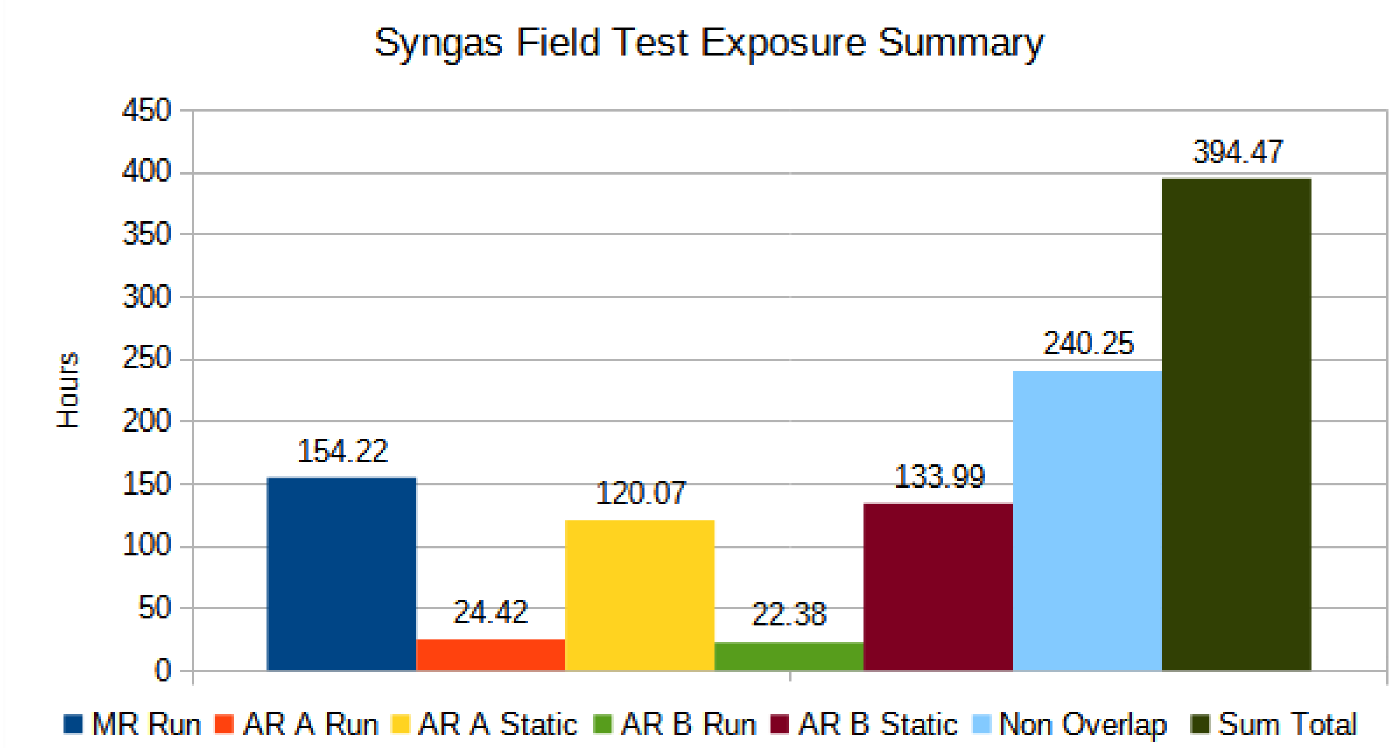
- AR ID: 2.5" (0.635 m)
- AR Length: 5' (1.524 m)
- Cat. loading: ~ 232g / vessel
- Ads. loading: ~ 1,638g /vessel
- Inert pellet loading: ~ 3,260g /vessel
- Run configuration: 2 or 3 beds in series

MR-AR assembled bench scale unit

Bench-Scale Experiments

Bench-Scale Experiments

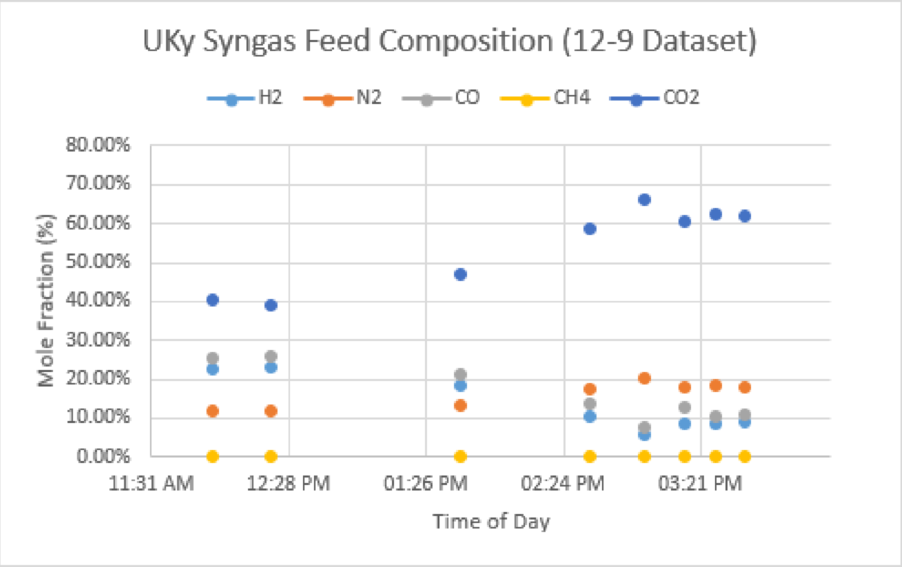
Field Test Period: 05-28-21 - Present

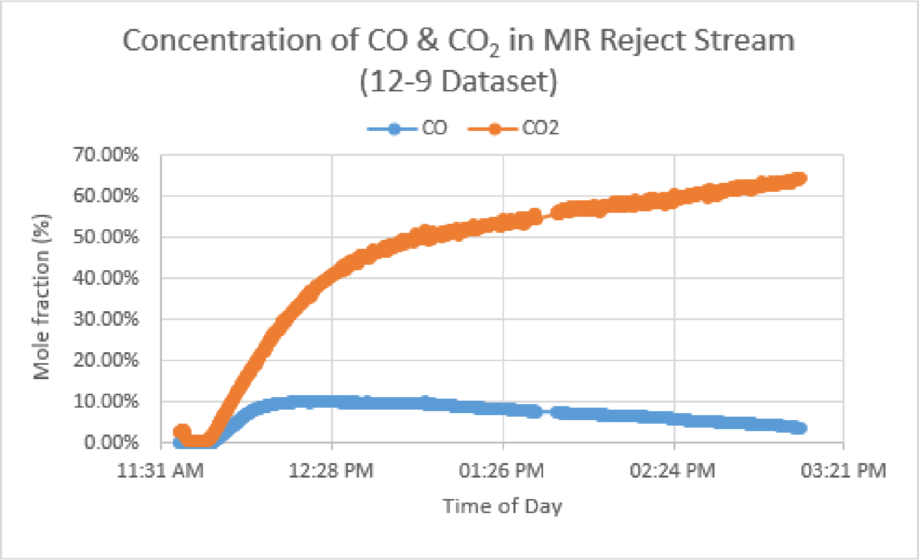


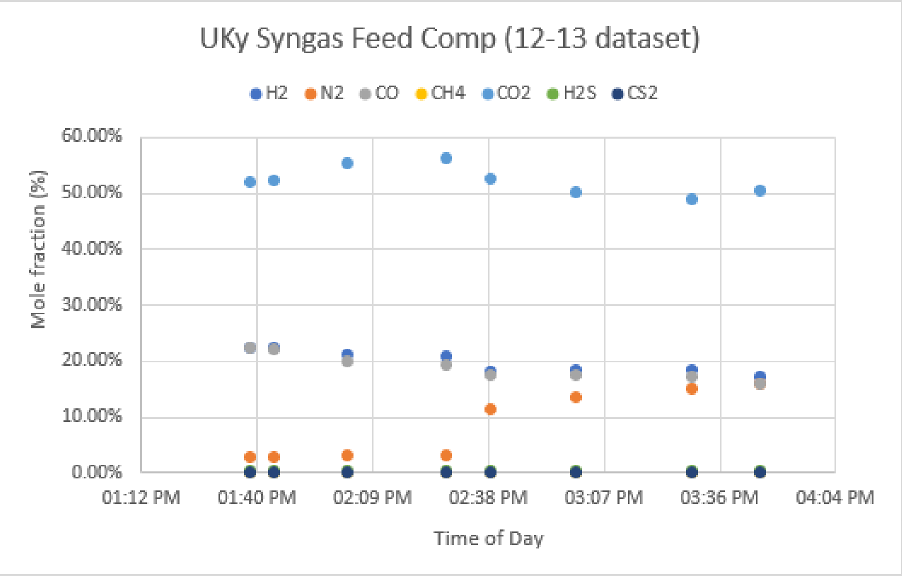
Total Exposure Hours

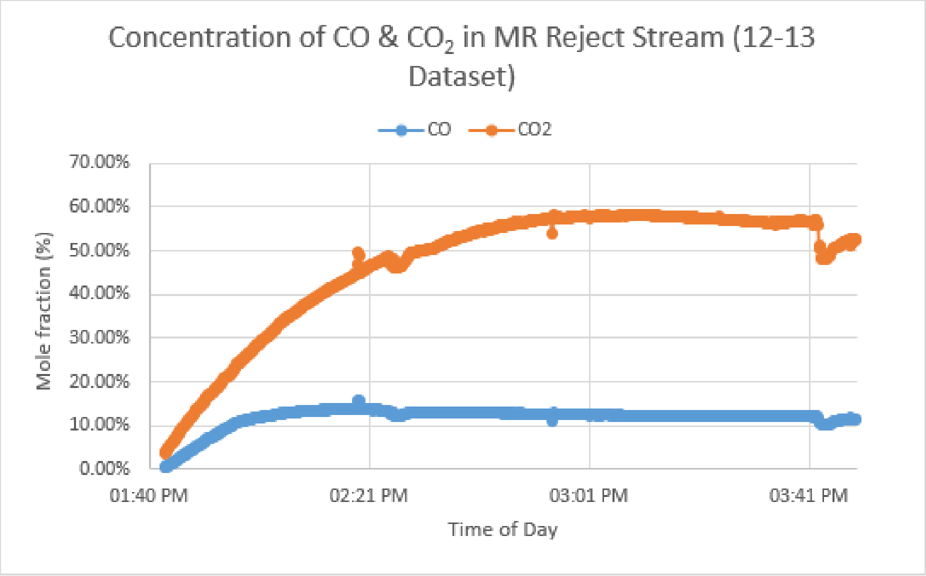
Non-overlap" refers to time which is only counted in one "mode" at a time (ie. if MR is running at the same time as an AR is sitting in static, it only counts once)

MR Experimental Data: MR Feed-Reject CO/CO_2 conc.

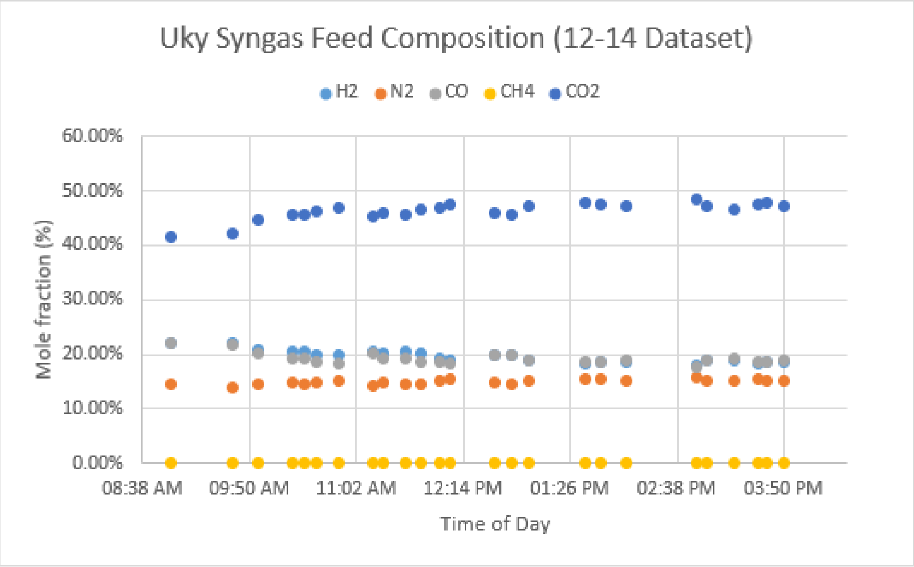


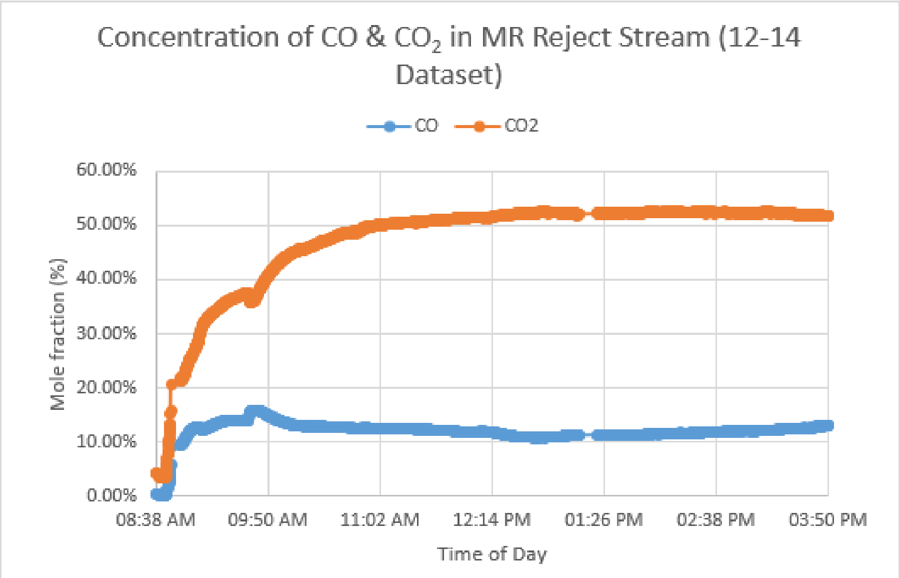


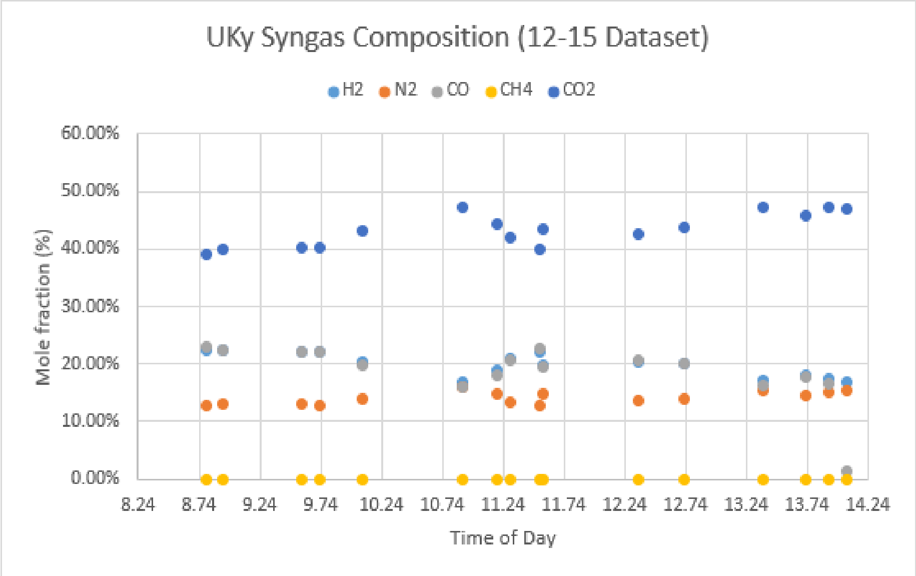


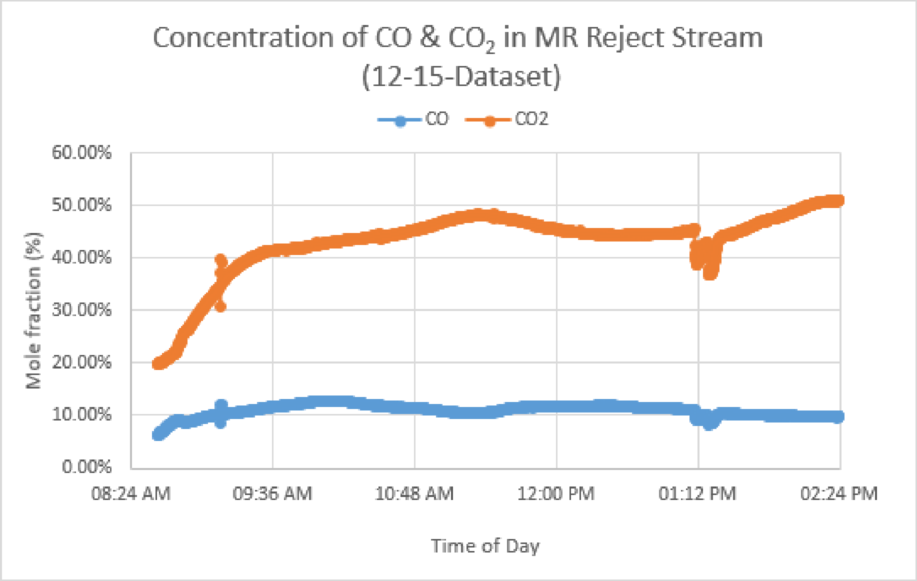


MR Experimental Data: MR Feed-Reject CO/CO_2 conc.









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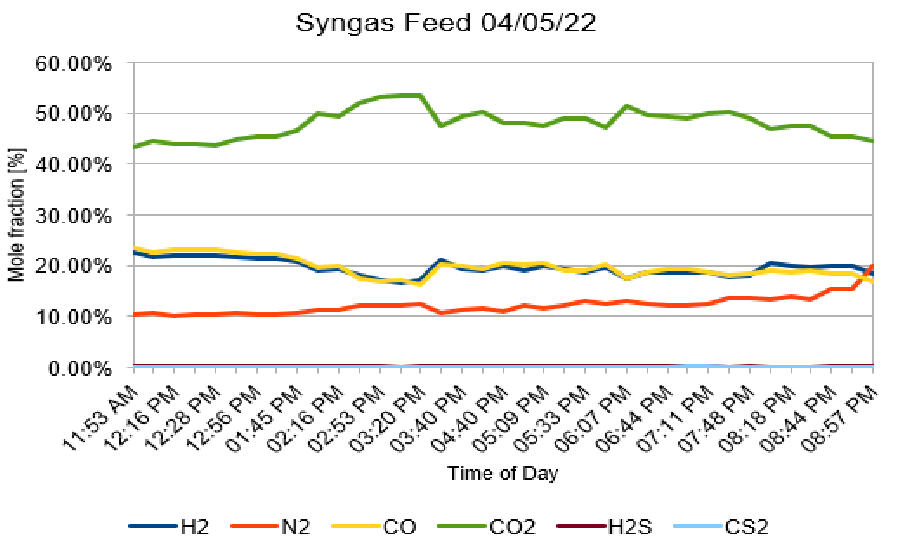

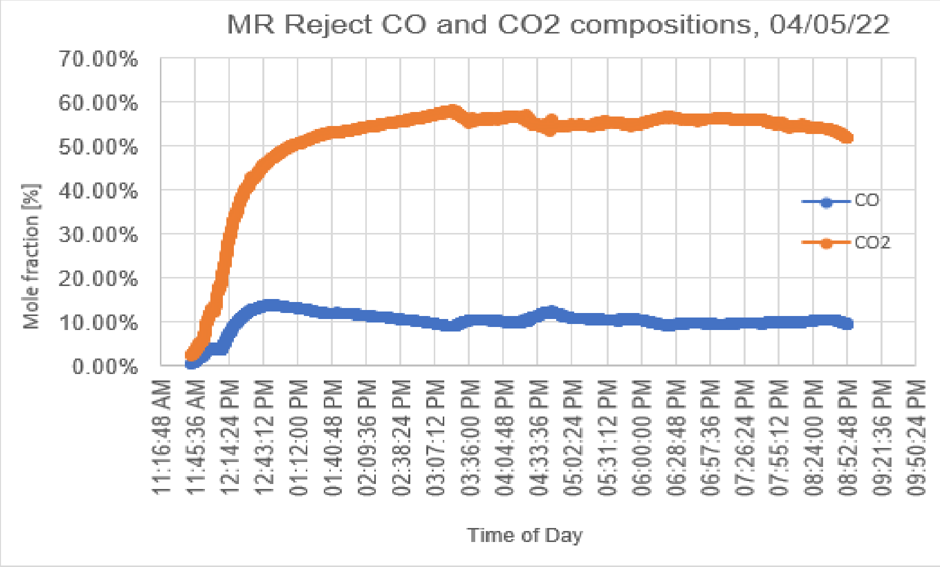

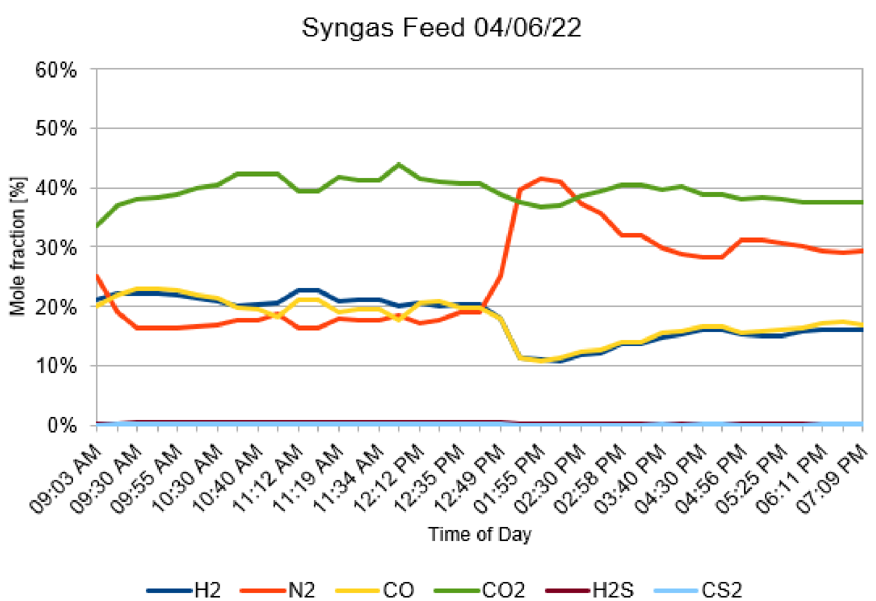

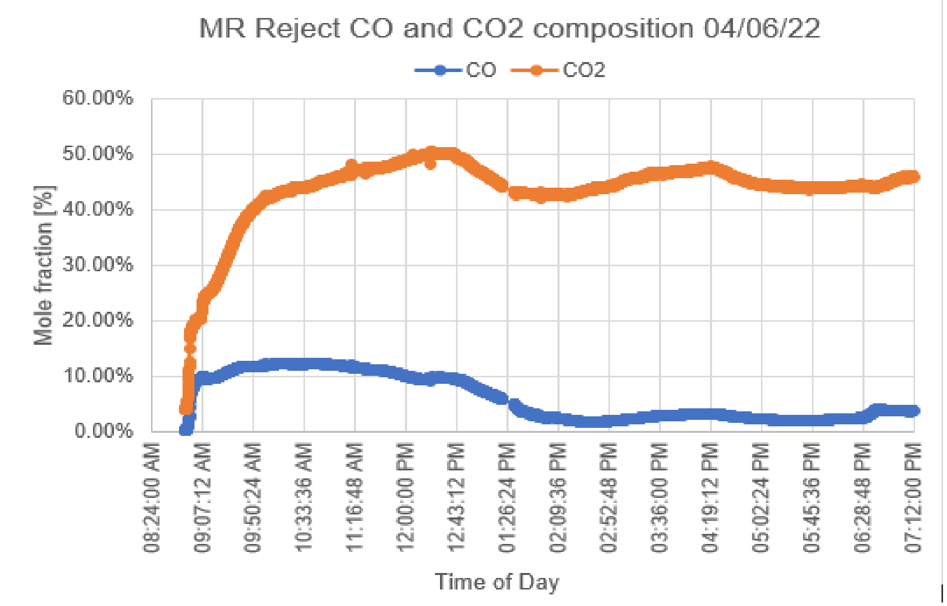

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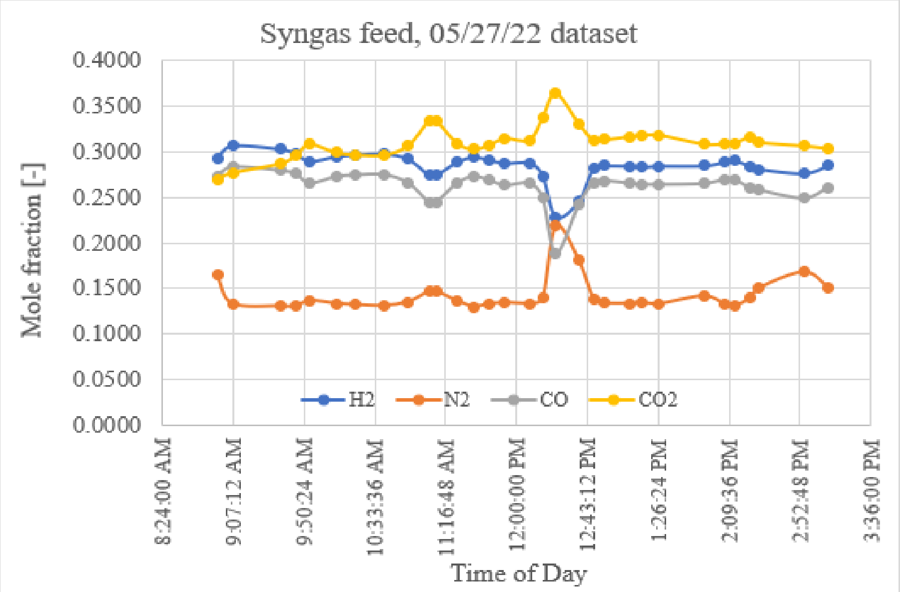
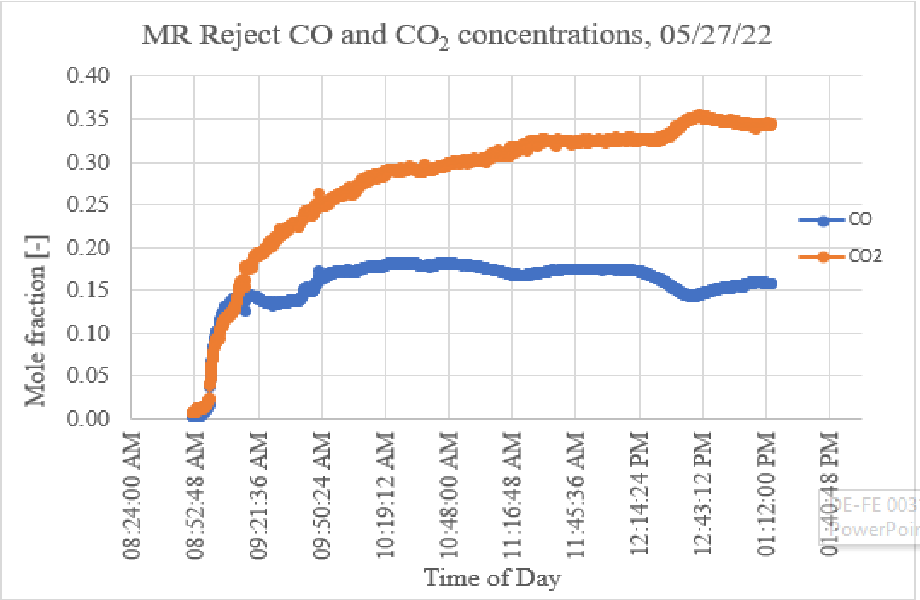
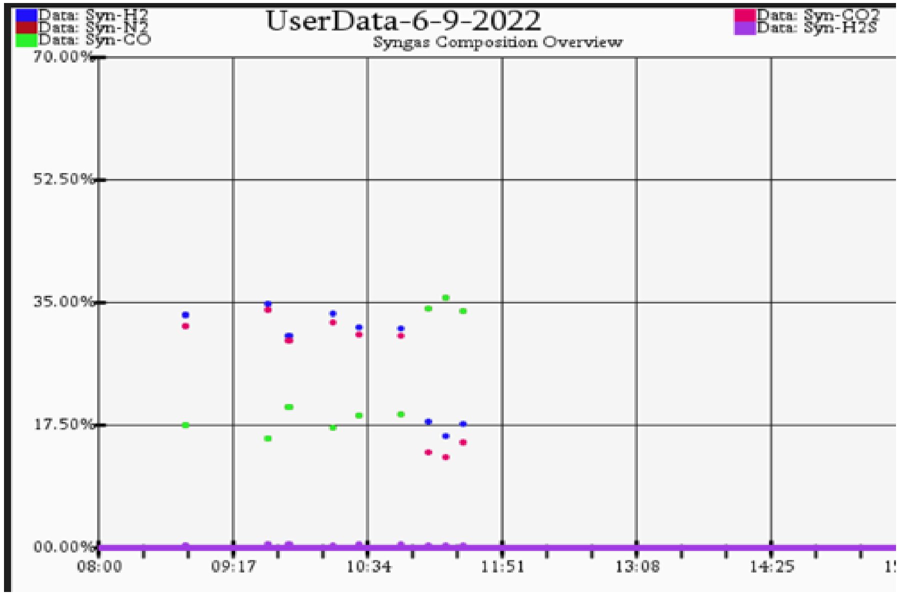
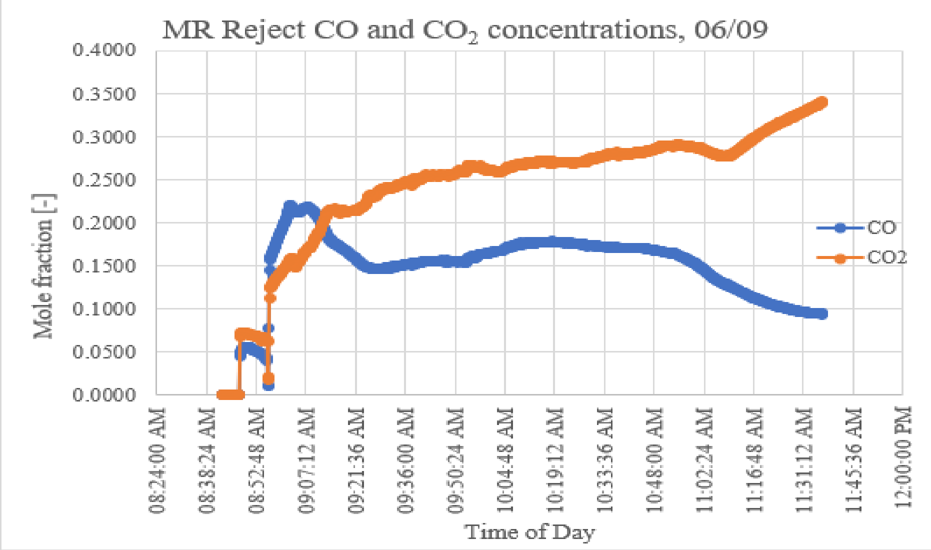
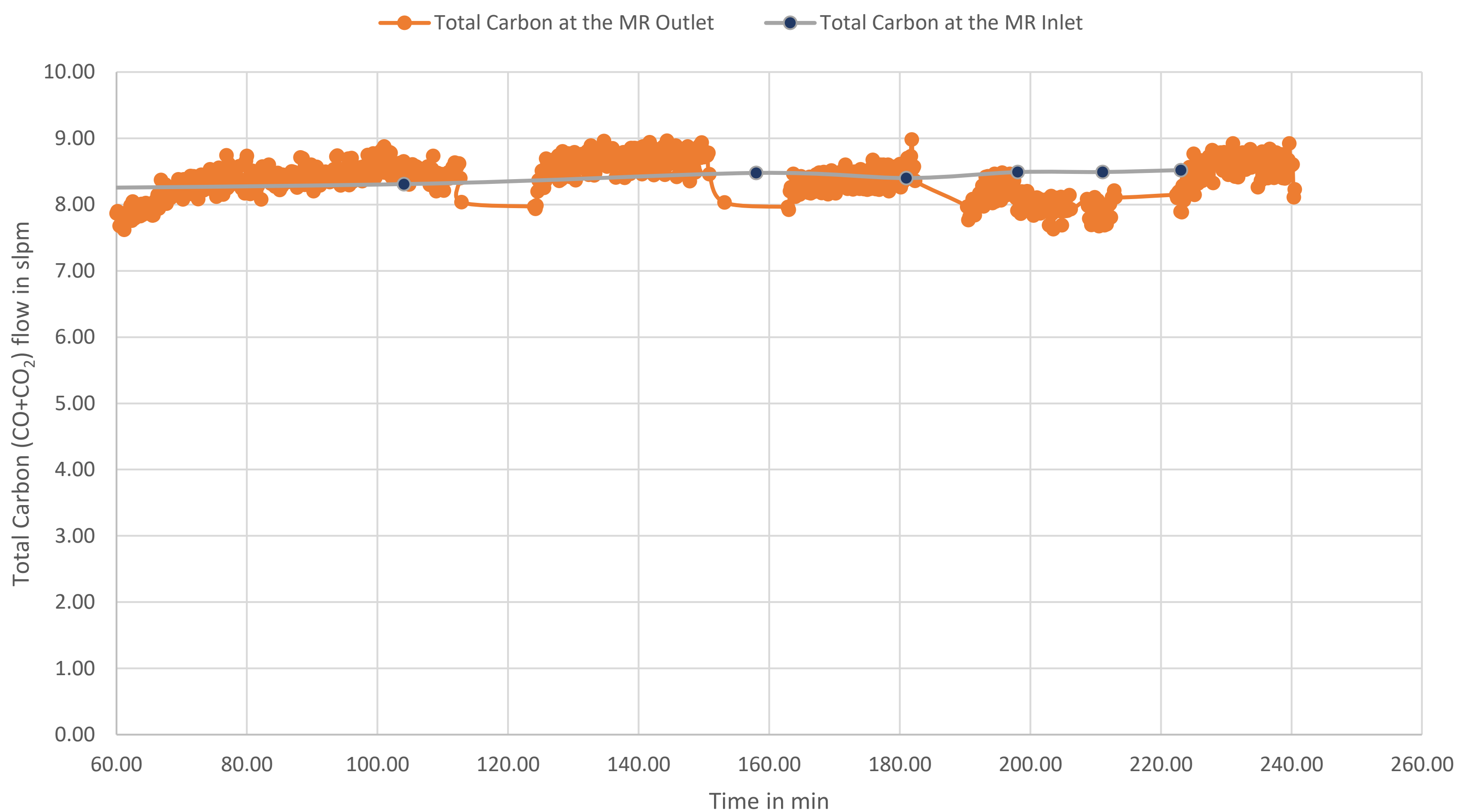






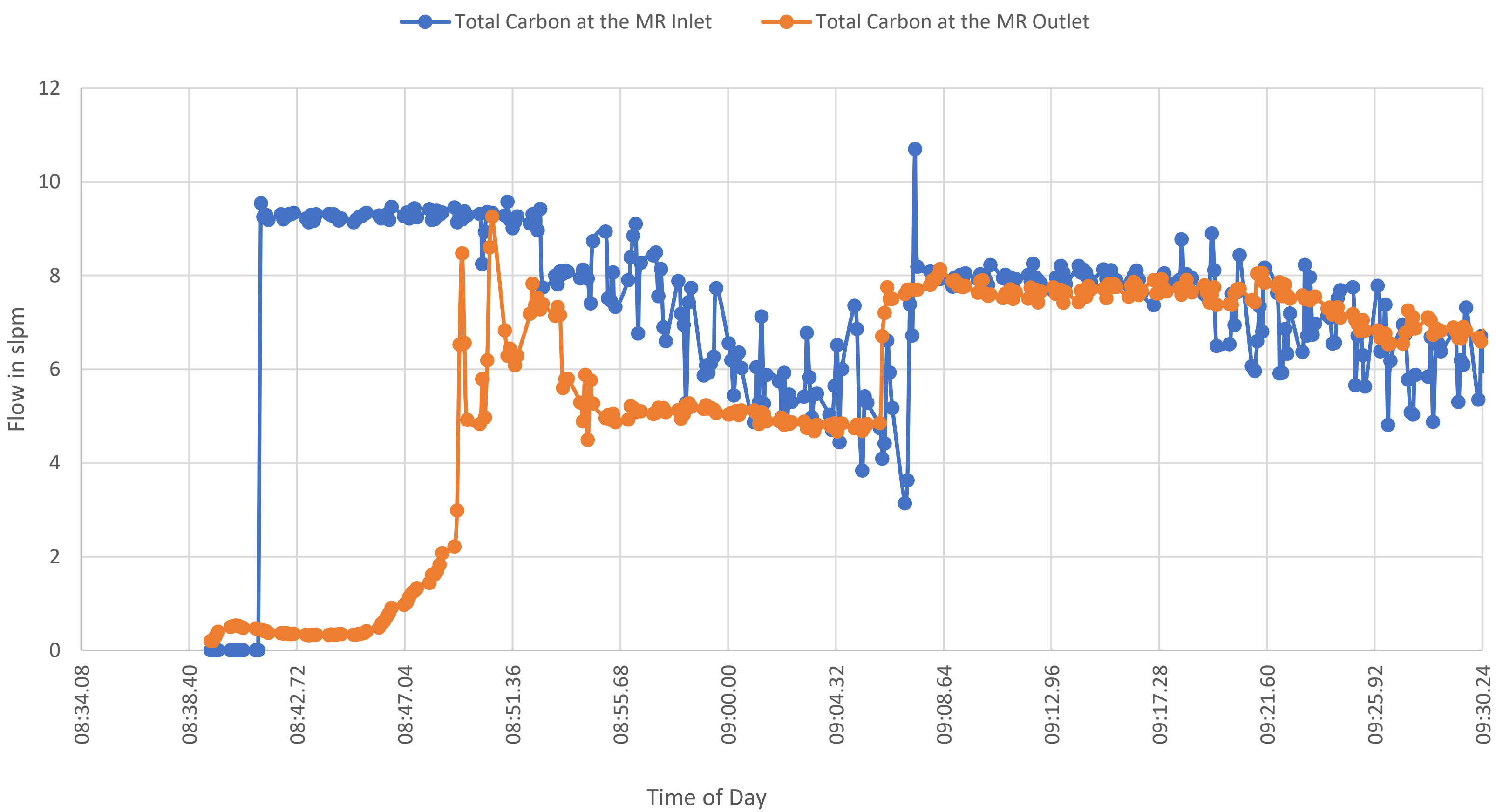


MR Experimental Data: MR Feed-Reject $CO+CO_2$ conc.



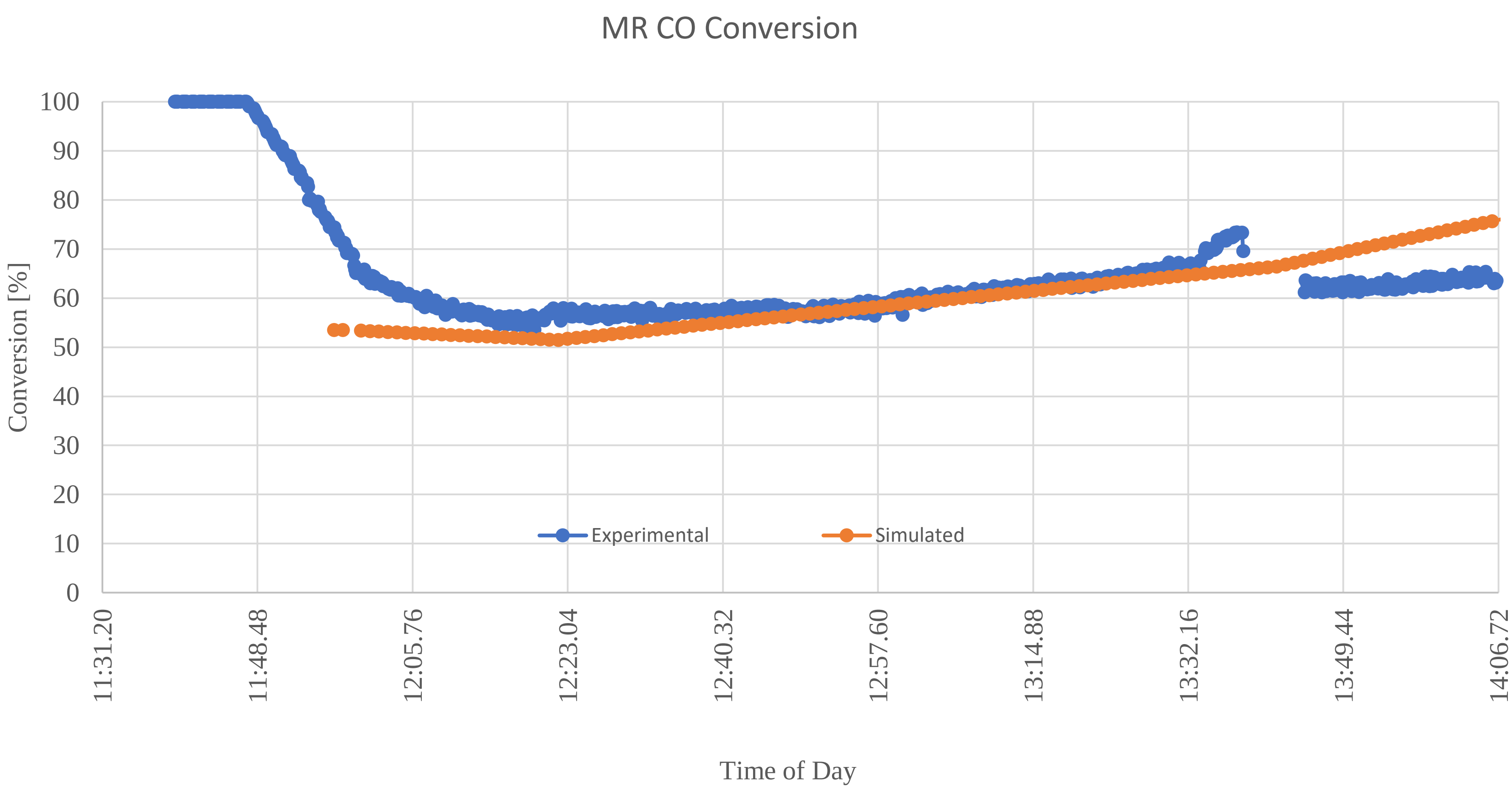
Total carbon ($CO + CO_2$) steady-state flow in the MR inlet and MR reject-side exit

MR Experimental Data: MR Feed-Reject $CO+CO_2$ conc.



Total carbon ($CO + CO_2$) dynamic N_2 to syngas pulse flow in the MR inlet and MR reject-side exit

MR Experimental - Simulated Conversions



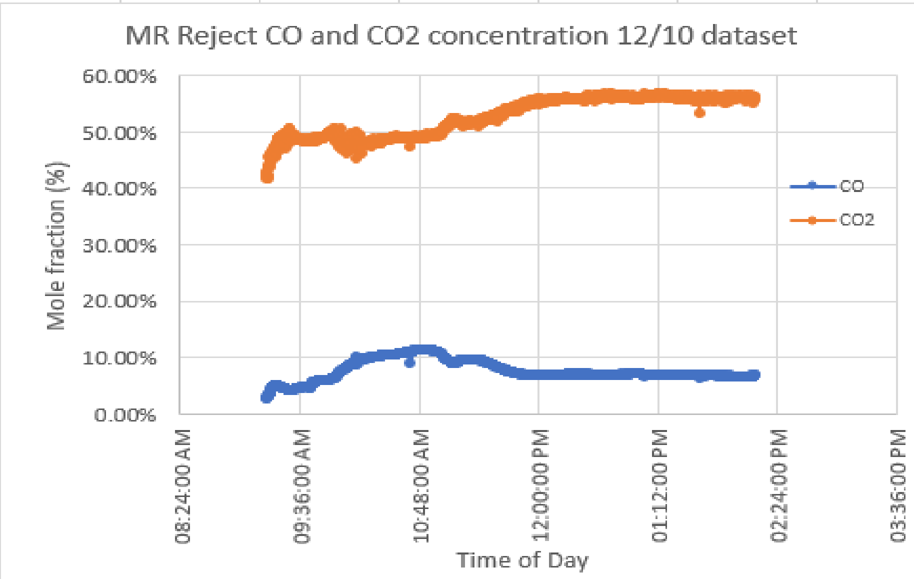
MR CO experimental (12/09/2021) and simulated conversions

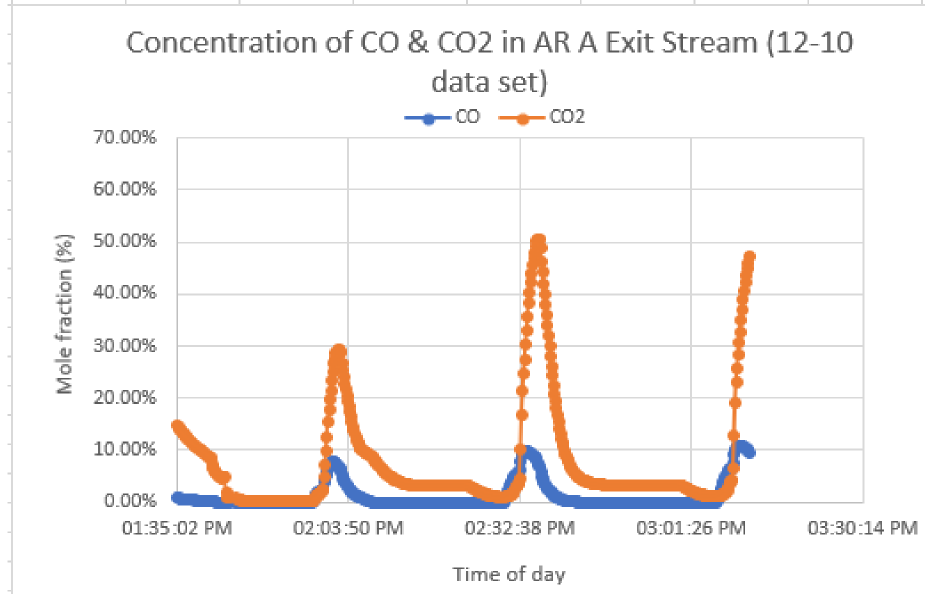
Experimental Data Analysis – MR CO conv. summary

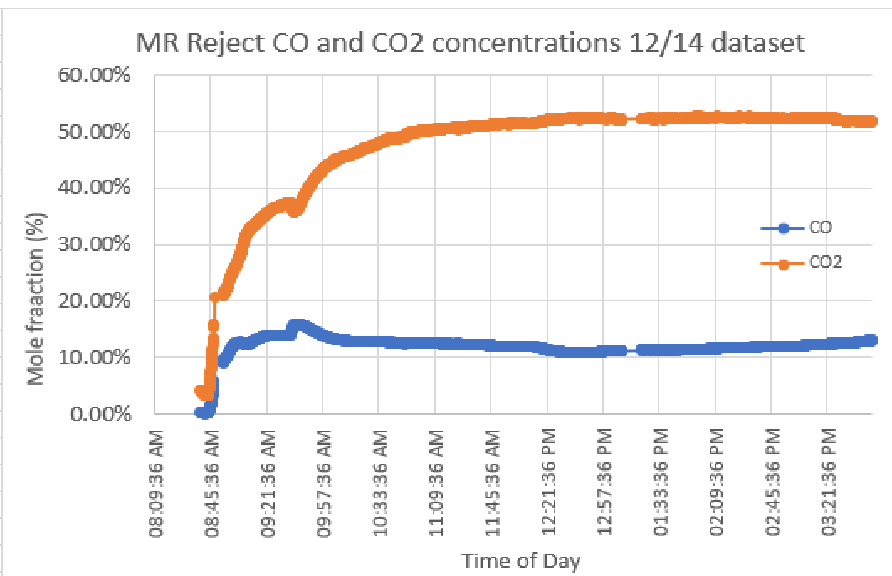
Data-set	Mean Feed Composition [$CO/CO_2/H_2/H_2O/N_2$]	Feed Pressure [psig]	Temp. [°C]	Flow rate [scfm]	Measured MR CO Conv. [%]	Simulated MR CO Conv. % (*%)
12-09-21	23.99 /36.25 /21.13 /7.57 /11.02	285	250	0.482	53	41 (80) - 46 (100)
12-13-21	16.35 /38.75 /16.57 /25.84 /2.21	249	240	0.585	39	35 (80) – 41 (100)
12-14-21	12.75 /32.76 /13.90 /30.10 /10.47	255	249	0.614	51	45 (80) - 52 (100)
12-15-21	14.58 /29.90 /14.37 /29.87 /9.64	245	263	0.626	52	39 (80) – 46 (100)
04-05-22	15.29 /37.09 /15.19 /22.94 /9.49	258	265	0.328	35	34 (80)
04-06-22	15.73 /30.80 /16.19 /23.60 /13.68	255	265	0.284	32	30 (80)
	9.34 /24.12 /9.05 /37.37 /20.12	220	265	0.284	75	74 (80)
06-09-22	9.67 /11.46 /10.51 /62.96 /5.40	260	253	0.611	64	69 (80)

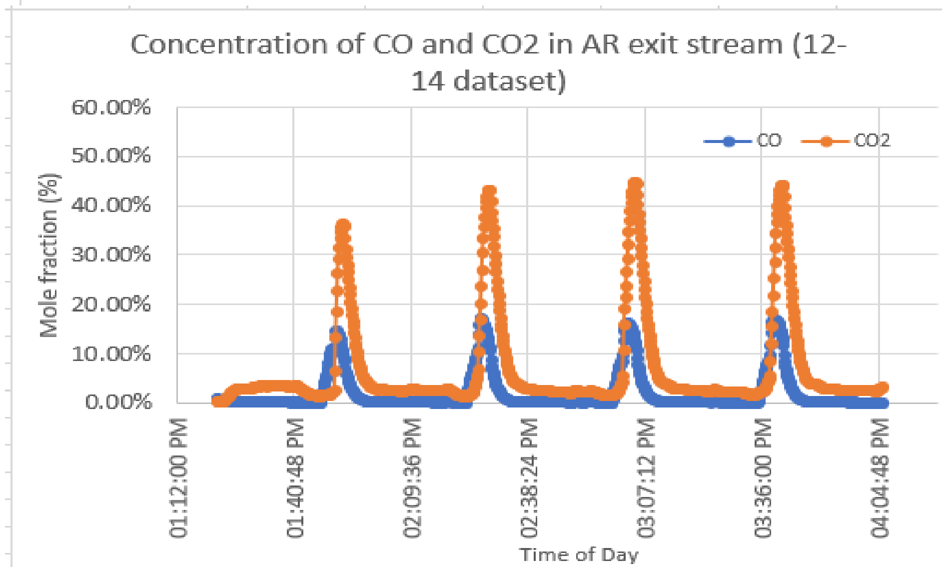
**Surface area of membrane exposed to gas flow (%)*

AR Reaction/Adsorption-Regeneration Experimental Data:
Feed: MR Reject – (H_2O, N_2) Exit: CO/CO_2 conc.

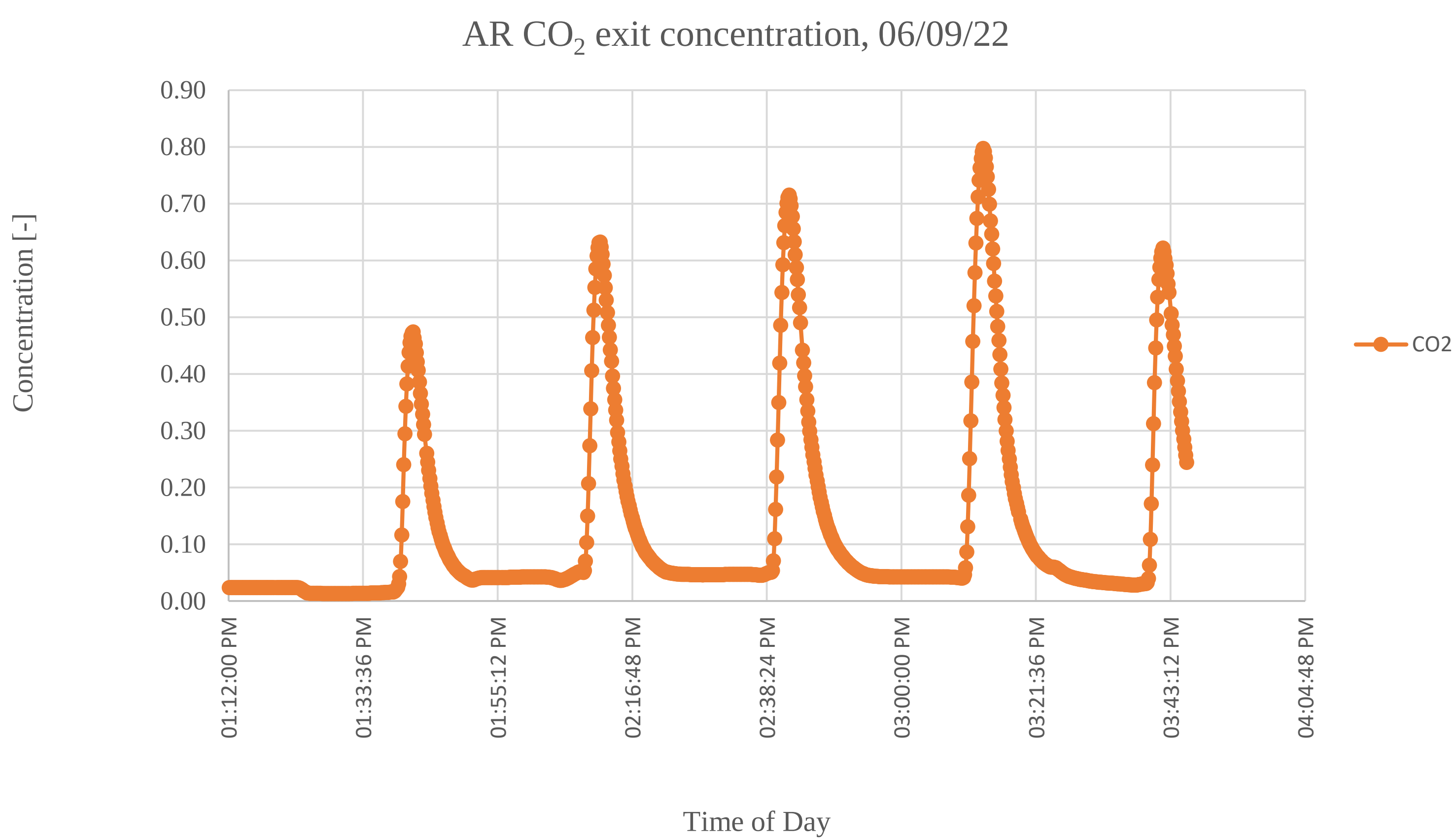




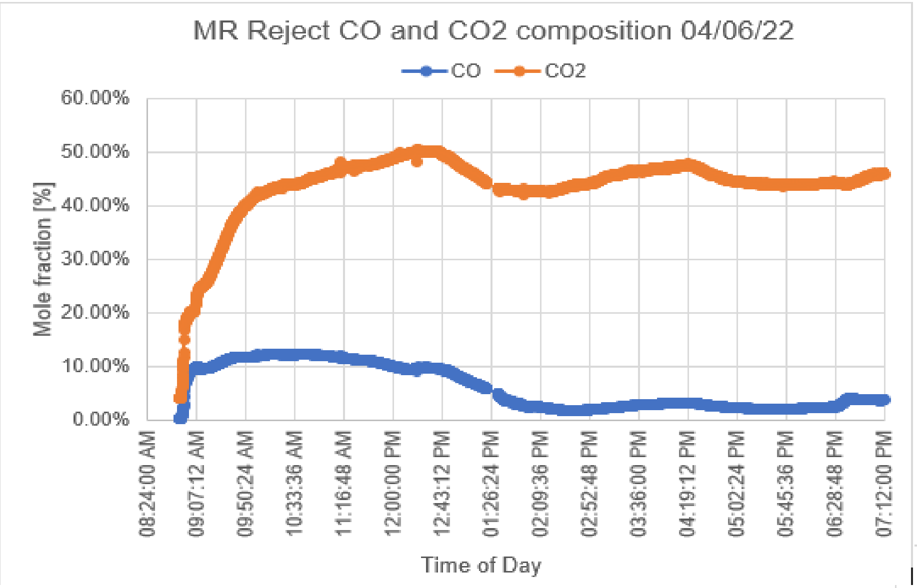




AR Adsorption-Regeneration Experimental Data: Feed: CO_2 – (H_2O, N_2) Exit: CO_2 conc.

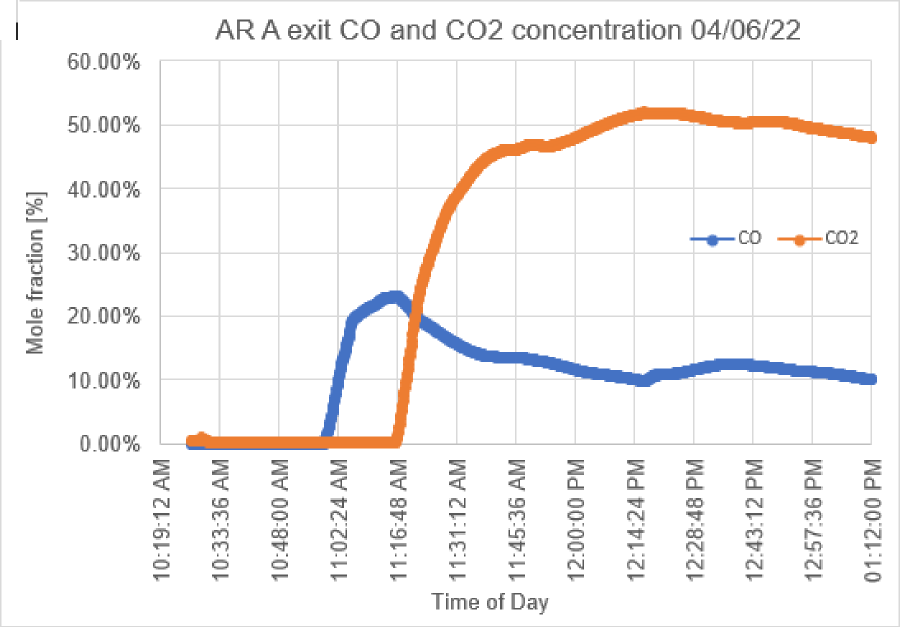


AR Experimental Data – AR breakthrough (syngas)

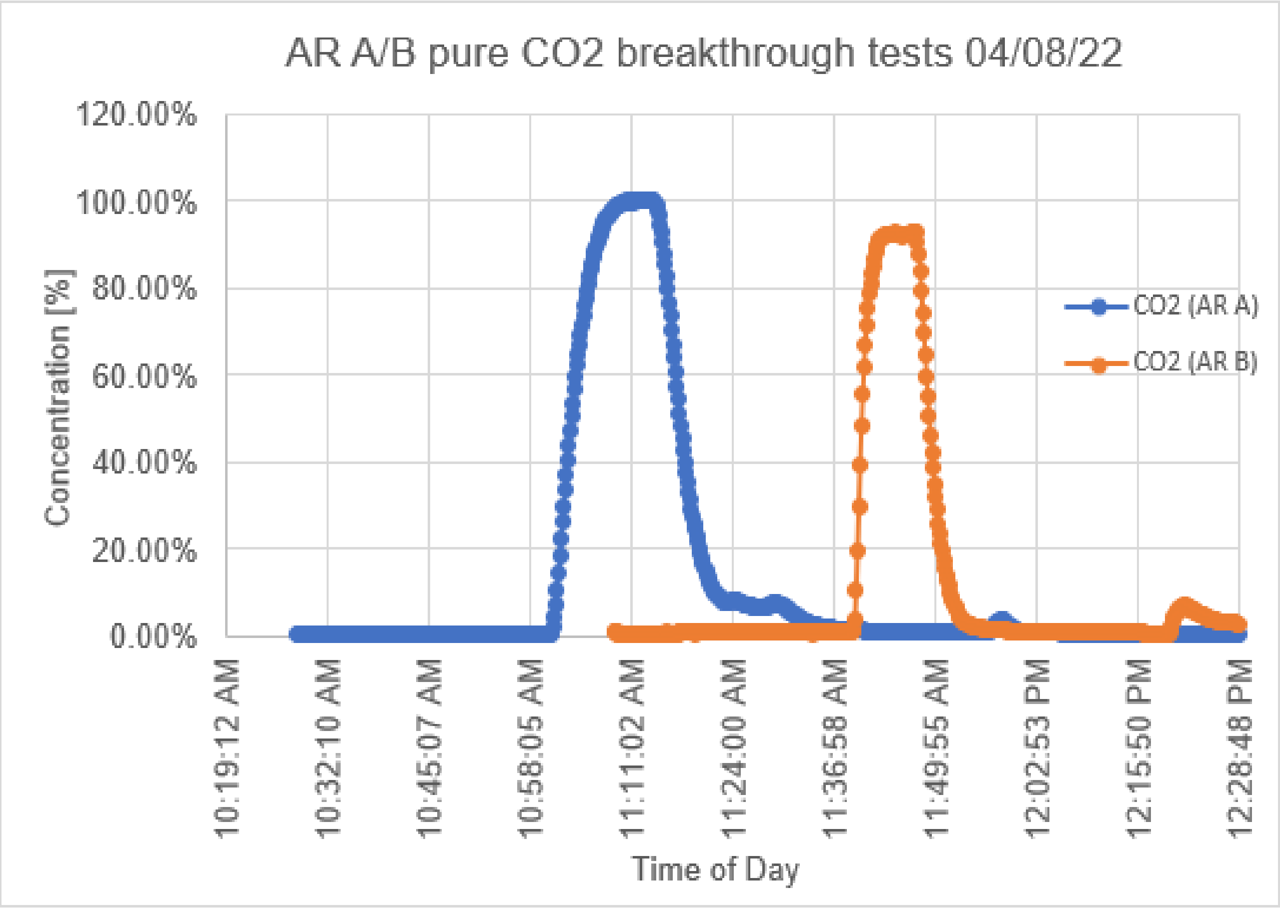


AR Feed (MR Reject)

AR Exit



AR Experimental CO_2 Breakthrough Data: Feed: CO_2 – N_2 Exit: CO_2 conc.



Operating Conditions:

AR A (2 beds in series)

- Feed T: 223^{o}C
- Feed P: 140 psi
- Flowrate: 4 slpm
- Mass of Ads.: 3505.9 g

AR B (2 beds in series)

- Feed T: 253^{o}C
- Feed P: 100 psi
- Flowrate: 4 slpm
- Mass of Ads.: 3325.4 g

AR Experimental Data – AR working/test capacity and W/F$_{CO2}$

Data set	AR	Feed gas	Working capacity (% wt.)	Test capacity (% wt.)
05/28/21	B	Syngas	3.73	-
07/23/21	B	Syngas	2.86	-
08/04/21	B	Syngas	2.54	-
	A	Syngas	1.14	-
12/10/21	B	Syngas	2.94	-
12/14/21	B	Syngas	1.50	-
12/15/21	B	Syngas	1.43	-
04/06/22	A	Syngas	-	2.49
04/07/22	A	Pure CO_2	-	4.90
04/08/22	A	Pure CO_2	-	7.30
04/08/22	B	Pure CO_2	-	4.16

Working capacity: *Ratio of the mass of CO_2 adsorbed to the mass of adsorbent in AR bed at CO_2 breakthrough.*

CO_2 breakthrough *is defined as the time for which the CO_2 exit molar flowrate, measured at the AR exit, becomes 1% of the CO_2 inlet molar flowrate.*

Test capacity: *Ratio of the mass of CO_2 adsorbed to the mass of adsorbent in AR bed past CO_2 breakthrough but before bed saturation.*

Data set	Target (g_{ads}/slpm CO_2)	Real AR A (g_{ads}/slpm CO_2)	Real AR B (g_{ads}/slpm CO_2)	Stream	Cycle Times	Cycles Run
05/24/22	10000	11772	11620	Syngas	20/20 mins	3
05/25/22	4250	4241	4142	Syngas	20/20 mins	4
05/27/22	5500	5741	5684	Syngas	15/15 mins	10
06/07/22	3500	3546	3572	Syngas	15/15 mins	4
06/08/22	4000	4100	4043	Syngas	15/15 mins	6
06/09/22	4500	4784	4267	Pure CO2	15/15 mins	3
06/10/22	1500	1518	1569	Pure CO2	15/15 mins	4

Experimental Data Analysis – AR Dispersion

- Residence time density (Rtd) experiments performed on the AR vessels

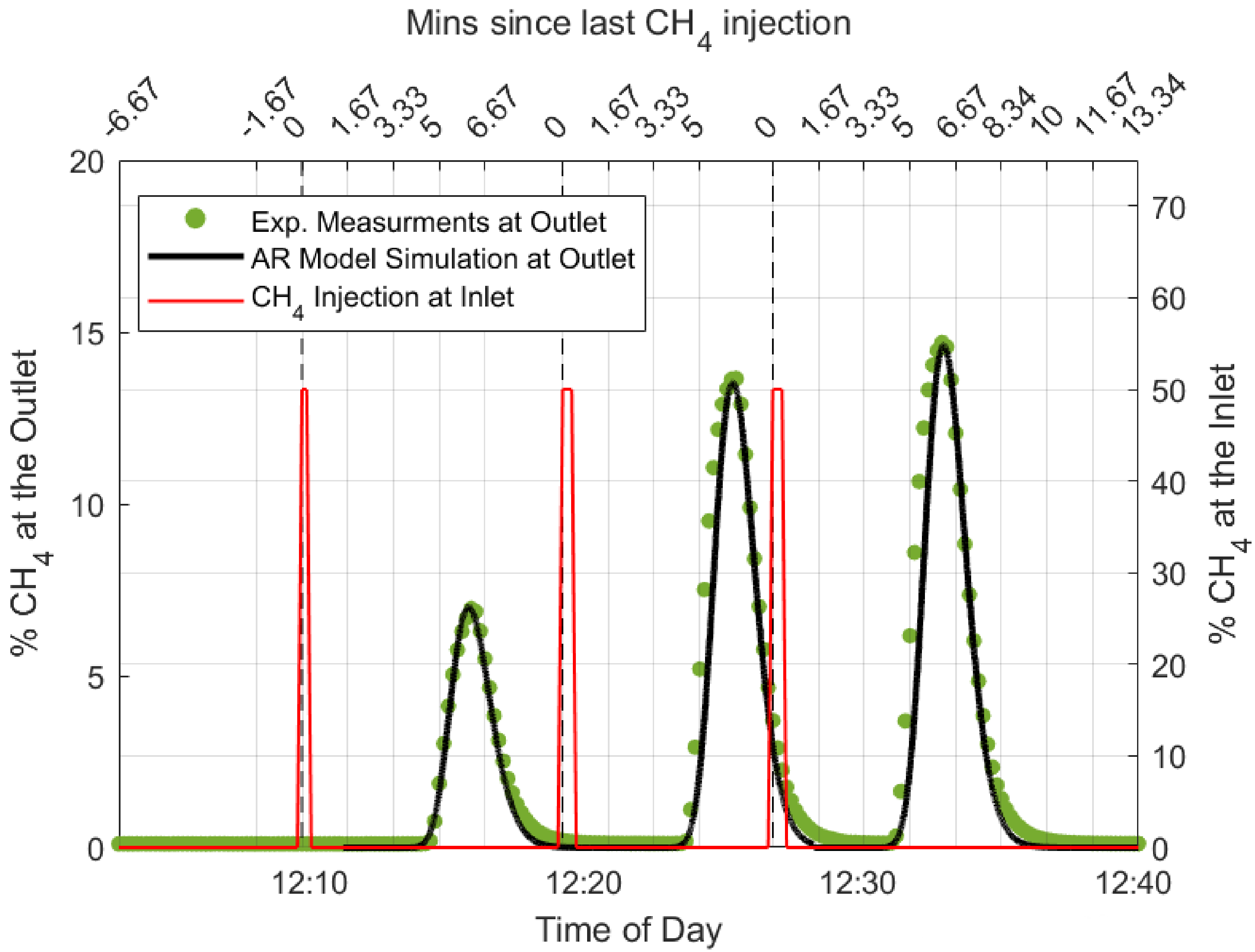
- AR vessels are filled with N_2 and CH_4 is used as a tracer (50/50 N_2/CH_4 blend)

- The tracer is injected at 3 subsequent, discrete time points for a duration of a few seconds (15 s – 35 s)

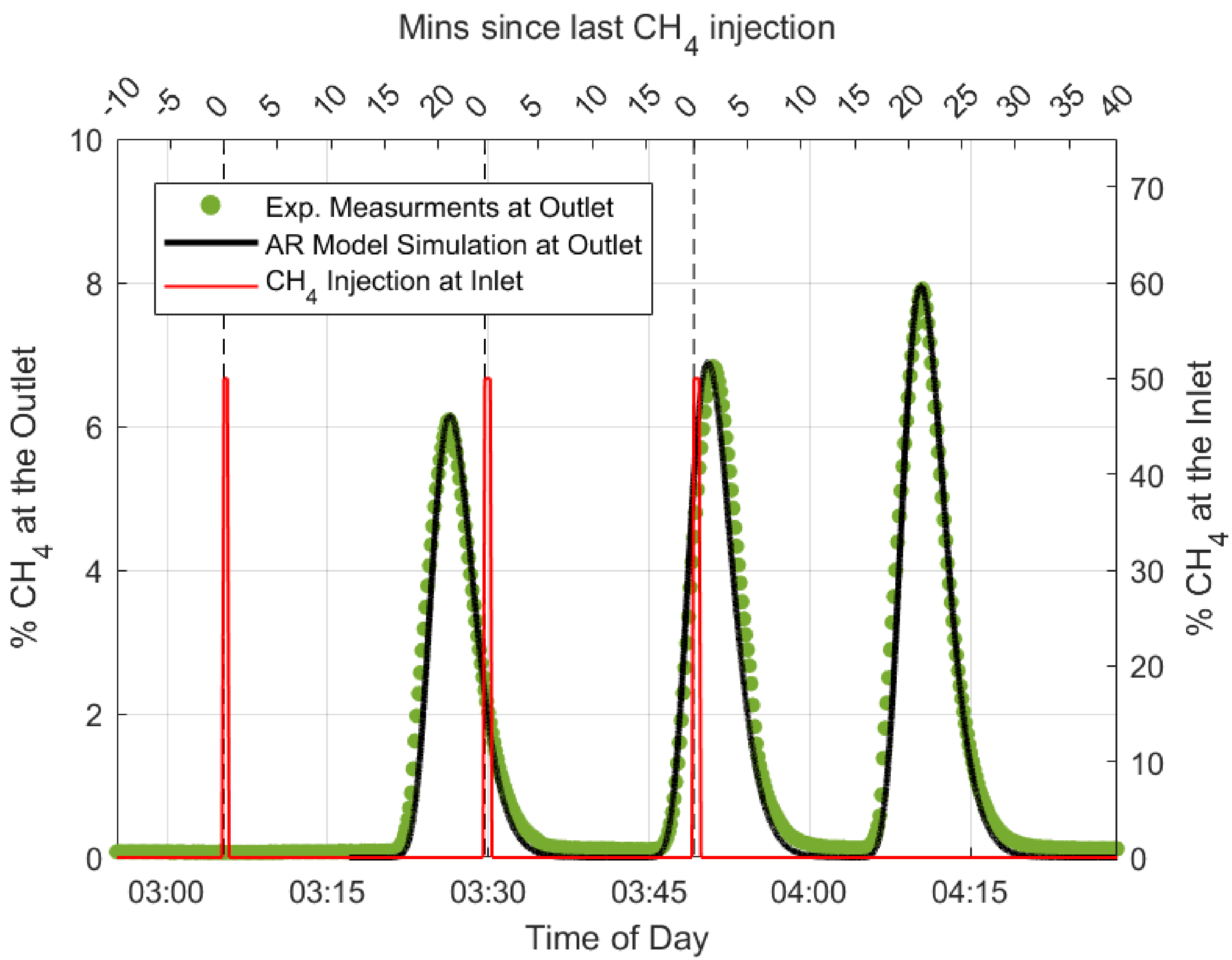
- CH4 concentration is measured at the AR outlet (Responses)

  - ➢ A dispersion coefficient for the AR model is identified that best approximates the response to the first tracer injection
  - ➢ The identified dispersion coefficient is used in simulations for the subsequent tracer responses
  - ➢ Resulting model predications show excellent agreement with the experimental data

Experimental Data Analysis – AR A Dispersion



Experimental Data Analysis – AR B Dispersion



Preliminary TEA

Preliminary TEA: Overall Performance Summary

	Case B5B	MR-AR (No Sales)	MR-AR (N2 Sales @ $30/ton)	MR-AR (Ar Sales @ $1.5/kg)	Target
Performance Summary					
Carbon Capture	90.0%	91.0%	91.0%	91.0%	N/A
CO_2 Purity	99.5%	99.7%	99.7%	99.7%	95%
Net Power Production (MWe)	543	629	593	629	N/A
COE (no T&S) [$/MWh]	135.4	109.8	89.8	89.1	94.78
CO_2 Captured Cost (no T&S) [$/ton]	63.2	37.4	9.6	9.2	N/A

Future Work

Experimental (on-going)

- Continue to assess MR and AR experimental unit performance under live syngas conditions.

Modeling (on-going)

- Continue to assess MR and AR unit model performance in regions of the parameter space compatible with carried out experiments.

Detailed TEA (Initiated)

- Update the baseline IGCC process simulation based on revised baseline document.

- Update MR-AR IGCC process simulation with experimentally validated model.

- Update all plant cost elements and assess plant economics.

Publications

- Margull Nicholas, Theodore T. Tsotsis and Vasilios I. Manousiouthakis. "On Multiscale Modeling and Simulation of a Novel Partial Pressure and Temperature Swing Adsorptive Reactor (PPTSAR) with Application to the Water Gas Shift Reaction." *Chemical Engineering Journal* (2022): 136161.

- Karagöz, Seçgin, Theodore T. Tsotsis, and Vasilios I. Manousiouthakis. "Multi-scale model based design of membrane reactor/separator processes for intensified hydrogen production through the water gas shift reaction." *International Journal of Hydrogen Energy* 45.12 (2020): 7339-7353.

- Pichardo, Patricia A., et al. "Techno-economic analysis of an intensified integrated gasification combined cycle (IGCC) power plant featuring a combined membrane reactor-adsorptive reactor (MR-AR) system." *Industrial & Engineering Chemistry Research* 59.6 (2019): 2430-2440.

- Karagöz, Seçgin, et al. "Multi-scale membrane reactor (MR) modeling and simulation for the water gas shift reaction." *Chemical Engineering and Processing-Process Intensification* 133 (2018): 245-262.

Publications

- Pichardo, Patricia A., et al. "Technical economic analysis of an intensified Integrated Gasification Combined Cycle (IGCC) power plant featuring a sequence of membrane reactors." *Journal of Membrane Science* 579 (2019): 266-282.

- Karagöz, Seçgin, et al. "Multiscale model based design of an energy-intensified novel adsorptive reactor process for the water gas shift reaction." *AIChE Journal* 65.7 (2019): e16608.

- Karagöz, Seçgin, Theodore T. Tsotsis, and Vasilios I. Manousiouthakis. "Multi-scale modeling and simulation of a novel membrane reactor (MR)/adsorptive reactor (AR) process." *Chemical Engineering and Processing-Process Intensification* 137 (2019): 148-158.

Acknowledgements

The contributions of Dr. Kunlei Liu, Dr. Dimitrios Koumoulis, and the whole University of Kentucky Center for Applied Energy Research (CAER) team, are gratefully acknowledged.

The financial support of the US Department of Energy, and the technical guidance by, and helpful discussions with, our Project Manager Katharina Daniels, and Mr. Andrew Jones, Mr. Walter W. Shelton, Mr. Travis R. Shultz, and Ms. Lynn Brickett are gratefully acknowledged.

Questions