Dynamic Modeling of a Solid-Sorbent CO_2 Capture System

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AIChE 2013 Annual Meeting
San Francisco, CA, USA, November 3-8, 2013

OUTLINE

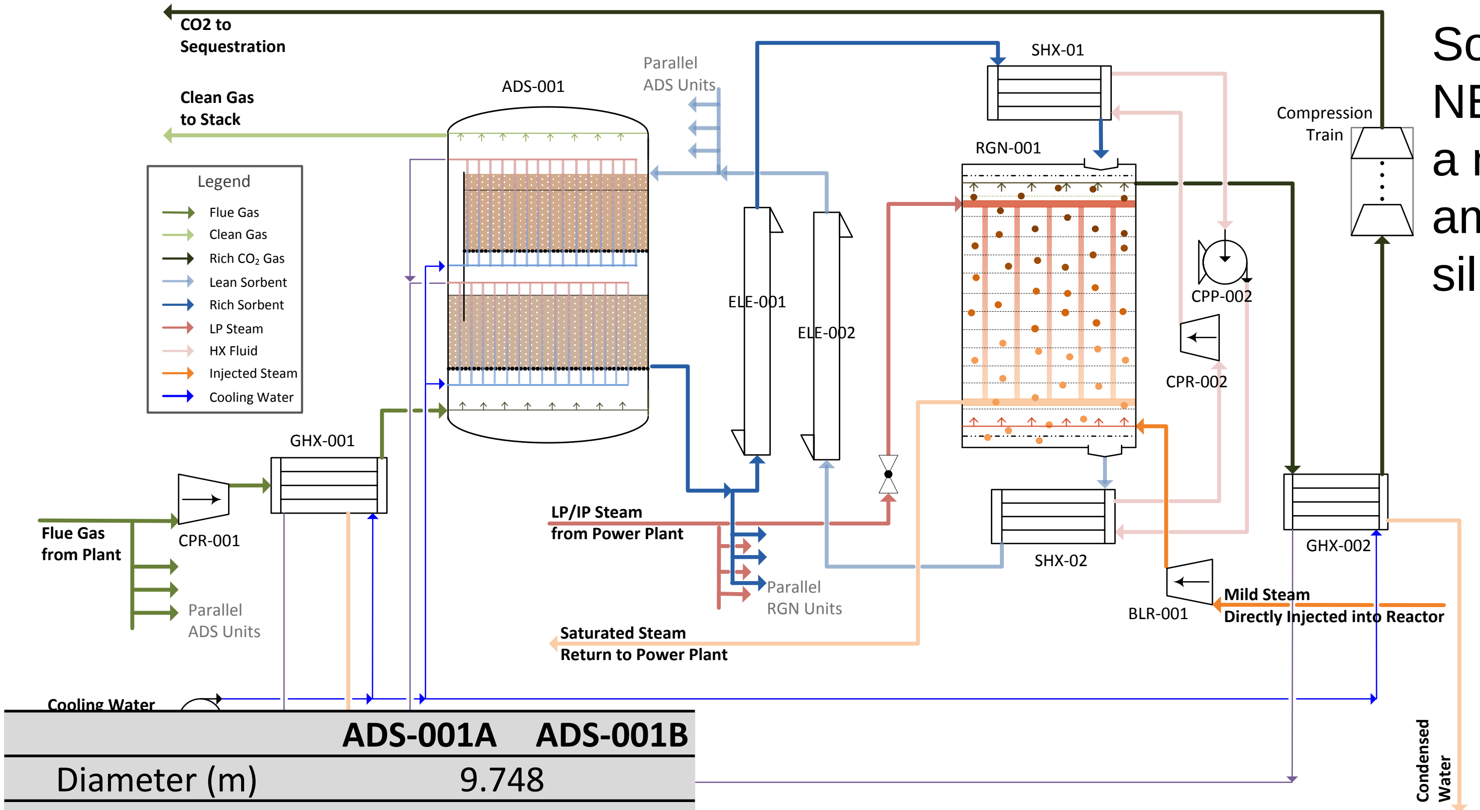
- Motivation
- Dynamic Model Development
- Results and Discussions
- Conclusions

MOTIVATION

- Under the auspices of US DOE's *Carbon Capture Simulation Initiative (CCSI),* we are developing computational models of various post-combustion CO_2 capture technologies

- As part of this project, our current focus is on the development of dynamic models and control systems for solid-sorbent CO_2 capture and compression system.

Optimized Process Developed using CCSI Toolset



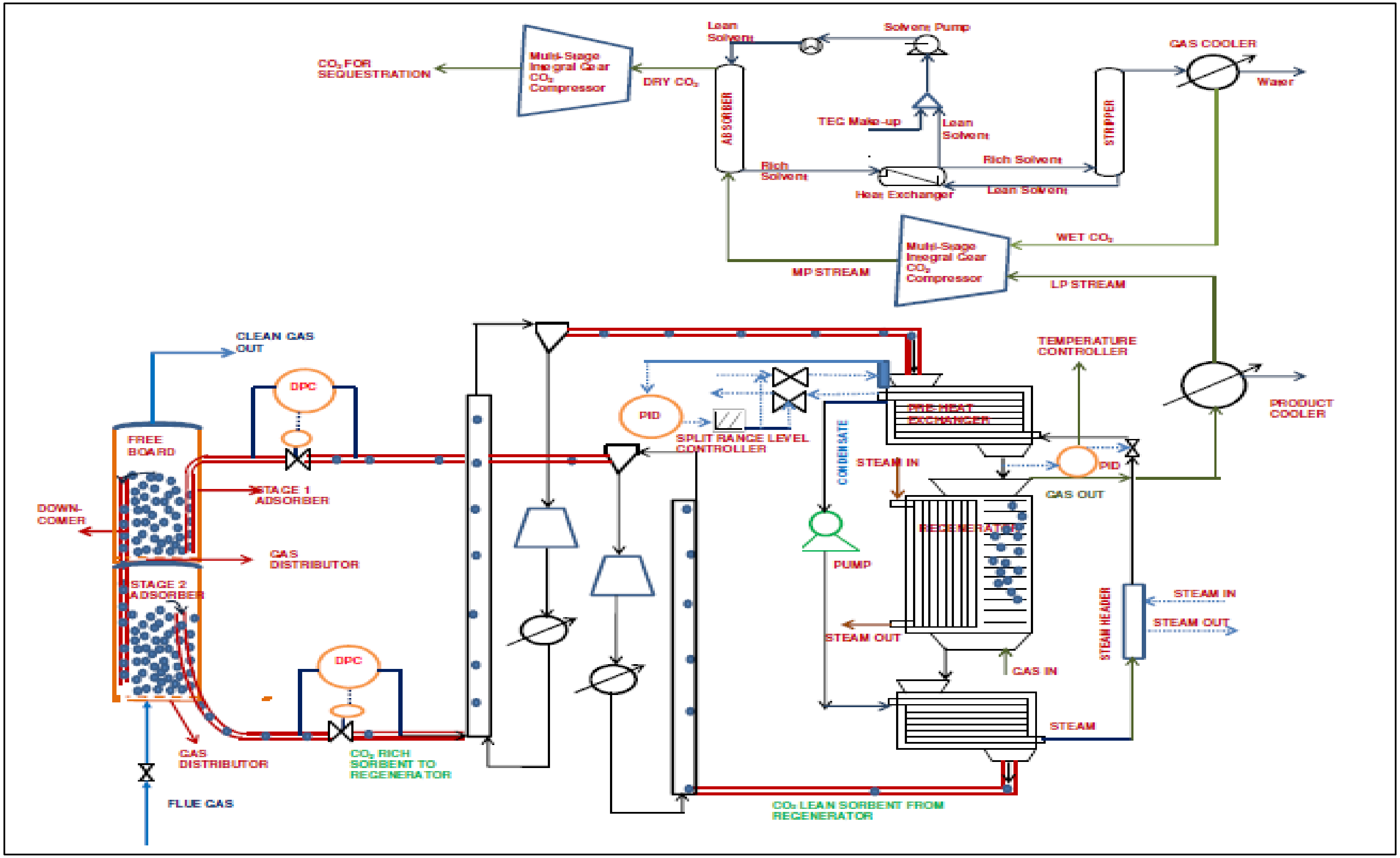
Solid Sorbent: NETL 32D, a mesoporous amine-impregnated silica substrate

	ADS-001A	ADS-001B
Diameter (m)	9.748	
Bed Depth (m)	7.232	4.854
Total HX Area (m^2)	1733.7	941.3

	RGN-001
Diameter (m)	7.147
Height (m)	4.592
Total HX Area (m^2)	1573.1

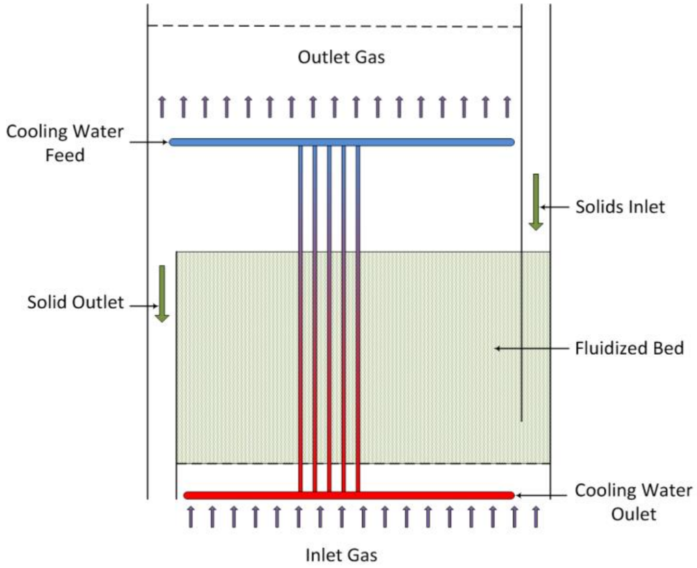
	Solid Sorbent	MEA[27] (Δ10°C HX)	MEA[27] (Δ5°C HX)
Q_Rxn (GJ/tonne CO2)	1.82	1.48	1.48
Q_Vap (GJ/tonne CO2)	0	0.61	0.74
Q_Sen (GJ/tonne CO2)	0.97	1.35	0.68
Total Q	2.79	3.44	2.90

Modeling Domain

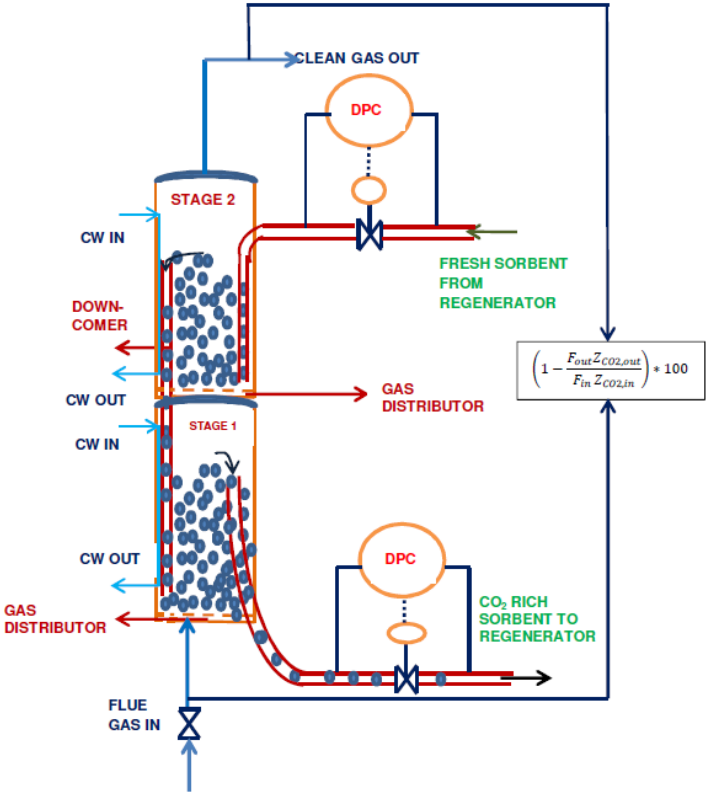


Bubbling Fluidized Bed Model Development

- 1-D two-phase pressure-driven non-isothermal dynamic model of a solid-sorbent CO_2 capture in a two-stage bubbling fluidized bed reactor system.
- Models are flexible such that it can be used as an adsorber or regenerator
- Embedded cooler/heater depending on the application
- Flexible configuration- solids can enter/leave at/from the top or bottom
- A 2-stage adsorption model with customized variables for uncertainty quantification capabilities has been developed



DYNAMIC MODEL – BUBBLING FLUIDIZED BED



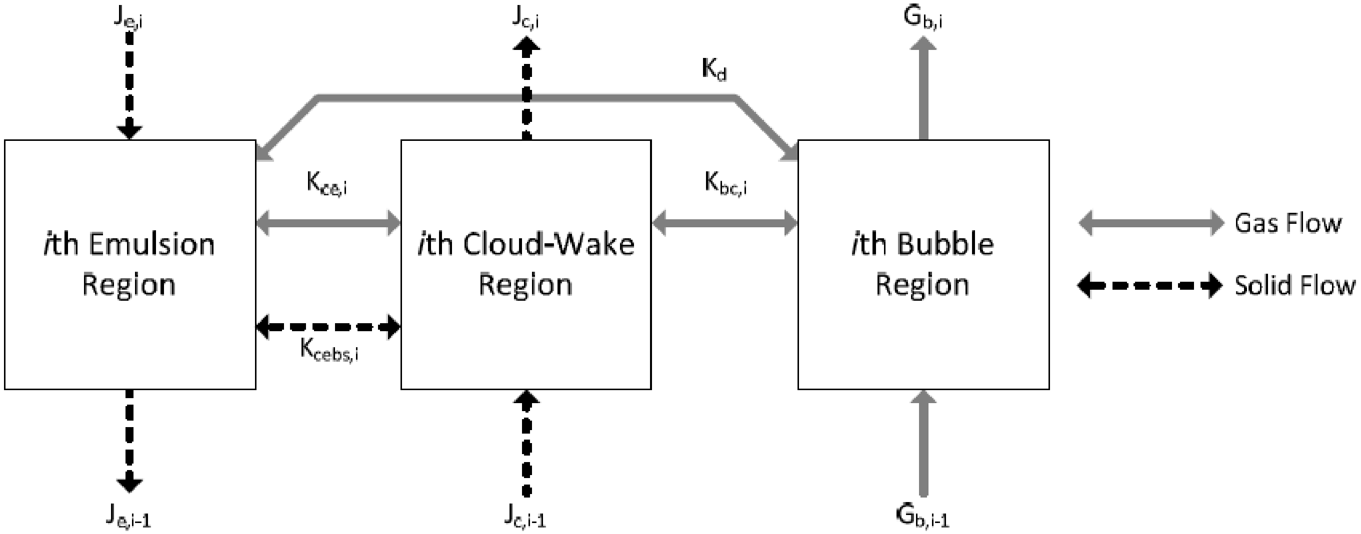
Model Assumptions

1. Each BFB consists of bubble, emulsion and cloud-wake regions.
2. Bubble region is free of solids.
3. Constant average particle properties throughout the bed
4. Adsorption-reaction takes place in solid-phase.
5. Solids leave at the top of the bed (Overflow-type configuration).
6. Transients of the immersed heat exchangers are neglected

*Lee, A.; Miller, D. A 1-D Three Region Model for a Bubbling Fluidized Bed Adsorber. *Ind. Eng. Chem. Res.* **, 52, 469-484, 2013**

* Modekurti, S.; Bhattacharyya, D., Zitney, S. E., Dynamic modeling and control studies of a two-stage bubbling fluidized bed adsorber-reactor for solid sorbent CO_2 capture, *Ind. Eng. Chem. Res.* **, 52, 10250-120260, 2013**

MODEL DEVELOPMENT



- Gaseous species : CO_2, N_2, H_2O
- Solid phase components: bicarbonate, carbamate, and physisorbed water.
- Transient species conservation and energy balance equations for both gas and solid phases in all three regions.

*Lee, A.; Miller, D. A 1-D Three Region Model for a Bubbling Fluidized Bed Adsorber. Submitted to *Ind. Eng. Chem. Res.* **2012**

CONSERVATION EQUATIONS

Bubble Region :

Gaseous Components

$$\frac{\partial\left(\delta_x A C_{b,j,x}\right)}{\partial t} = -\frac{\partial\left(y_{b,j,i} G_{b,x}\right)}{\partial x} - \delta_x A K_{bc,j,x}\left(C_{b,j,x} - C_{c,j,x}\right) + K_{g,bulk,j,x}$$

$$\begin{aligned}&\frac{\partial\left(C_{bt,x} A \delta_x C_{p,g,b,x}\left(T_{g,b,x} - T_{ref}\right)\right)}{\partial t}\\ &\quad = -\frac{\partial\left(G_{b,x} C_{p,g,b,x}\left(T_{g,b,x} - T_{ref}\right)\right)}{\partial x} - A\delta_x H_{bc,x}\left(T_{g,b,x} - T_{g,c,x}\right) + H_{g,bulk,x}\end{aligned}$$

Cloud-wake Region :

Gaseous Components

$$\begin{aligned}&\frac{\partial\left(\delta_x \alpha_x A C_{c,j,x}\right)}{\partial t}\\ &\quad = \delta_x A K_{bc,j,x}\left(C_{b,j,x} - C_{c,j,x}\right) - \delta_x A K_{ce,j,x}\left(C_{c,j,x} - C_{e,j,x}\right)\\ &\quad + \alpha_x \delta_x \left(1 - \varepsilon_{d,x}\right) A r_{g,c,j,x}\end{aligned}$$

$$\begin{aligned}&\frac{\partial\left(C_{ct,x} A \alpha_x \delta_x \varepsilon_d C_{p,g,c,x}\left(T_{g,c,x} - T_{ref}\right)\right)}{\partial t}\\ &\quad = A\delta_x H_{bc,x}\left(T_{g,b,x} - T_{g,c,x}\right) - A\delta_x H_{ce,x}\left(T_{g,c,x} - T_{g,e,x}\right)\\ &\quad - A\alpha_x \delta_x \left(1 - \varepsilon_{d,x}\right)\rho_s a_p h_{p,x}\left(T_{g,c,x} - T_{s,c,x}\right)\\ &\quad + \alpha_x \delta_x \left(1 - \varepsilon_{d,x}\right) A \sum_j \left(r_{g,c,j,x} C_{p,g,j,c,x}\left(T_{g,c,x} - T_{ref}\right)\right)\end{aligned}$$

CONSERVATION EQUATIONS

Cloud Wake Region :

Adsorbed Species

$$
\begin{aligned}
&\frac{\partial\left(A\alpha_x\delta_x\left(1-\varepsilon_{d,x}\right)\rho_s n_{c,i,x}\right)}{\partial t}\\
&\qquad = -A\frac{\partial\left(J_{c,x}n_{c,i,x}\right)}{\partial x} - K_{s,bulk,x} - A\delta_x\rho_s K_{ce,bs,x}\left(n_{c,i,x}-n_{e,i,x}\right)\\
&\qquad + A\alpha_x\delta_x\left(1-\varepsilon_{d,x}\right)r_{s,c,i,x}
\end{aligned}
$$

$$
\begin{aligned}
&\frac{\partial\left(A\alpha_x\delta_x\left(1-\varepsilon_{d,x}\right)\rho_s C_{p,s}\left(T_{s,c,x}-T_{ref}\right)\right)}{\partial t}\\
&\qquad = -A\frac{\partial\left(J_{c,x}\left(C_{p,s}\left(T_{s,c,x}-T_{ref}\right)+h_{ads,c,x}\right)\right)}{\partial x} - H_{s,bulk,x}\\
&\qquad - A\delta_x\rho_s K_{ce,bs,x}\left(C_{p,s}\left(T_{s,c,x}-T_{ref}\right)+h_{ads,c,x}-\left(C_{p,s}\left(T_{s,e,x}-T_{ref}\right)+h_{ads,e,x}\right)\right)\\
&\qquad - \alpha_x\delta_x\left(1-\varepsilon_{d,x}\right)A\sum_j\left(r_{g,c,j,x}C_{p,g,j,c,x}\left(T_{g,c,x}-T_{ref}\right)\right)\\
&\qquad + A\alpha_x\delta_x\left(1-\varepsilon_{d,x}\right)\rho_s a_p h_{p,x}\left(T_{g,c,x}-T_{s,c,x}\right)
\end{aligned}
$$

CONSERVATION EQUATIONS CONTD.

Emulsion Region :

Gaseous Components

$$\frac{\partial\left(A\left(1-\alpha_x\delta_x-\delta_x\right)\varepsilon_d C_{e,j,x}\right)}{\partial t} = \delta_x A K_{ce,j,x}\left(C_{c,j,x}-C_{e,j,x}\right)-K_{g,bulk,j,x}+\left(1-\alpha_x\delta_x-\delta_x\right)\left(1-\varepsilon_{d,x}\right)A r_{g,e,j,x}$$

$$\begin{aligned}\frac{\partial\left(C_{et,x}A\left(1-\alpha_x\delta_x-\delta_x\right)\varepsilon_d C_{p,g,e,x}\left(T_{g,e,x}-T_{ref}\right)\right)}{\partial t} &= A\delta_x H_{ce,x}\left(T_{g,c,x}-T_{g,e,x}\right)-H_{g,bulk,x}\\ &-A\left(1-\alpha_x\delta_x-\delta_x\right)\left(1-\varepsilon_{d,x}\right)\rho_s a_p h_{p,x}\left(T_{g,e,x}-T_{s,e,x}\right)\\ &+A\left(1-\alpha_x\delta_x-\delta_x\right)\left(1-\varepsilon_{d,x}\right)\sum_j\left(r_{g,e,j,x}C_{p,g,j,e,x}\left(T_{g,e,x}-T_{ref}\right)\right)\end{aligned}$$

CONSERVATION EQUATIONS CONTD.

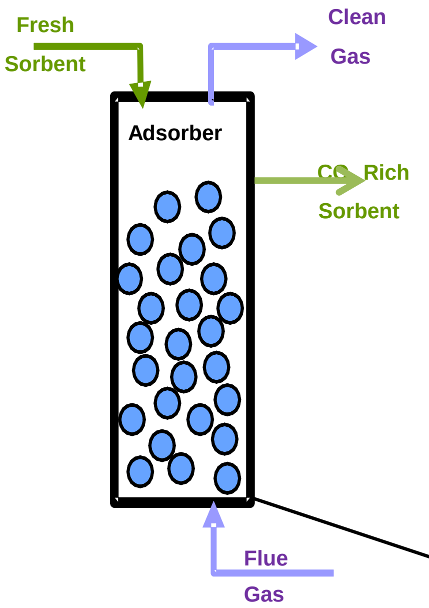
Emulsion Region :

Adsorbed Species

$$\begin{aligned}\frac{\partial\left(A(1-\alpha_x\delta_x-\delta_x)(1-\varepsilon_{d,x})\rho_s n_{e,i,x}\right)}{\partial t}\\ &= -A\frac{\partial\left(J_{e,x}n_{e,i,x}\right)}{\partial x}+K_{s,bulk,x}+A\delta_x\rho_s K_{ce,bs,x}\left(n_{c,i,x}-n_{e,i,x}\right)\\ &+A(1-\alpha_x\delta_x-\delta_x)(1-\varepsilon_{d,x})r_{s,e,i,x}\end{aligned}$$

$$\begin{aligned}\frac{\partial\left(A(1-\alpha_x\delta_x-\delta_x)(1-\varepsilon_{d,x})\rho_s C_{p,s}\left(T_{s,e,x}-T_{ref}\right)\right)}{\partial t}\\ &= -A\frac{\partial\left(J_{e,x}\left(C_{p,s}\left(T_{s,e,x}-T_{ref}\right)+h_{ads,e,x}\right)\right)}{\partial x}+H_{s,bulk,x}\\ &+A\delta_x\rho_s K_{ce,bs,x}\left(C_{p,s}\left(T_{s,c,x}-T_{ref}\right)+h_{ads,c,x}-\left(C_{p,s}\left(T_{s,e,x}-T_{ref}\right)+h_{ads,e,x}\right)\right)\\ &-A(1-\alpha_x\delta_x-\delta_x)(1-\varepsilon_{d,x})\sum_j\left(r_{g,e,j,x}C_{p,g,j,e,x}\left(T_{g,e,x}-T_{ref}\right)\right)\\ &+A(1-\alpha_x\delta_x-\delta_x)(1-\varepsilon_{d,x})\rho_s a_p h_{p,x}\left(T_{g,e,x}-T_{s,e,x}\right)\\ &+\pi d_{HX}h_{t,x}\Delta T_{HX,x}N_{HX}C_r\end{aligned}$$

HYDRODYNAMIC MODEL



$$\left(\frac{\sqrt{d_{b,u,x}}-\sqrt{d_{b,e,x}}}{\sqrt{d_{b,0}}-\sqrt{d_{b,e,x}}}\right)^{\left(1-\frac{\gamma_1}{\gamma_{3,x}}\right)}\left(\frac{\sqrt{d_{b,u,x}}-\sqrt{\gamma_{2,x}}}{\sqrt{d_{b,0}}-\sqrt{\gamma_{2,x}}}\right)^{\left(1+\frac{\gamma_1}{\gamma_{3,x}}\right)}=e^{\left(\frac{0.3x}{D_t}\right)}$$

where $\gamma_1=\frac{2.56\times10^{-2}}{v_{mf}}\sqrt{\frac{D_t}{g}}$ and $\gamma_{3,x}=\sqrt{\gamma_1{}^2+4\frac{d_{b,m,x}}{D_t}}$

$$d_{b,e,x}=\frac{D_t}{4}\left(-\gamma_1+\gamma_{3,x}\right)^2$$

$$d_{b,m,x}=2.59\,g^{-0.2}\left(A_x\left[v_{g,x}-v_{e,x}\right]\right)^{0.4}$$

$$d_{b,0}=1.38\,g^{-0.2}\left(a_o\left[v_{g,0}-v_{e,0}\right]\right)^{0.4}$$

Mori and Wen (1975)

$$v_{b,x}=v_{g,x}-v_{mf}+0.35\sqrt{gD_{t,h}}$$

$$K_{bc,j,x}=1.32\times4.5\frac{v_{mf}}{d_{b,x}}+5.85\frac{D_{j,x}{}^{0.5}g^{0.25}}{d_{b,x}{}^{5/4}}$$

$$K_{ce,j,x}=6.78\sqrt{\frac{\varepsilon_{d,x}{}^2D_{j,x}v_{b,x}}{d_{b,x}{}^3}}$$

Sit and Grace (1981)

REACTION KINETICS

$$H_2O_{(g)} \leftrightarrow H_2O_{(phys)}$$

$$2R_2NH + CO_{2,(g)} \leftrightarrow R_2NH_2^+ + 2R_2NCO_2^-$$

$$R_2NH + CO_{2,(g)} + H_2O_{(phys)} \leftrightarrow R_2NH_2^+ + HCO_3^-$$

$$r_{1,r,i} = k_{1,r,i}\left(\frac{P_i C_{r,H_2O,i}}{C_{r,t,i}} - \frac{n_{r,H_2O,i}}{K_{1,r,i}}\right)$$

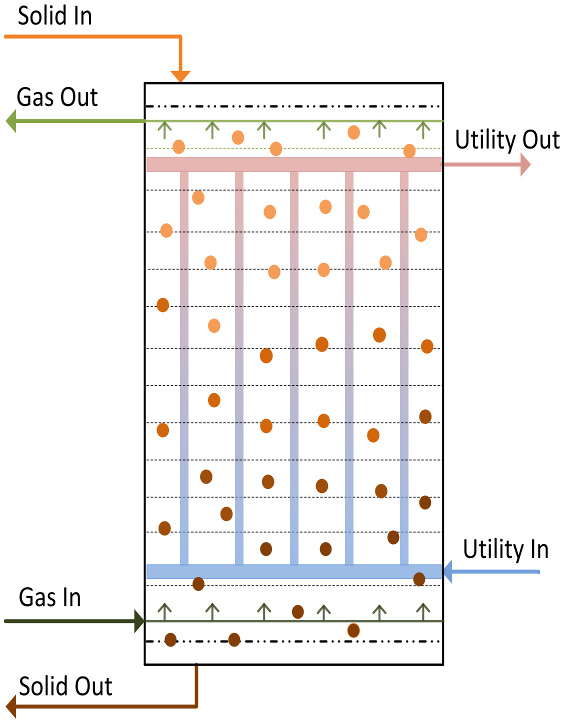
$$r_{2,r,i} = k_{2,r,i}\left(\left[1 - 2\frac{n_{r,carb,i}}{n_v} - \frac{n_{r,bicarb,i}}{n_v}\right] n_{r,H_2O,i}\left[\frac{P_i C_{r,CO_2,i}}{C_{r,t,i}}\right] - \left[\frac{\left\{\frac{n_{r,carb,i}}{n_v} + \frac{n_{r,bicarb,i}}{n_v}\right\} n_{r,bicarb,i}}{K_{2,r,i}}\right]\right)$$

$$r_{3,r,i} = k_{3,r,i}\left(\left[1 - 2\frac{n_{r,carb,i}}{n_v} - \frac{n_{r,bicarb,i}}{n_v}\right]^2 \left[\frac{P_i C_{r,CO_2,i}}{C_{r,t,i}}\right] - \left[\frac{\left\{\frac{n_{r,carb,i}}{n_v} + \frac{n_{r,bicarb,i}}{n_v}\right\} n_{r,carb,i}}{K_{3,r,i}}\right]\right)$$

*Lee et al. A model for the Adsorption Kinetics of CO_2 on Amine-Impregnated Mesoporous Sorbents in the Presence of Water, 28th International Pittsburgh Coal Conference 2011, Pittsburgh, PA, USA.

Dynamic Model–Moving Bed Reactor

- ➢ 1-D two-phase pressure-driven non-isothermal dynamic model of a moving bed reactor mainly for the regenerator application



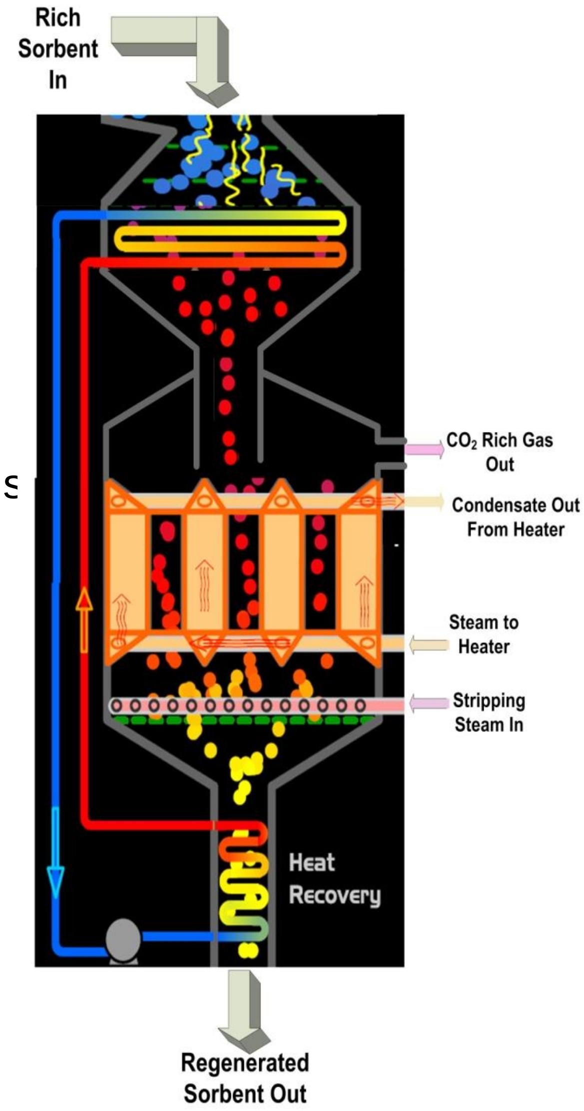
Model Assumptions

- ➢ Vertical shell & tube type reactor
- ➢ Gas and solids flows are modeled by plug flow model with axial dispersion.
- ➢ Particles are uniformly dispersed through the reactor with constant voidage
- ➢ Particle attrition ignored
- ➢ Temperature is uniform within the particles

- Gaseous species : CO_2, N_2, H_2O
- Solid phase components: bicarbonate, carbamate, and physisorbed water.

Development of Moving Bed Model

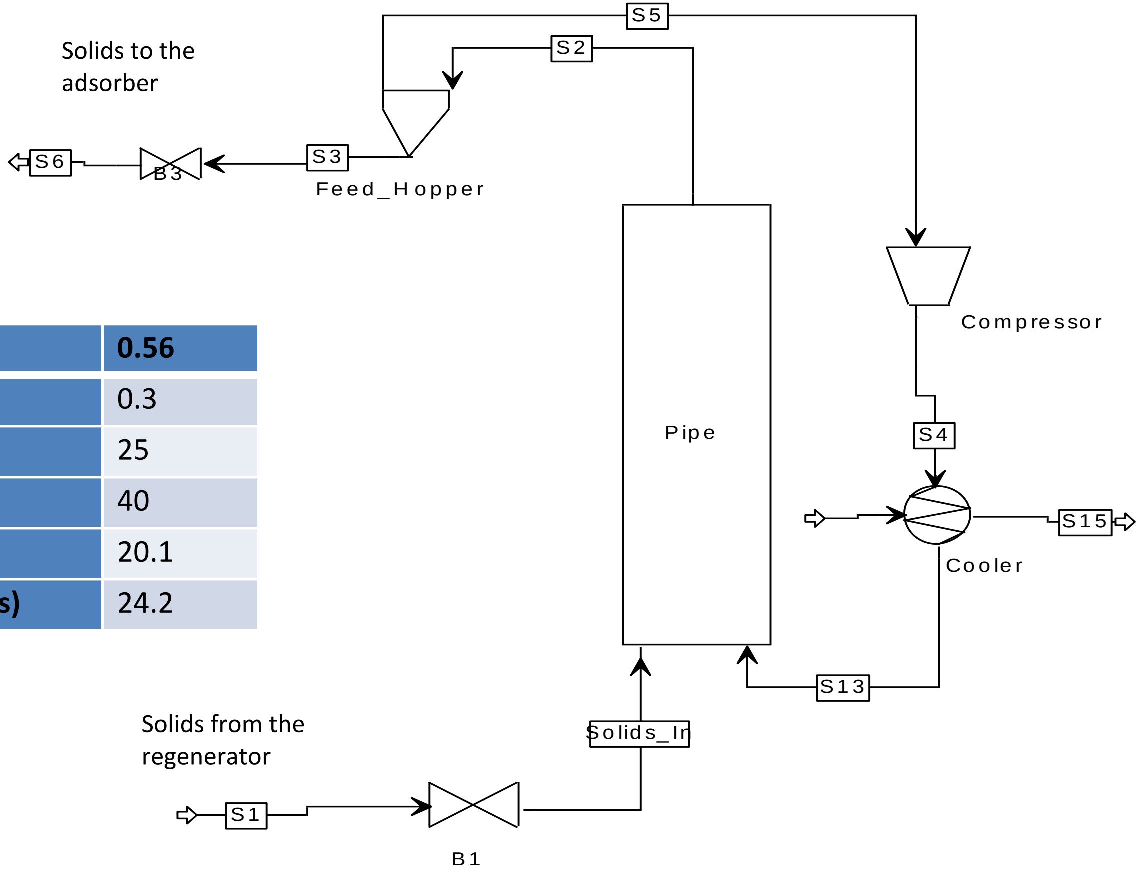
- Integrated pre and post-heat exchangers are considered for heat recovery
- Gas and solids flows are modeled by plug flow model with axial dispersion
- For pressure drop calculation, a modified Ergun equation by using the slip velocity between the solids and gas is used instead of the s velocity
- Energy balance equations consider heat transfer between solid and gas and tube wall and the mixed phase
- Heat transfer coefficient between the mixed phase and the tube wall is calculated by a modified packet-renewal theory
- Bed hydrodynamics are described by analogy to fixed bed and fluidized bed systems
- Reaction kinetics are similar to the bubbling bed model



Pneumatic Transport Modeling

- Assumptions
  - Isothermal
  - Ideal separation of gases and solids. Therefore, transport gas is free of solids after separation.
  - No mass transfer and reactions during the transport
- Options considered for the transport medium
  - Unclean flue gas from the adsorber inlet
  - Clean flue gas from the adsorber outlet
  - **A recycling transport medium with makeup from the clean gas**
  - CO_2 from the outlet of the regenerator
- Calculation of the overall pressure drop in the vertical pipe
  - Pressure drop due to gas acceleration
  - Pressure drop due to solids acceleration
  - Pressure drop due to gas to pipe friction
  - Pressure drop due to solids to pipe friction
  - Pressure drop due to static head of the solids

Pneumatic Transport Modeling: Regenerator to Adsorber

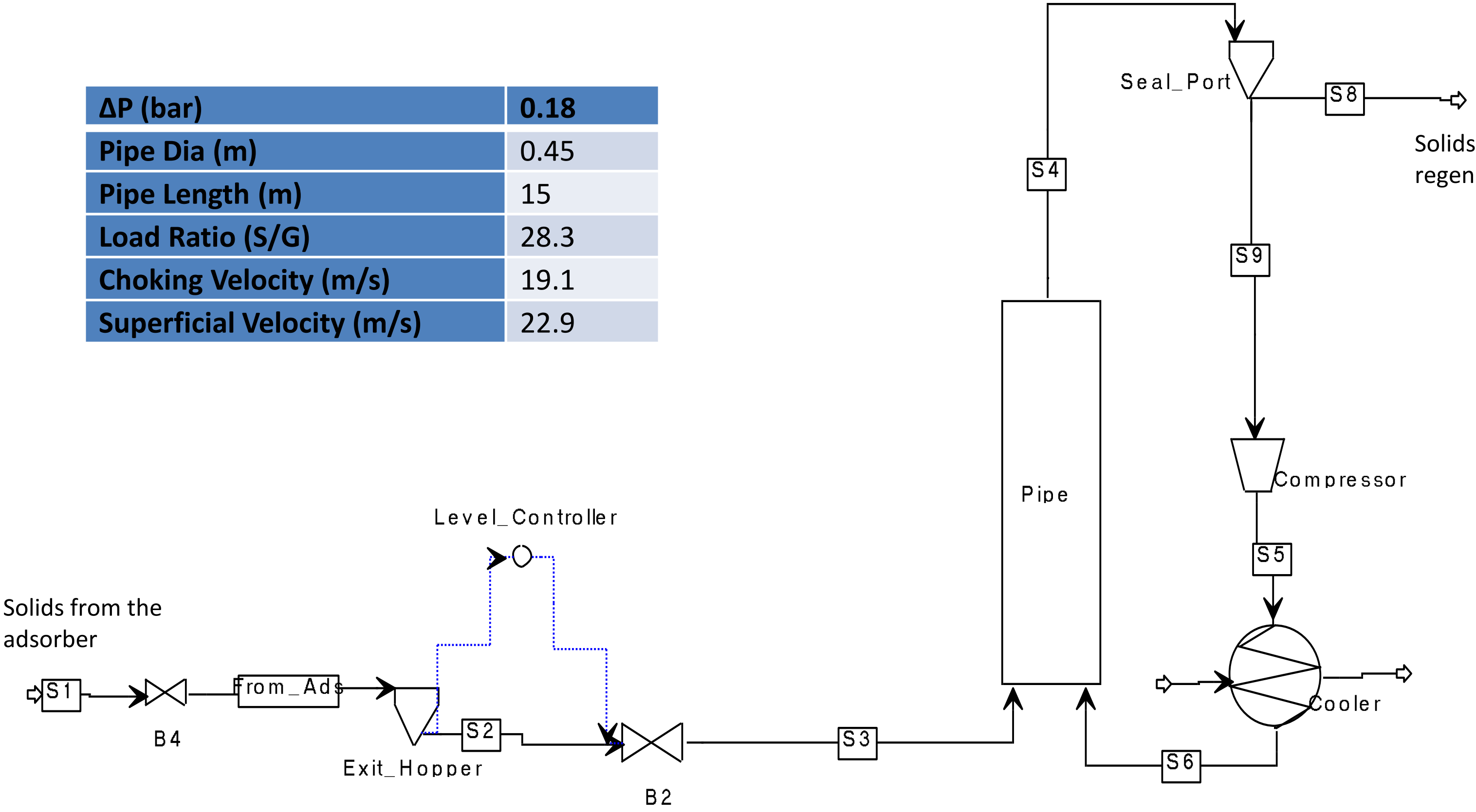

Solids to the adsorber

Solids from the regenerator

ΔP (bar)	**0.56**
Pipe Dia (m)	0.3
Pipe Length (m)	25
Load Ratio (S/G)	40
Choking Velocity (m/s)	20.1
Superficial Velocity (m/s)	24.2

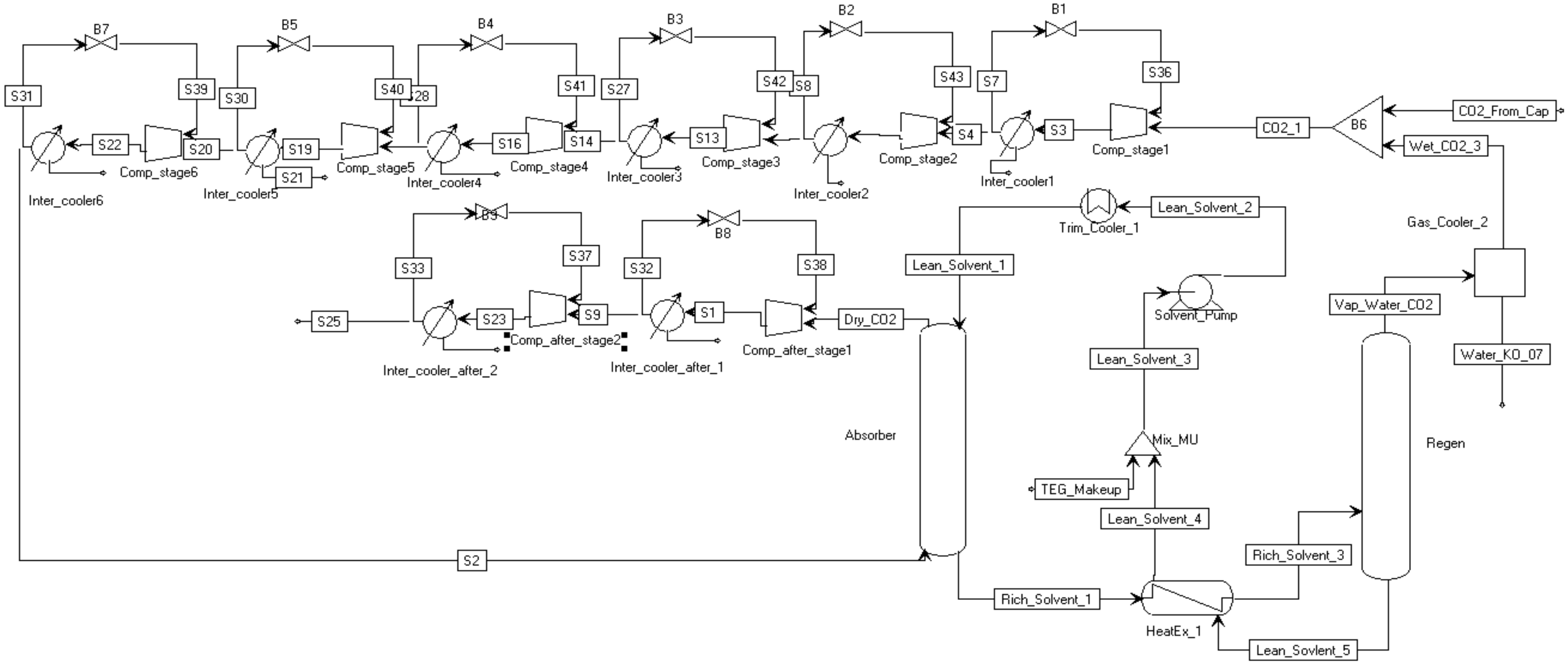
Pneumatic Transport Modeling: Adsorber to Regenerator

ΔP (bar)	0.18
Pipe Dia (m)	0.45
Pipe Length (m)	15
Load Ratio (S/G)	28.3
Choking Velocity (m/s)	19.1
Superficial Velocity (m/s)	22.9



CO_2 Compression System Model

- Dynamic model of a multi-stage integral gear compressor system with inter-stage coolers, knock-out drums, and TEG absorption system has been developed.
- Performance curves obtained from a commercial vendor has been used for calculating off-design performance.



CO_2 Compression System Model

Dimensionless Exit Flow Coefficient

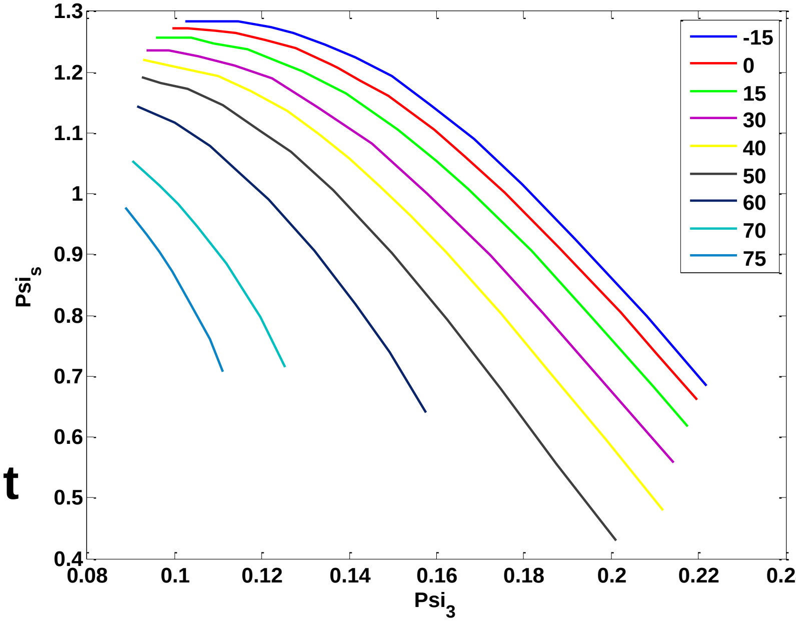
$$\varphi_3 = \frac{\dot{V}_3}{\pi d_2 b_2 u_2}$$

$$\dot{V}_3 = \dot{V}_s \frac{z_d T_d P_s}{P_d z_s T_s}$$

$$T_d = T_s \left(\frac{P_d}{P_s}\right)^{\frac{k-1}{k\eta}}$$

Dimensionless Isentropic Head Coefficient

$$\varphi_s = \frac{2 y_s}{u_2^2}$$



y_s = Isentropic head = $z_s R T_s \frac{k}{k-1}\left(\left(\frac{P_d}{P_s}\right)^{\frac{k-1}{k}} - 1\right)$

$$\varphi_s = A\varphi_3^2 + B\varphi_3 + C$$

CO$_2$ Compressor Load Control

IGV Model

$$y = ae^{bx} + ce^{dx}$$

Surge Detection and Control

$$\frac{\partial}{\partial \dot{V}}\left({}^{P_d}/_{P_s}\right) = 0$$

$$\frac{\partial \varphi_s}{\partial \varphi_3} = 0$$

$$PS = \frac{\varphi_3^{op} - \varphi_3^*}{\varphi_3^*}$$

Gain Scheduling Controller

$$\sigma_\lambda(\xi) = \begin{cases} 0 & if\, 0 \le \xi \le \lambda \\ \xi - \lambda & if\, \xi > \lambda \end{cases}$$

$$\begin{aligned} u(t) &= k(t)y(t) + u_0 \\ k(t) &= \alpha\sigma_\lambda\left(|y(y)|\right) \\ k(0) &= k_0 \end{aligned}$$

Modeling of Balance of the Plant

1. Pressure flow-network along with the control valves

2. Gas and Solid distributors

3. Downcomer and Exit-hopper

4. Other components such as flue-gas stack etc.

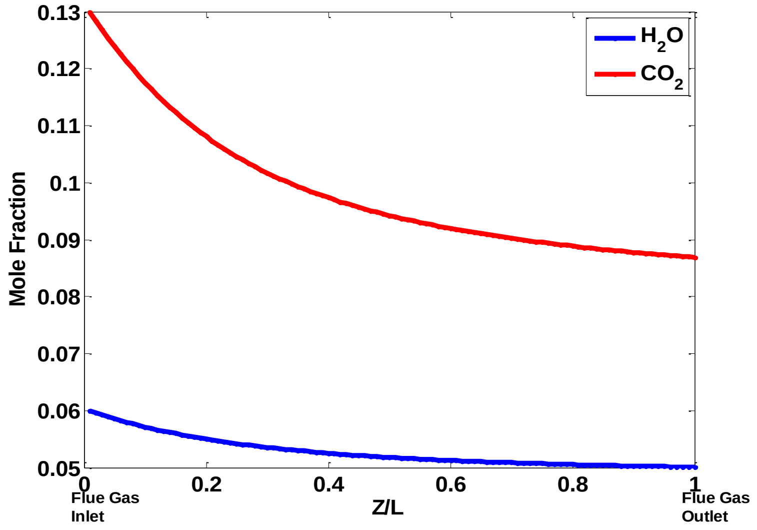
5. Pre-heater, post-heat exchanger, post-cooler, steam and BFW system for heat recovery

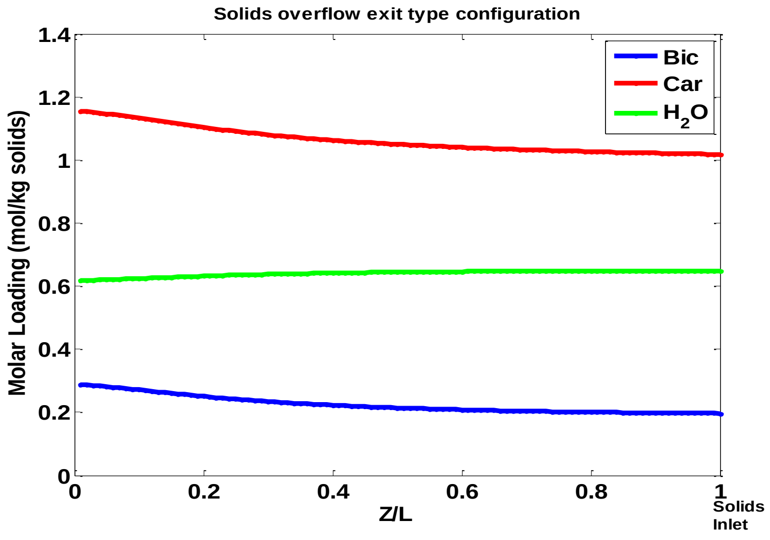
SOLUTION METHODOLOGY

- All models are set up in Aspen Custom Modeler
- The dynamic model is solved by using the Method of Lines
- ACM model is embedded in Simulink for LMPC implementation.

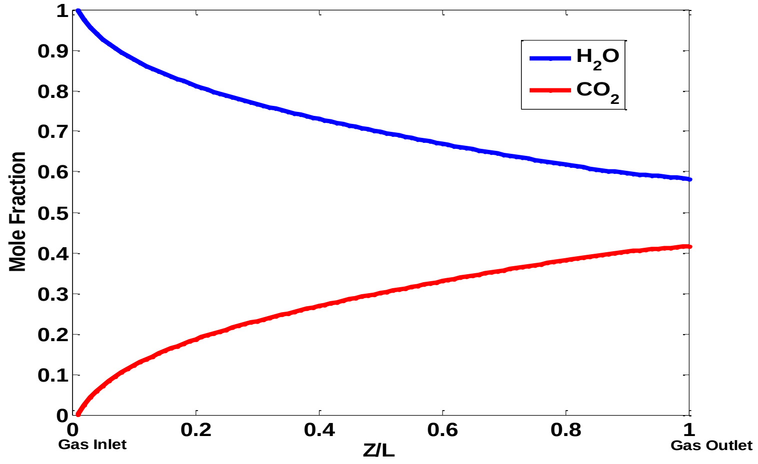
Bubbling Bed Model : Results from Single Stage

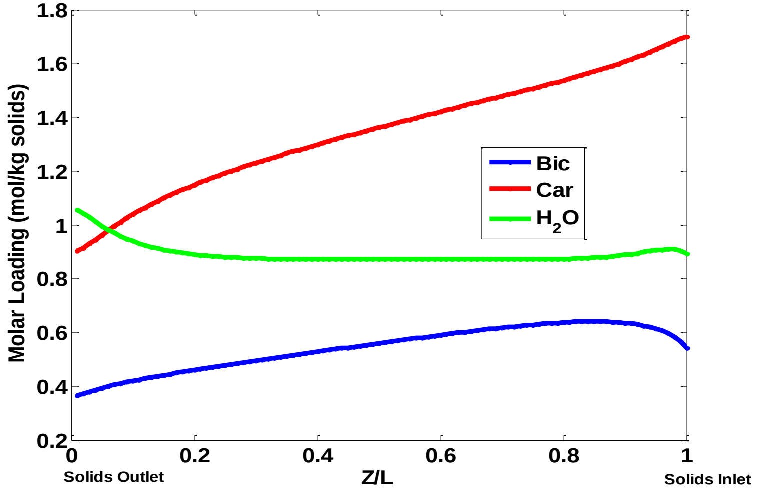
Adsorber



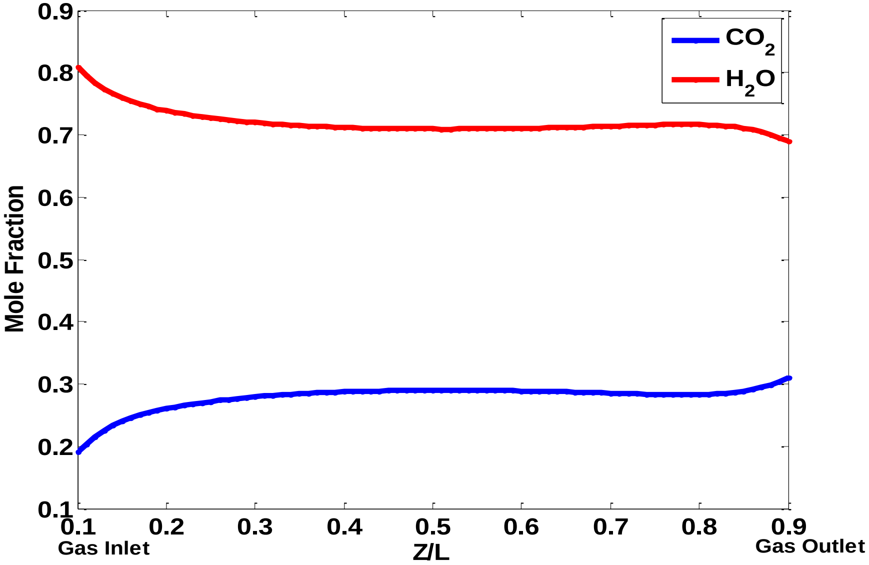


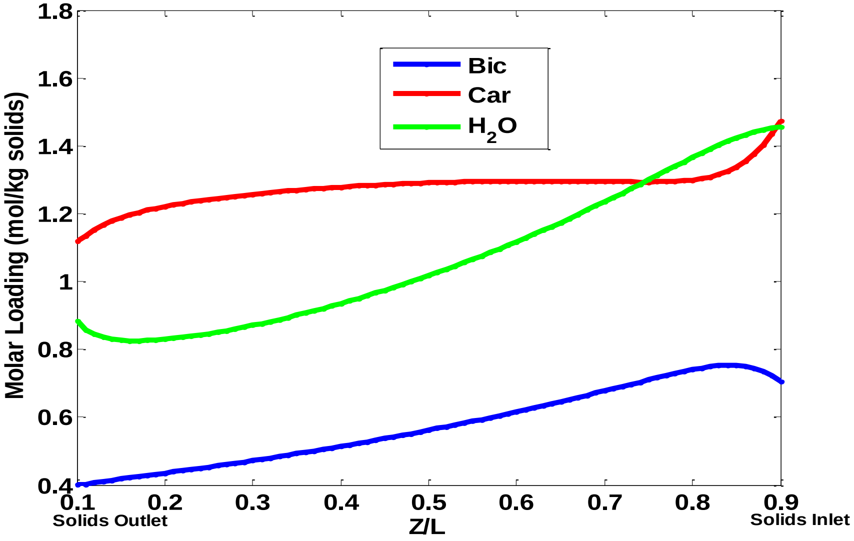
Regenerator

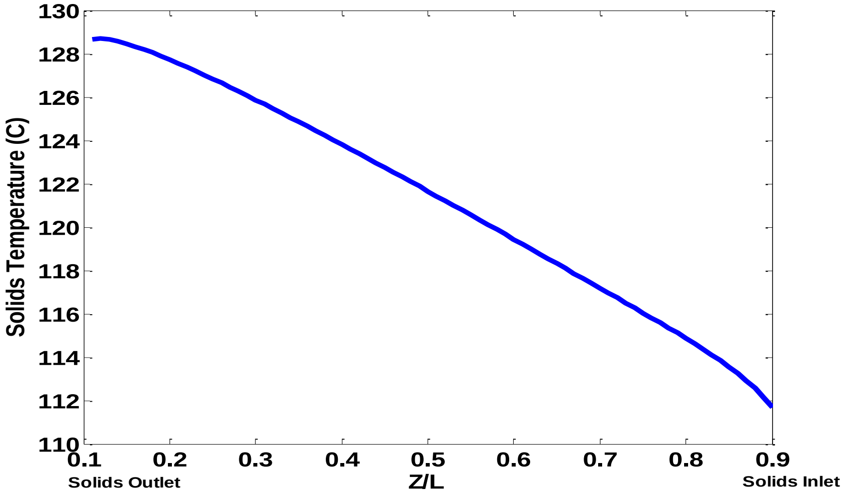


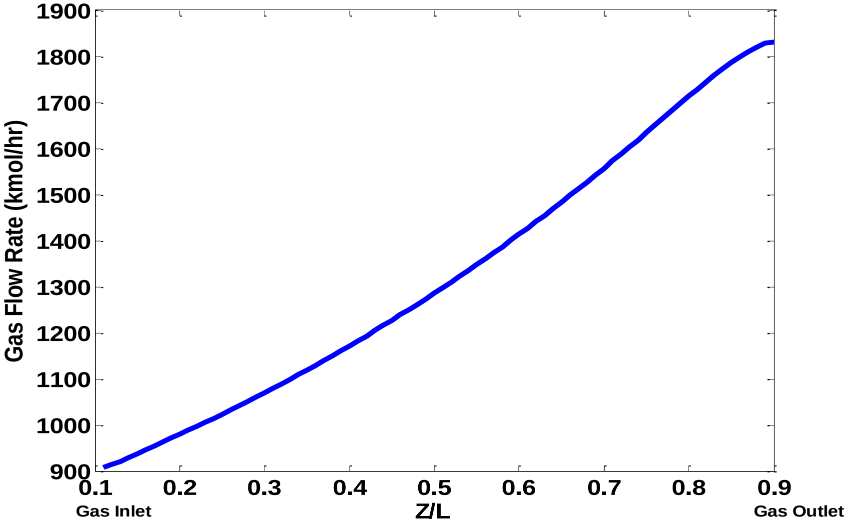


Moving Bed Regenerator: Results





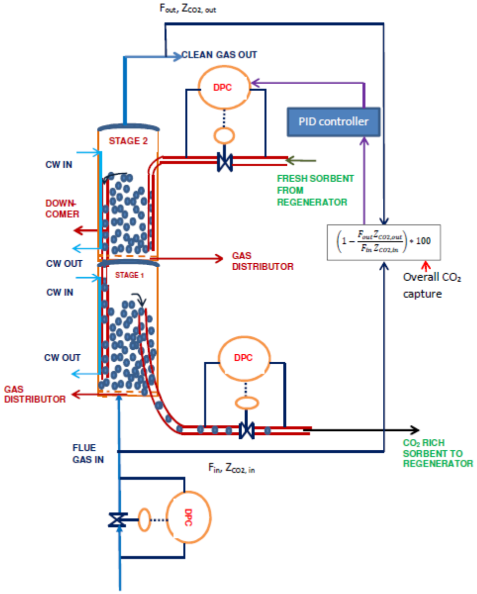


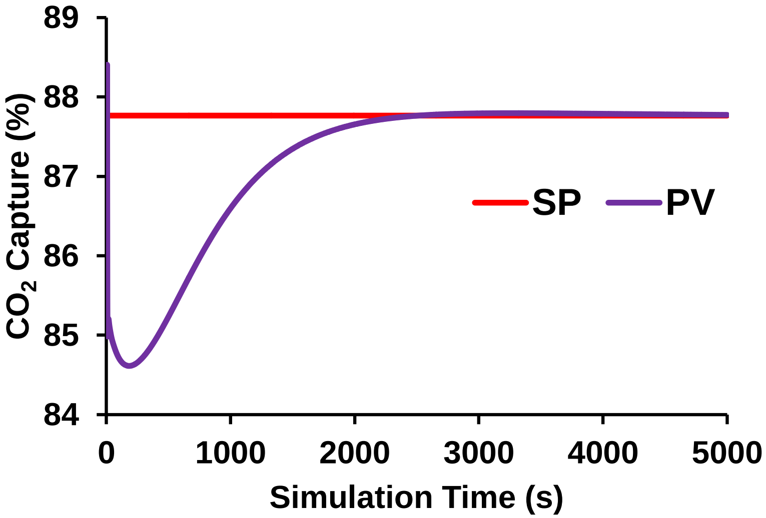


CONTROLLER DESIGNS FOR MAINTINING CO_2 CAPTURE – ADSORBER-ONLY (20% step increase in flue gas flowrate)

1. PID CONTROLLER

- PID controller for controlling CO_2 capture by manipulating the solid sorbent flowrate.
- Note the large undershoot and long settling time.





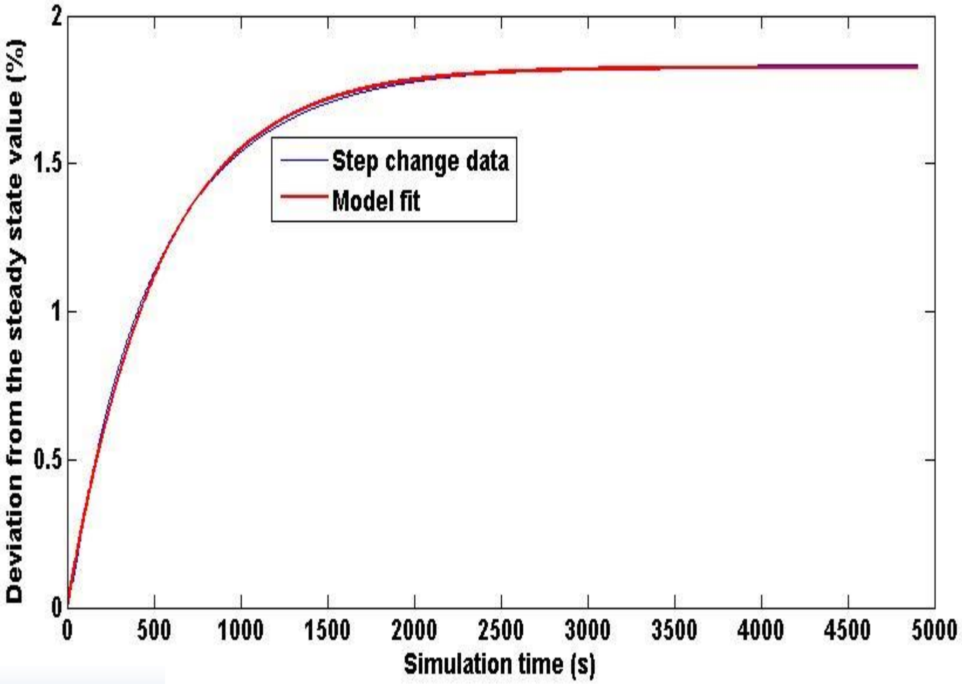
Configuration and Performance of the PID Controller

CONTROLLER DESIGN CONTD.

2.FEEDBACK-AUGMENTED FEEDFORWARD CONTROLLER

- Data for the process and disturbance models are generated by implementing step changes in the sorbent flowrate and the flue gas flowrate, respectively.

- Process and disturbance models are identified in MATLAB as first-order and pure-gain-plus-second–order models, respectively.



Comparison of the process model to the data from ACM®

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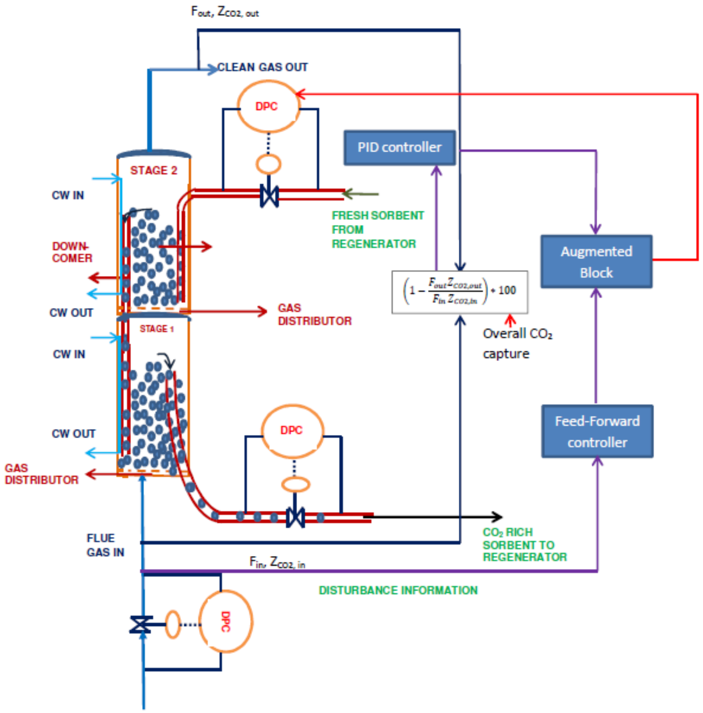
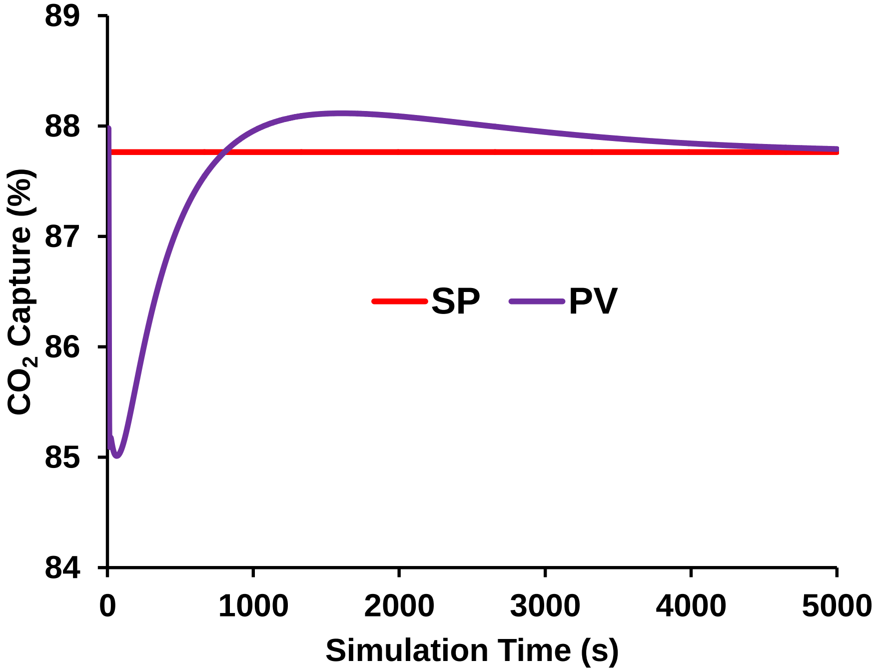
2.FEEDBACK-AUGMENTED FEEDFORWARD CONTROLLER

- Note the smaller/shorter undershoot with large overshoot and settling time





Configuration and Performance of the Feedback-Augmented Feedforward Controller

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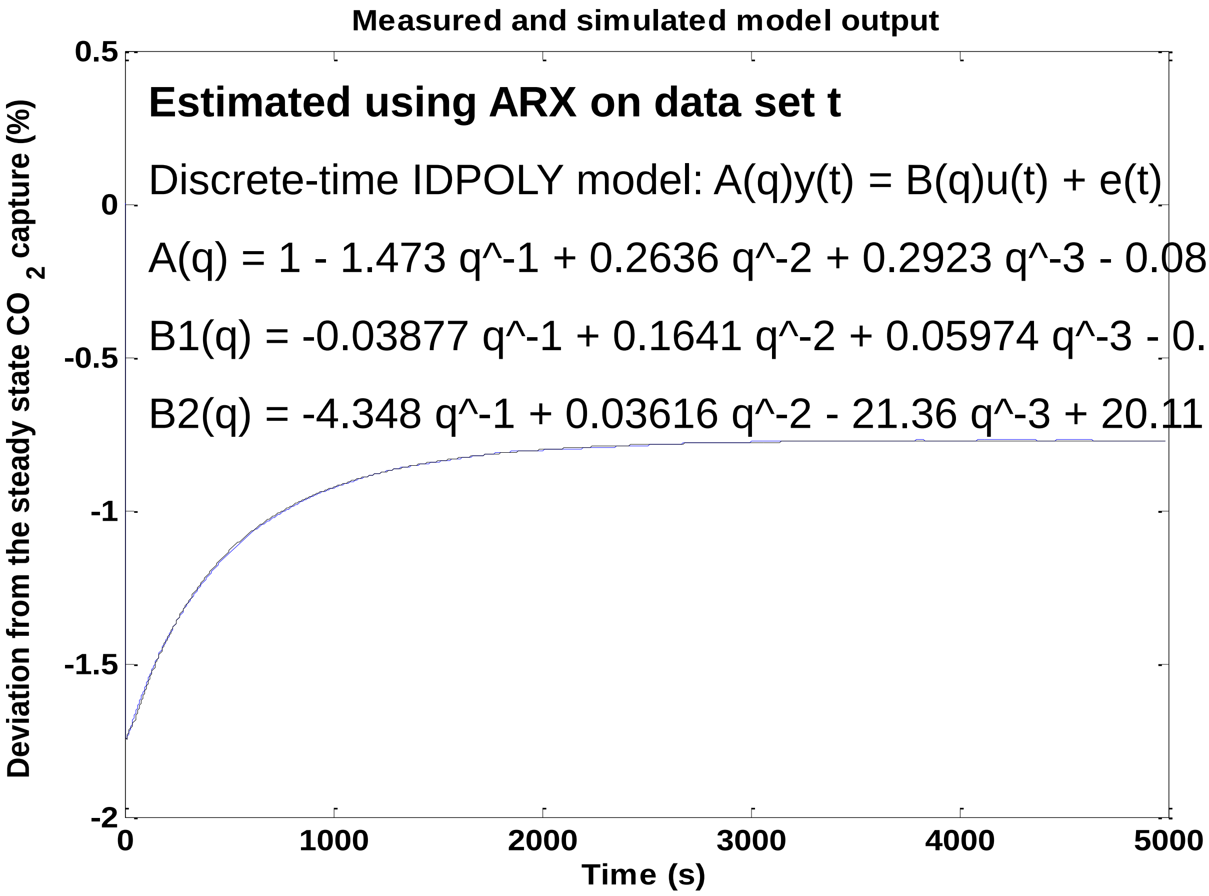
3.LINEAR MODEL PREDICTIVE CONTROLLER



Estimated using ARX on data set t

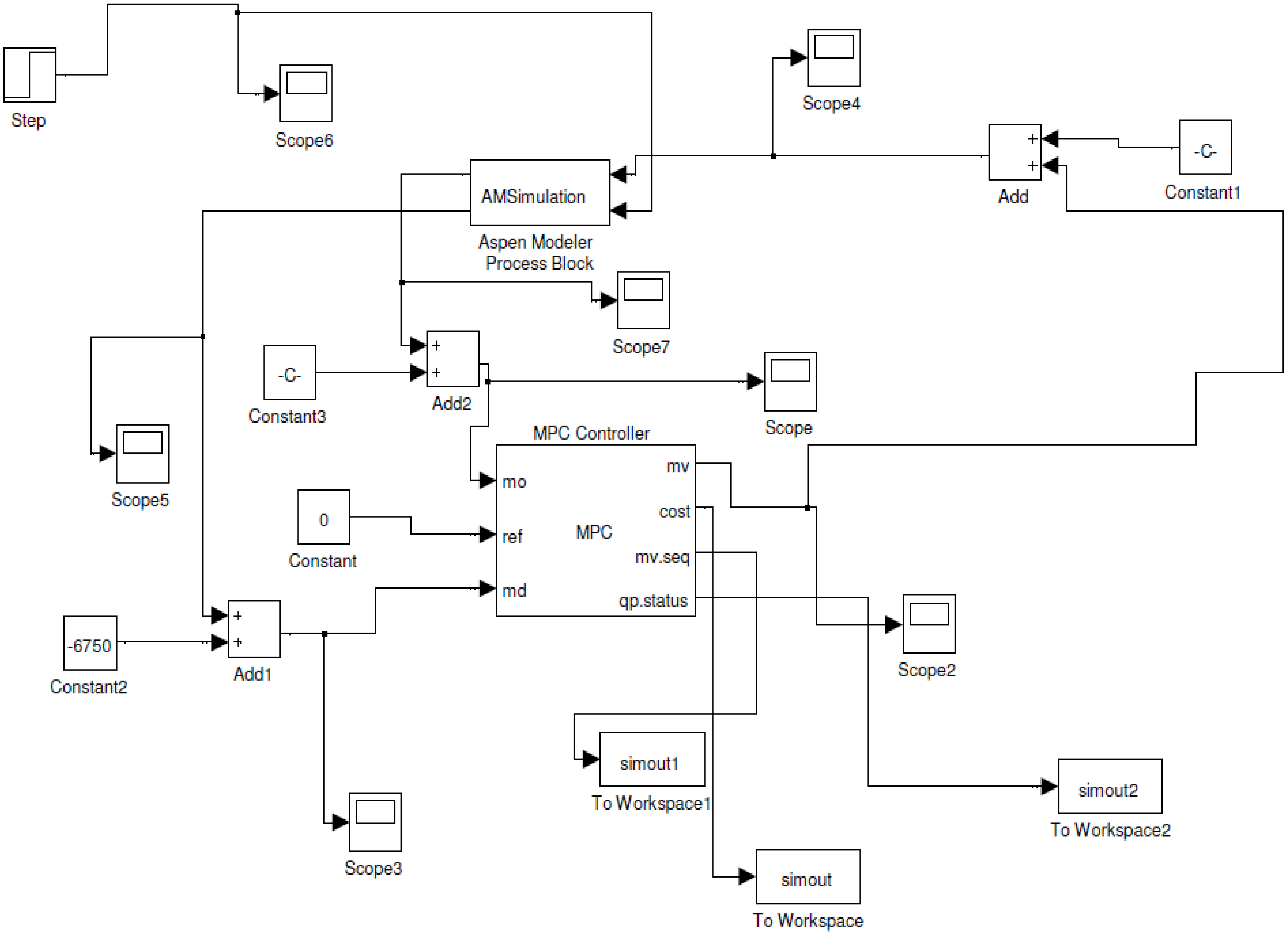
Discrete-time IDPOLY model: A(q)y(t) = B(q)u(t) + e(t)

A(q) = 1 - 1.473 q^-1 + 0.2636 q^-2 + 0.2923 q^-3 - 0.08314 q^-4

B1(q) = -0.03877 q^-1 + 0.1641 q^-2 + 0.05974 q^-3 - 0.1471 q^-4

B2(q) = -4.348 q^-1 + 0.03616 q^-2 - 21.36 q^-3 + 20.11 q^-4

ARX model as the disturbance model



Simulink block diagram for LMPC implementation

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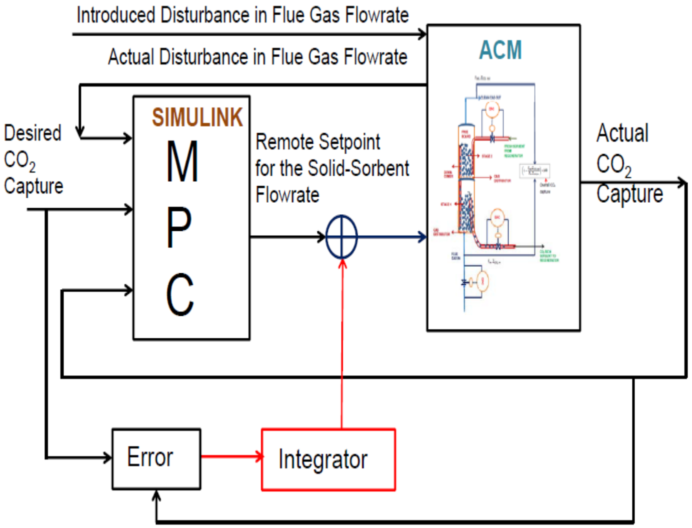
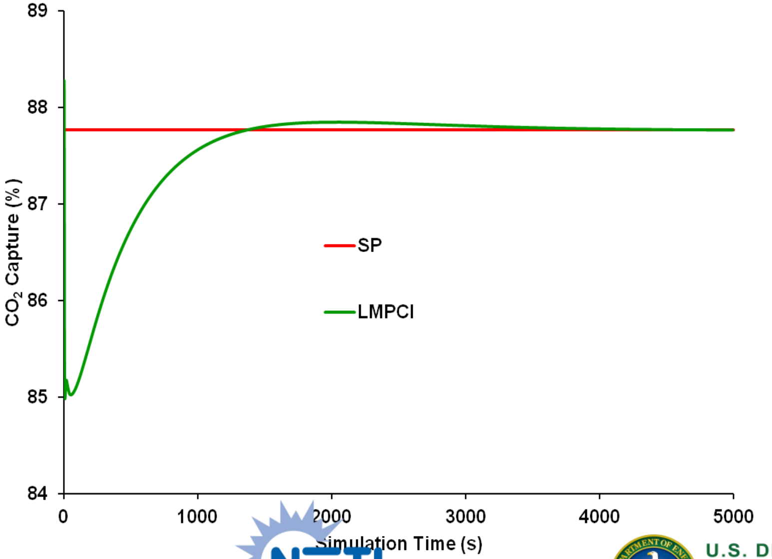
3.1 Offset-free LMPC Using an Integrator



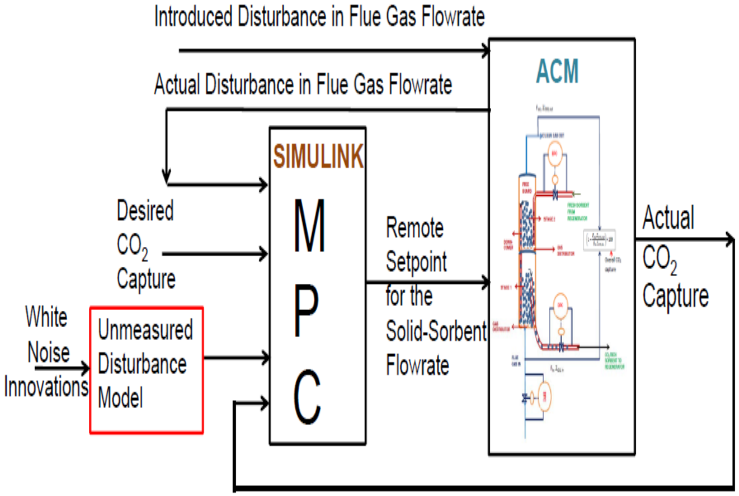
Configuration of LMPC with Additional Integrator

- Manipulated variable is sorbent flowrate.
- ACM model is embedded in SIMULINK for MPC implementation.
- 20% step increase in flue gas flowrate as disturbance.



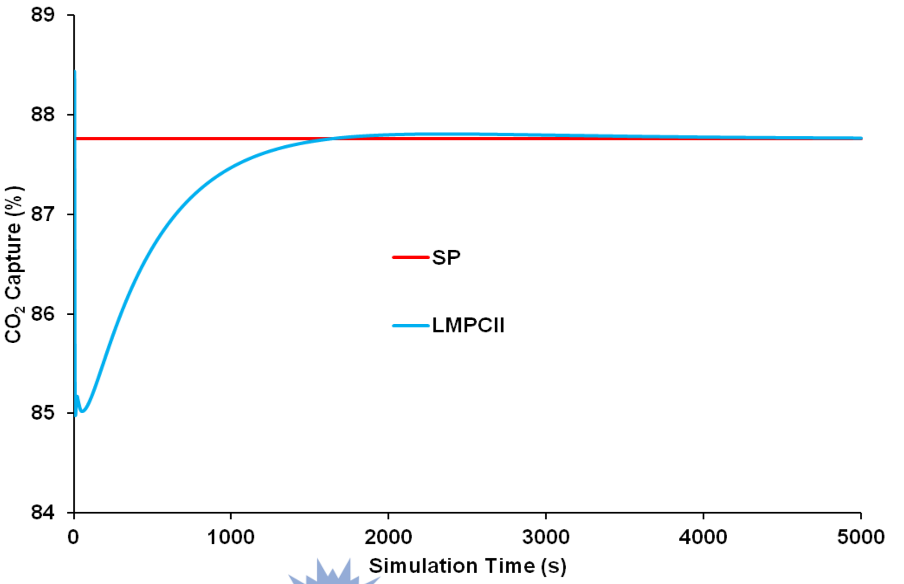
CONTROLLER DESIGN CONTD.

3.2 Offset-free LMPC Using Unmeasured Disturbance

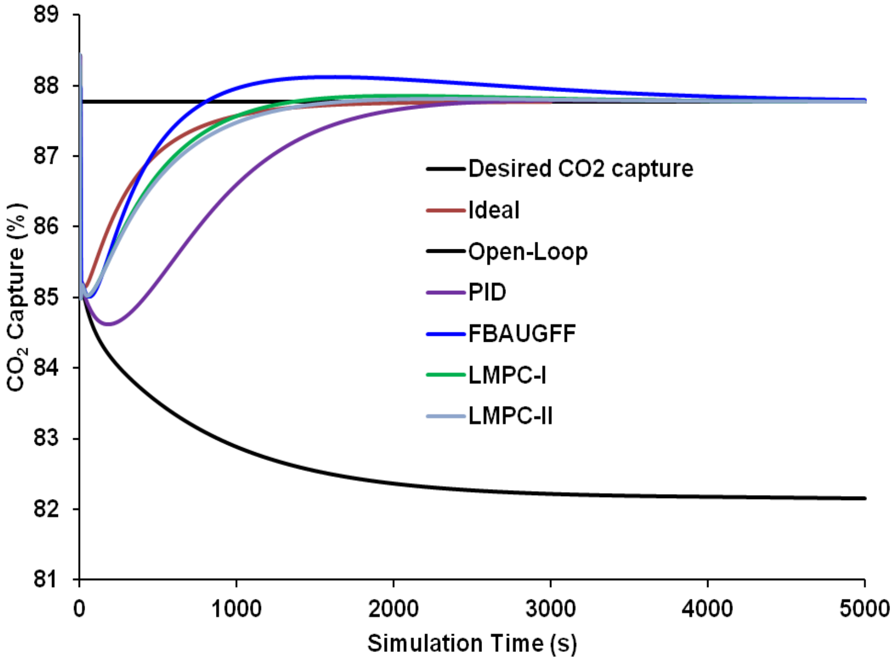


Configuration and performance of LMPC with estimation of unmeasured disturbance

- ➢ Estimation of unmeasured disturbance using advanced Controllers of MPC toolbox in MATLAB ®.
- ➢ The ACM model is embedded in SIMULINK for MPC implementation.
- ➢ 20% step increase in flue gas flowrate.
- ➢ Performance is satisfactory even for other disturbances.



CONTROLLER PERFORMANCE COMPARISON

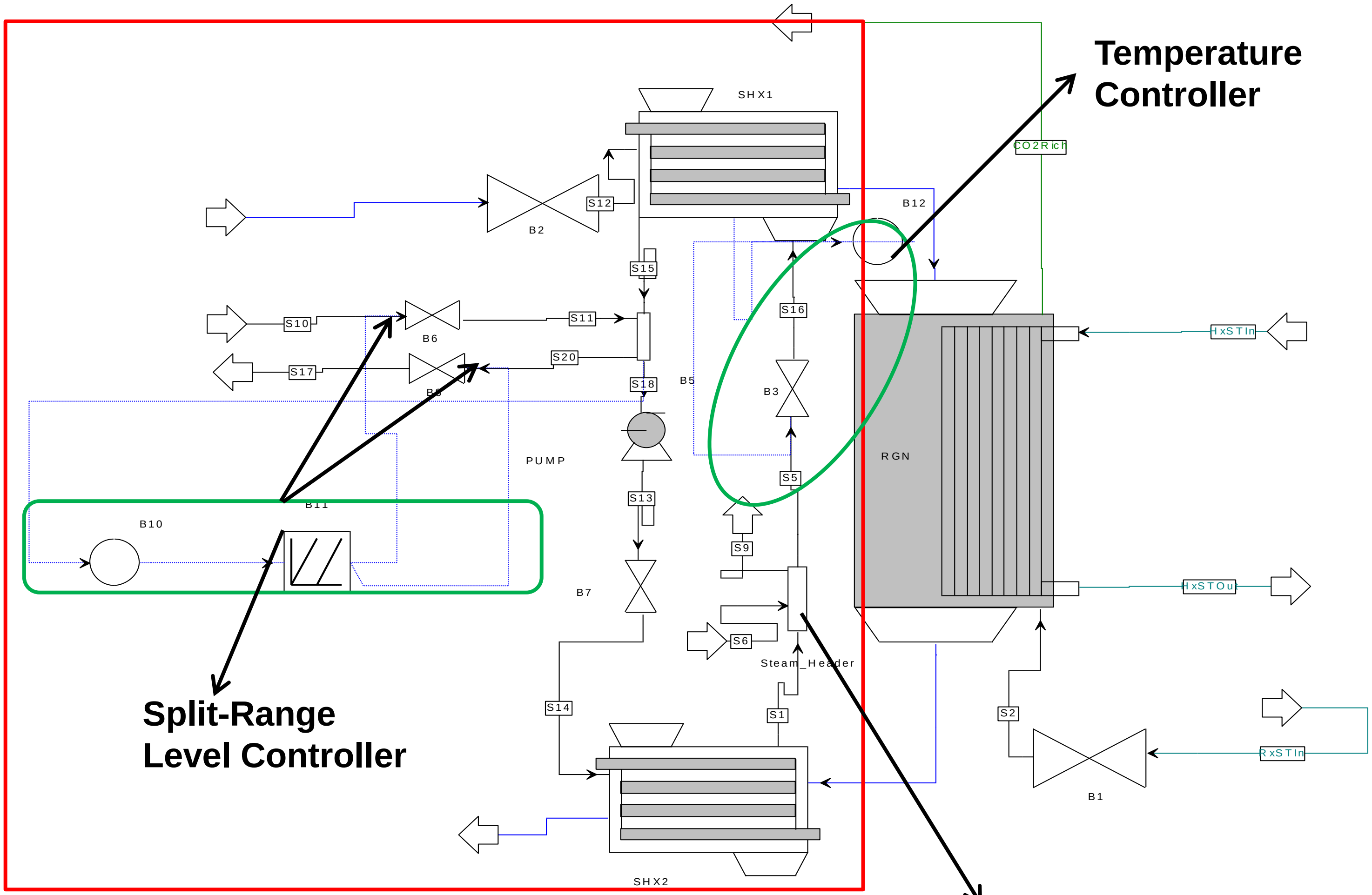


Control performances of LMPC-I and LMPC-II are superior to others

Control Performance Table

CONTROLLER	IAE	ISE	ITAE
	(hr)	(hr)	(hr^2)
(1) PID	0.8111	1.7551	1.12E-04
(2) FBAUGFF	0.4751	**0.5502**	6.60E-05
(3) LMPC-I	**0.3913**	0.6138	**5.57E-05**
(4) LMPC-II	0.4007	0.6386	6.30E-05

Control Configuration of the Regenerator System



Temperature Controller

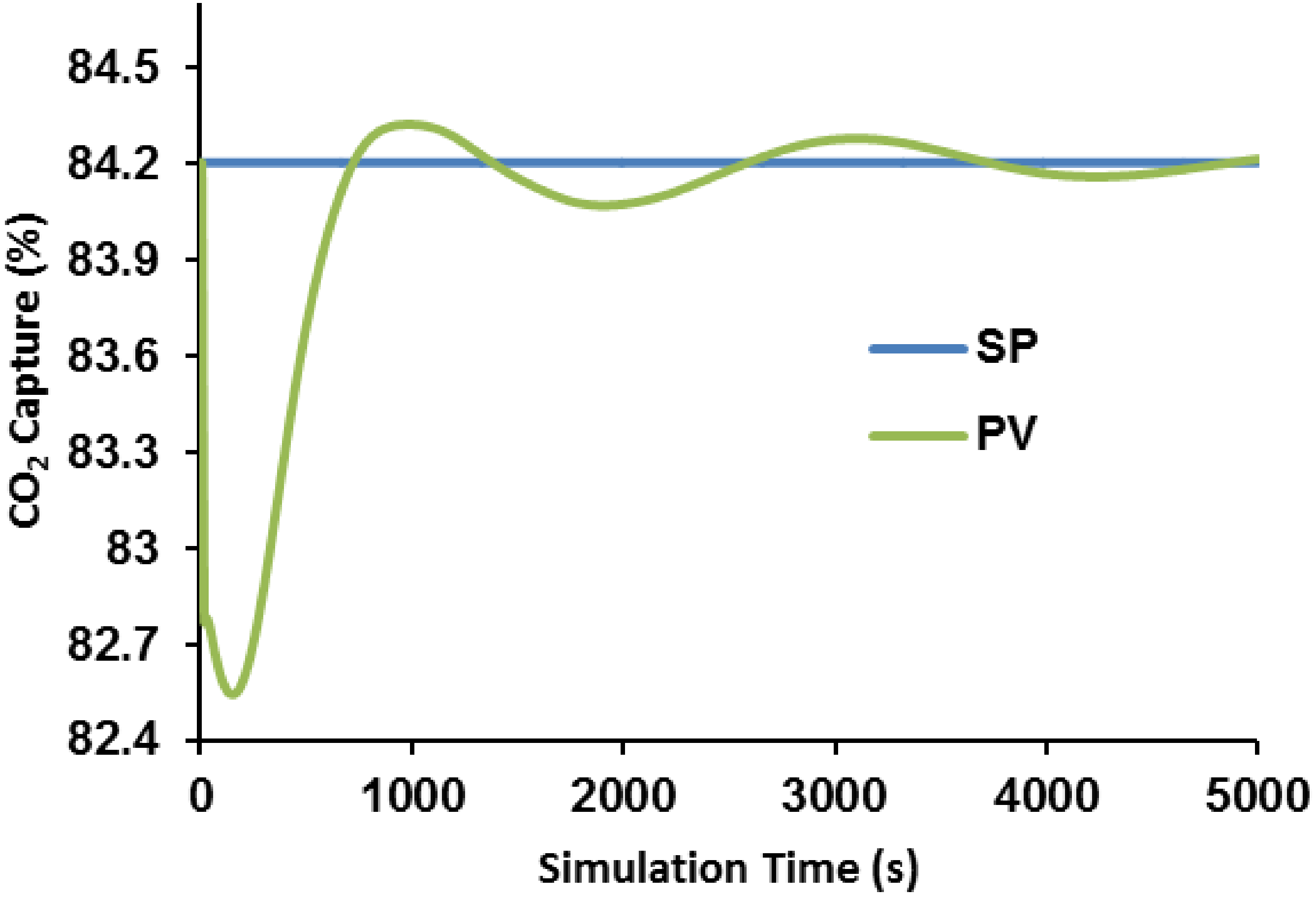
Split-Range Level Controller

Steam Header

Schematic of the ACM flow sheet of the moving bed regenerator with steam/BFW system

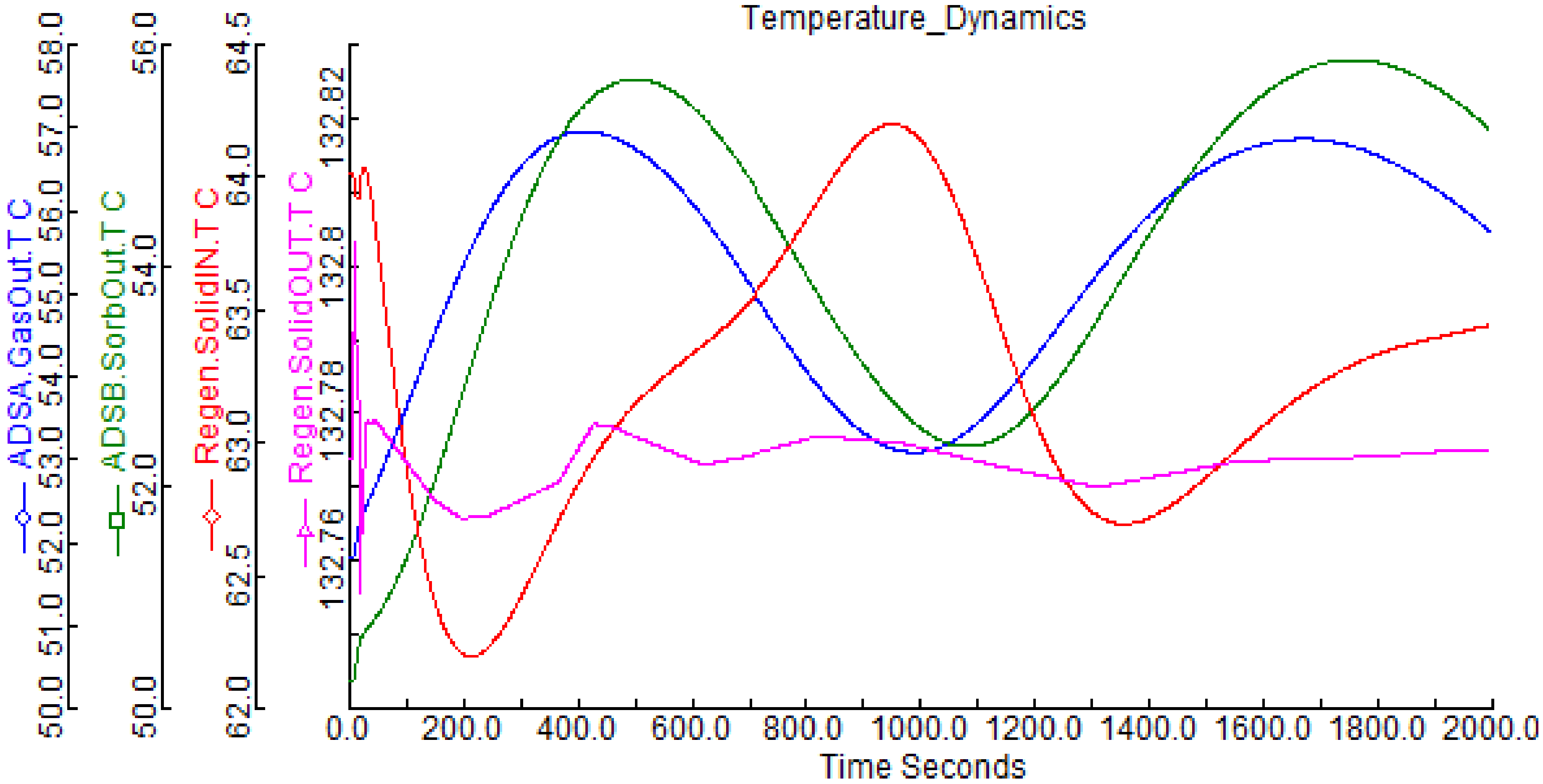
Integrated Adsorber-Regenerator Dynamic Model: PID Controller

<u>Disturbance</u>: 10% Ramp Increase in Flue Gas Flowrate

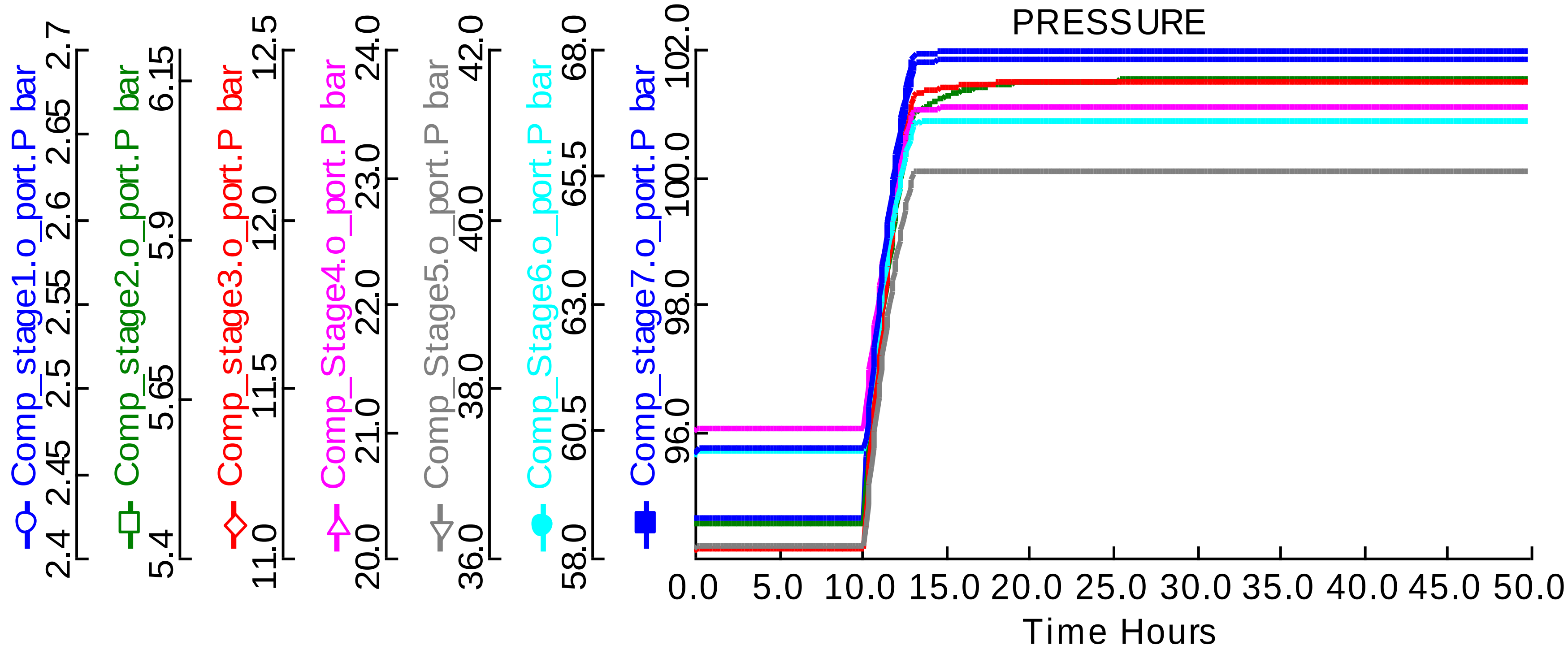


Integrated Adsorber-Regenerator Dynamic Model: PID Controller

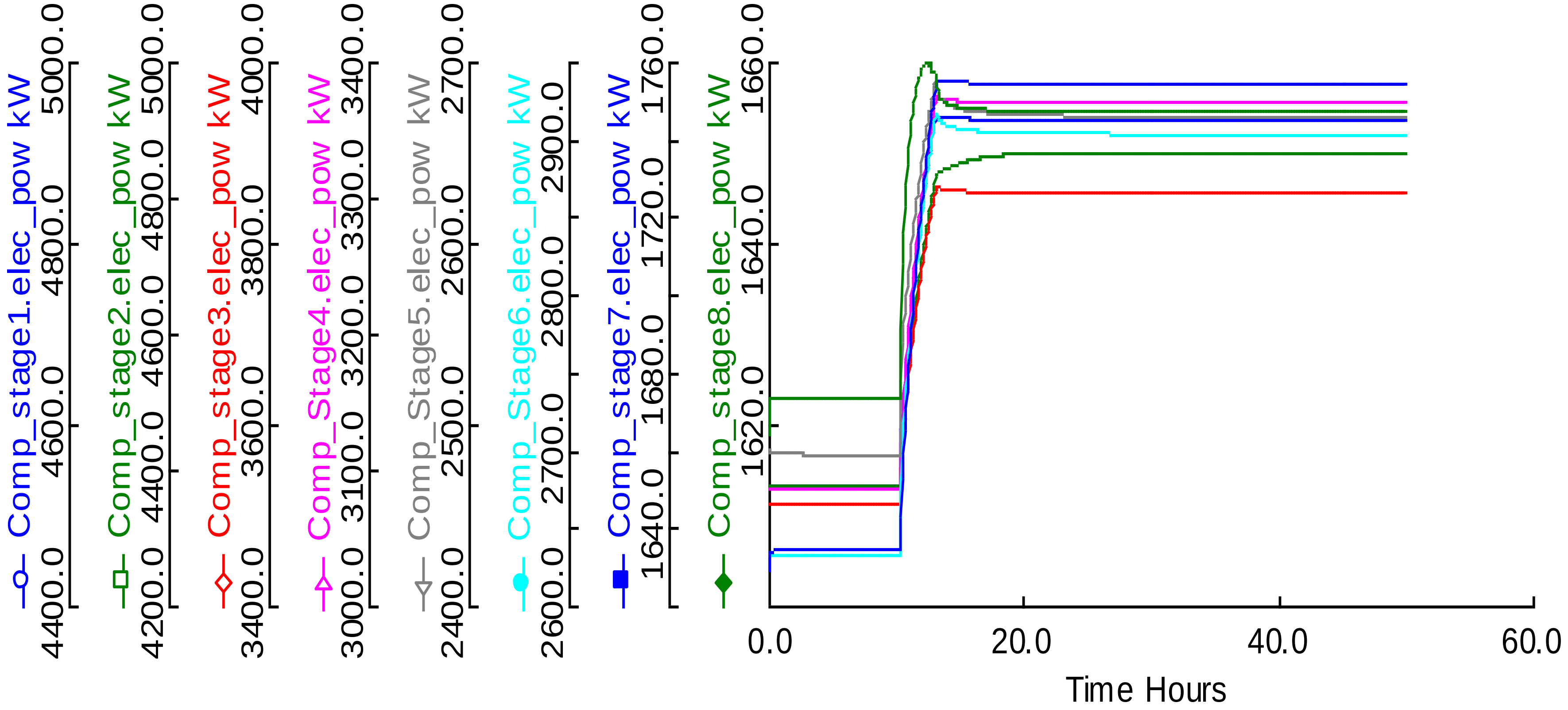
<u>Disturbance</u>: 10% Ramp Increase in Flue Gas Flowrate



Pressure Dynamics in CO_2 Compression System: 10% Ramp Change in flowrate



Power Dynamics in CO_2 Compression System: 10% Ramp Change in flowrate



CONCLUSIONS

1. One-dimensional, non-isothermal, pressure-driven dynamic models of a two-stage BFB adsorber-reactor, a moving bed regenerator, an integral gear CO_2 compression system along with the balance of the plant has been developed in ACM for solid-sorbent CO_2 capture.

2. For adsorber-only case, the performances of both LMPC strategies are satisfactory and superior to other control strategies.

3. The response of the coupled adsorber-regenerator system is slow and oscillatory due to interactions between the systems. Advanced control strategies should be considered for satisfying the overall CO_2 capture target over a period of time.

Acknowledgements:

- As part of the National Energy Technology Laboratory’s Regional University Alliance (NETL-RUA), a collaborative initiative of the NETL, this technical effort was performed under the RES contract DEFE0004000.

Disclaimer:

Thank you

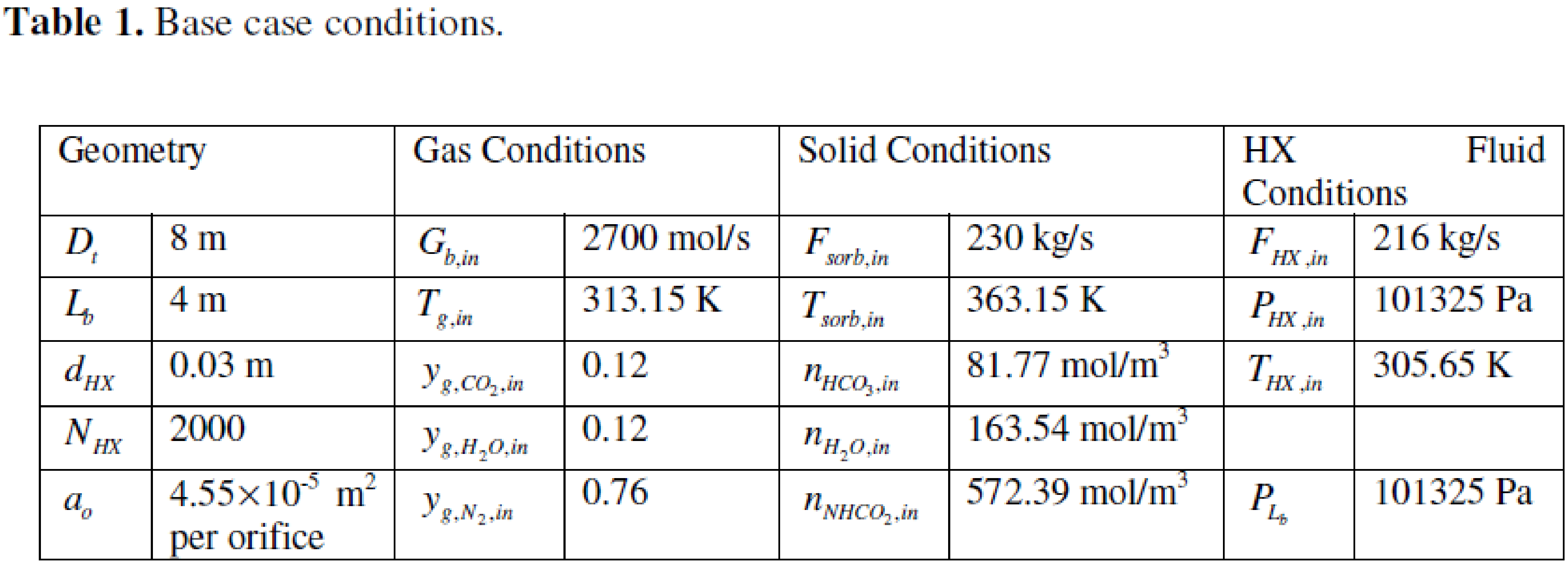


Table 1. Base case conditions.

Geometry		Gas Conditions		Solid Conditions		HX Fluid Conditions	
D_t	8 m	$G_{b,in}$	2700 mol/s	$F_{sorb,in}$	230 kg/s	$F_{HX,in}$	216 kg/s
L_b	4 m	$T_{g,in}$	313.15 K	$T_{sorb,in}$	363.15 K	$P_{HX,in}$	101325 Pa
d_{HX}	0.03 m	$y_{g,CO_2,in}$	0.12	$n_{HCO_3,in}$	81.77 mol/m^3	$T_{HX,in}$	305.65 K
N_{HX}	2000	$y_{g,H_2O,in}$	0.12	$n_{H_2O,in}$	163.54 mol/m^3		
a_o	4.55×10^{-5} m^2 per orifice	$y_{g,N_2,in}$	0.76	$n_{NHCO_2,in}$	572.39 mol/m^3	P_{L_b}	101325 Pa

Pneumatic Transport Modeling

Terminal Velocity of the particles:

$$u_t = u_t^* \left(\left(\mu_g (\rho_s - \rho_g) g \right) / \rho_g^2 \right)^{-1/3}$$

$$u_t^* = \frac{1}{18 / D_p^2} + \frac{(2.335 - 1.744\phi_s)}{(D_p^*)^{0.5}}$$

$$D_p^* = D_p \left(\left(\rho_g (\rho_s - \rho_g) g \right) / \mu_g^2 \right)^{1/3}$$

Choking Velocity, Voidage at Choking, and Superficial Velocity

$$G_s = \frac{F_s / 3600}{\pi D^2 / 4}$$

$$\frac{u_{ch}}{\varepsilon_{ch}} - u_t = \frac{G_s}{\rho_s (1 - \varepsilon_{ch})}$$

$$\rho_g^{0.77} = 2250D \frac{((\varepsilon_{ch})^{-4.7} - 1)}{\left(\frac{u_{ch}}{\varepsilon_{ch}} - u_t \right)^2}$$

$$u = 1.2u_{ch}$$

Pneumatic Transport Modeling

Load Ratio, Gas and Solid Velocities

$$u_g = {}^{u}/_{\varepsilon_p}$$

$$u_s = u_g - u_t$$

$$G_s = \rho_s(1 - \varepsilon_p)u_s$$

$$G_g = \rho_g \varepsilon_p u_g$$

$$Load\ Ratio = {}^{G_s}/_{G_g}$$

Reynold’s Number and Gas Friction Factor

$$f_g = 0.079 Re^{-0.25}$$

$$Re = \frac{Du\rho_g}{\mu_g}$$