NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL-RUA Regional University Alliance

NETL Carnegie Mellon PENNSTATE University of Pittsburgh VirginiaTech WestVirginiaUniversity URS

Dynamic Modeling and Control of a Solid-Sorbent CO_2 Capture Process with Two-stage Bubbling Fluidized Bed Adsorber-Reactor

Srinivasarao Modekurti, Debangsu Bhattacharyya
West Virginia University
Stephen E. Zitney
National Energy Technology Laboratory

U.S. DEPARTMENT OF ENERGY

AIChE Annual Meeting 2012, Pittsburgh, PA, USA, October 28-Nov 2, 2012

OUTLINE

- Motivation
- Dynamic Model Development
- Transient Studies
- Controller Design
  - Proportional-Integral-Derivative (PID) Controller
  - Feedback-Augmented Feedforward Controller
  - Linear Model Predictive (LMPC) Controller
- Conclusions

MOTIVATION

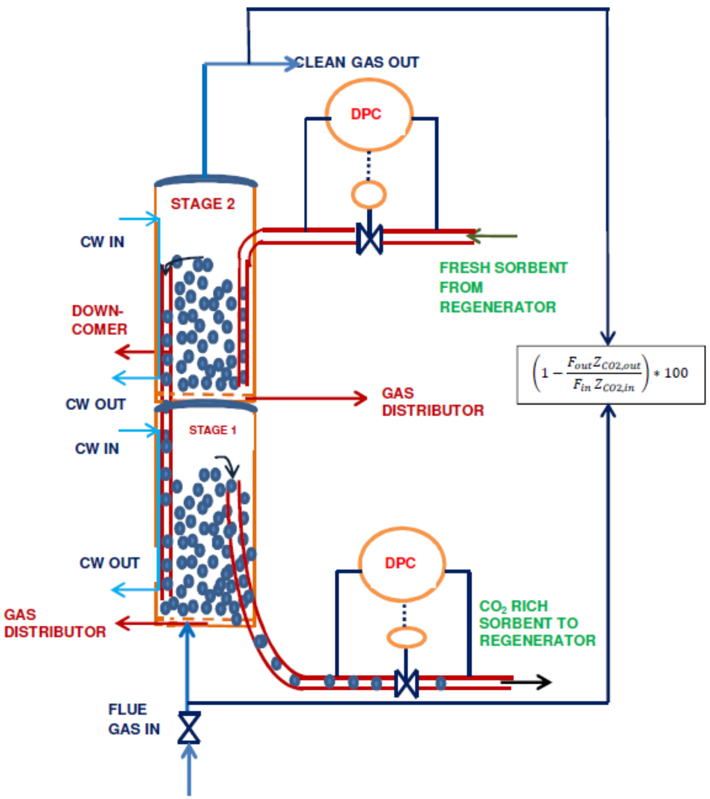
- **To meet the environmental regulations for CO_2 emissions, it is required that power plants have to satisfy certain amount of CO_2 capture over a period of time.**

- **Under *Carbon Capture Simulation Initiative (CCSI),* the US DOE is working on various post-combustion CO_2 capture technologies, e.g. solid-sorbent based CO_2 capture.**

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

DYNAMIC 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.**

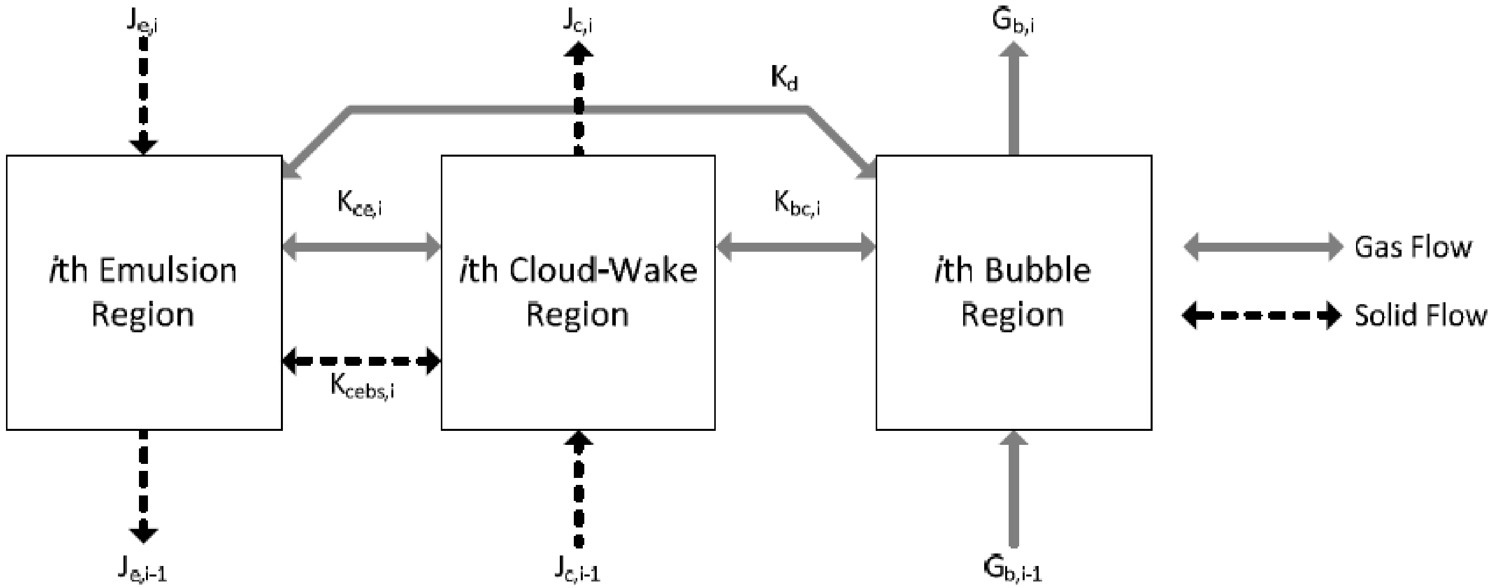


Model Assumptions

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. No accumulation in the embedded heat exchangers in the bed.

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

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

$$\frac{\partial(\delta V C_{b,i})}{\partial t} + \frac{V}{A}\frac{\partial(y_{b,i}G_{b,i})}{\partial x} + \delta V K_{bc,i}(C_{b,i} - C_{c,i}) + K_{g,bulk} = 0$$

$$\frac{\partial(C_{P,g}C_{bt}\delta V(T_{g,b} - T_{ref}))}{\partial t} + \frac{\partial(C_{P,g}G_b(T_{g,b} - T_{ref}))}{\partial x} + \delta A H_{bc}(T_{g,b} - T_{g,c}) - H_{g,bulk} = 0$$

Cloud-wake Region :

Gaseous Components

$$\frac{\partial(f_{cw}\delta\varepsilon_d V C_{c,i})}{\partial t} - V\delta K_{bc,i}(C_{b,i} - C_{c,i}) + V\delta K_{ce,i}(C_{c,i} - C_{e,i}) + V\delta(1-\varepsilon_d)f_{cw}r_{g,c} = 0$$

$$\frac{\partial(C_{P,g}C_{ct}V\delta f_{cw}e_d(T_{g,c} - T_{ref}))}{\partial t} - A\delta H_{bc}(T_{g,b} - T_{g,c}) + A\delta H_{ce}(T_{g,c} - T_{g,e}) + Af_{cw}\delta(1-\varepsilon_d)\rho_s a_p h_p(T_{g,c} - T_{s,c}) - f_{cw}\delta(1-\varepsilon_d)A\sum_j r_{g,c,i}C_{p,g,c,i}(T_{g,c} - T_{ref}) = 0$$

Adsorbed Species

$$\frac{\partial(Vf_{cw}\delta(1-\varepsilon_d)n_{c,j})}{\partial t} - \frac{V}{\rho_s}\frac{\partial(n_{c,j}J_c)}{\partial x} + K_{s,bulk,j} + V\delta K_{cebs}(n_{c,j} - n_{e,j}) - Vf_{cw}\delta(1-\varepsilon_d)r_{s,c} = 0$$

$$\frac{\partial\left(A\Delta x f_{cw}\delta\rho_s C_{P,s}(1-\varepsilon_d)(T_{s,c} - T_{ref})\right)}{\partial t} + A\frac{\partial(J_c C_{P,s}(T_{s,c} - T_{ref}) + h_{ads,c})}{\partial x} + H_{s,bulk} + A\delta\rho_s K_{cebs}(C_{P,s}(T_{s,c} - T_{ref}) + h_{ads,c} - C_{P,s}(T_{s,e} - T_{ref}) + h_{ads,e}) + f_{cw}\delta(1-\varepsilon_d)A\sum_j r_{g,c,i}C_{p,g,c,i}(T_{g,c} - T_{ref}) - Af_{cw}\delta(1-\varepsilon_d)\rho_s a_p h_p(T_{g,c} - T_{s,c}) = 0$$

CONSERVATION EQUATIONS CONTD.

Emulsion Region :

Gaseous Components

$$\frac{\partial\left(V(1-f_{cw}\delta-\delta)\varepsilon_d C_{e,i}\right)}{\partial \mathrm{t}} - \delta A \mathrm{K}_{\mathrm{ce,i}}\left(\mathrm{C}_{\mathrm{c,i}}-\mathrm{C}_{\mathrm{e,i}}\right) - \mathrm{K}_{\mathrm{g,bulk}} + (1-f_{cw}\delta-\delta)A(1-\varepsilon_d)\mathrm{r}_{\mathrm{g,e}} = 0$$

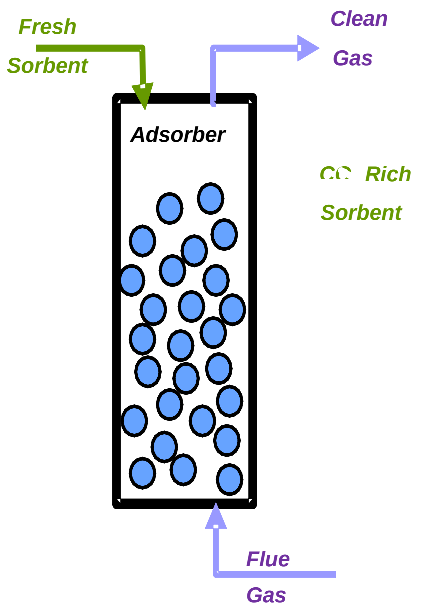
$$\frac{\partial\left(\mathrm{C}_{\mathrm{P,g}}\mathrm{C}_{\mathrm{et}}V(1-f_{cw}\delta-\delta)\varepsilon_d\left(T_{g,e}-T_{ref}\right)\right)}{\partial \mathrm{t}} - A\delta \mathrm{H}_{\mathrm{ce}}\left(\mathrm{T}_{\mathrm{g,c}}-\mathrm{T}_{\mathrm{g,e}}\right) + H_{g,bulk} + (1-f_{cw}\delta-\delta)(1-\varepsilon_d)A\rho_s a_p h_p\left(\mathrm{T}_{\mathrm{g,e}}-\mathrm{T}_{\mathrm{s,e}}\right)$$
$$-(1-f_{cw}\delta-\delta)(1-\varepsilon_d)A\sum_j r_{g,e,i}C_{p,g,e,i}\left(T_{g,e}-T_{ref}\right) = 0$$

Adsorbed Species

$$\frac{\partial\left(V(1-f_{cw}\delta-\delta)(1-\varepsilon_d)n_{e,j}\right)}{\partial \mathrm{t}} + \frac{V}{\rho_s}\frac{\partial\left(n_{e,j}J_e\right)}{\partial x} - \mathrm{K}_{\mathrm{s,bulk,j}} - \mathrm{V}\delta\mathrm{K}_{\mathrm{cebs}}\left(n_{\mathrm{c,j}}-\mathrm{n}_{\mathrm{e,j}}\right) - V(1-f_{cw}\delta-\delta)(1-\varepsilon_d)r_{s,e} = 0$$

$$\frac{\partial\left(\mathrm{C}_{\mathrm{P,s}}\rho_s A(1-f_{cw}\delta-\delta)(1-\varepsilon_d)\left(T_{s,e}-T_{ref}\right)\right)}{\partial t} + A\frac{\partial\left(J_e\mathrm{C}_{\mathrm{P,s}}\left(T_{s,e}-T_{ref}\right)+h_{ads,e}\right)}{\partial x} - \mathrm{H}_{\mathrm{s,bulk}}$$
$$-\ A\delta\rho_s K_{cebs}\left(C_{P,s}\left(T_{s,c}-T_{ref}\right)+h_{ads,c}-C_{P,s}\left(T_{s,e}-T_{ref}\right)+h_{ads,e}\right)$$
$$+(1-f_{cw}\delta-\delta)(1-\varepsilon_d)A\sum_j r_{g,e,i}C_{p,g,e,i}\left(T_{g,e}-T_{ref}\right) - (1-f_{cw}\delta-\delta)(1-\varepsilon_d)A\rho_s a_p h_p\left(\mathrm{T}_{\mathrm{g,e}}-\mathrm{T}_{\mathrm{s,e}}\right)$$
$$-\ \pi d_{HX}h_{t,x}\Delta T_{hx}N_{HX}C_r = 0$$

HYDRODYNAMIC MODEL



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

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

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

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

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

Mori and Wen (1975)

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

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

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

Sit and Grace (1981)

REACTION KINETICS

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

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

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

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

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

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

Modeling of balance of the Plant

1. **Pressure flow-network along with the control valves**

$$Q = C_v x \sqrt{\frac{\Delta P}{\rho}}$$

2. **Gas and Solid distributors**

$$\Delta P_d = (0.2\text{-}0.3)\ \Delta P_{bed}$$

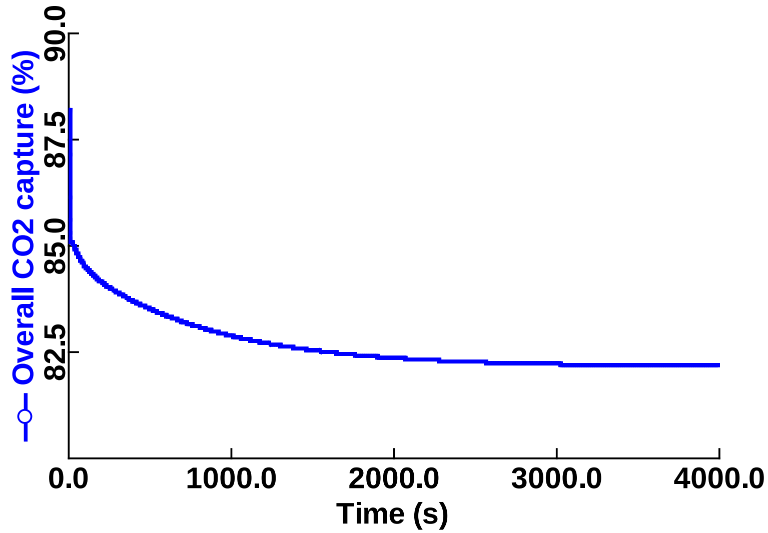
3. **Downcomer and Exit-hopper**

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

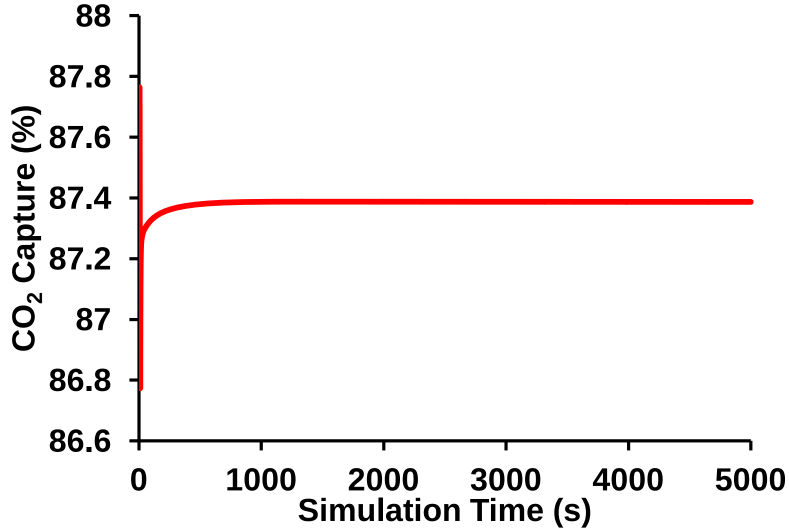
SOLUTION METHODOLOGY

- **Integration of sub-models with the adsorber-reactor model in ACM.**
- **Setting up initial and boundary conditions.**
- **ACM model is embedded in Simulink for LMPC implementation.**

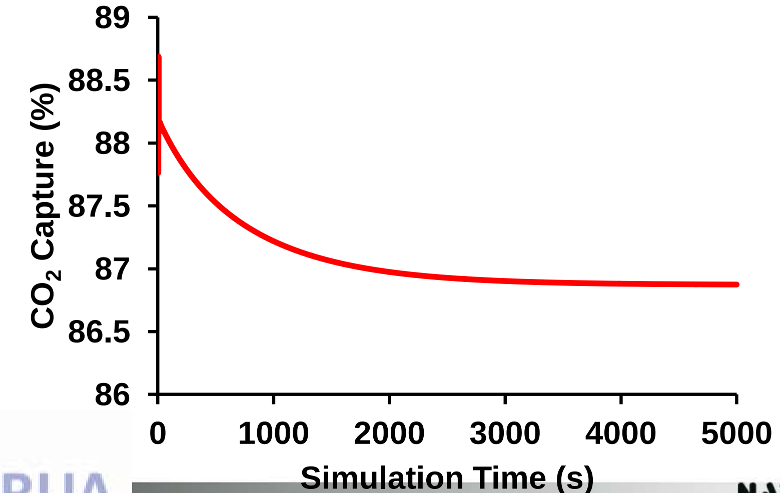
TRANSIENT STUDIES



Transient in CO_2 capture due to a 20% step increase in the flue gas flowrate



Transient in CO_2 capture due to an increase of 10 C in the flue gas inlet temperature

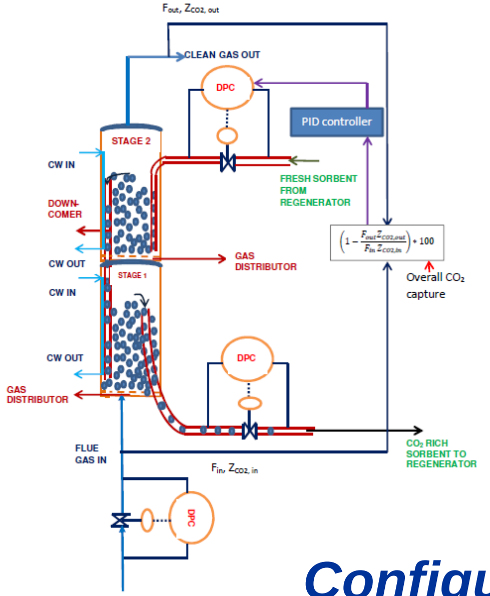


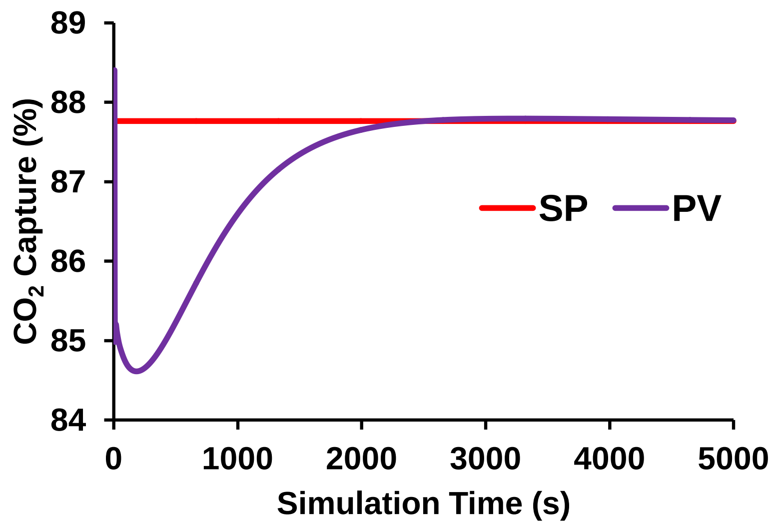
Transient in CO_2 capture due to an increase of 10% CO2 mole fraction in the flue gas inlet composition

CONTROLLER DESIGNS

1. PID CONTROLLER

- **Process models and the controllers are the same as open-loop case.**
- **An additional PID controller for controlling CO_2 capture by manipulating the solid sorbent flowrate.**
- **Note the large undershoot and long settling time.**



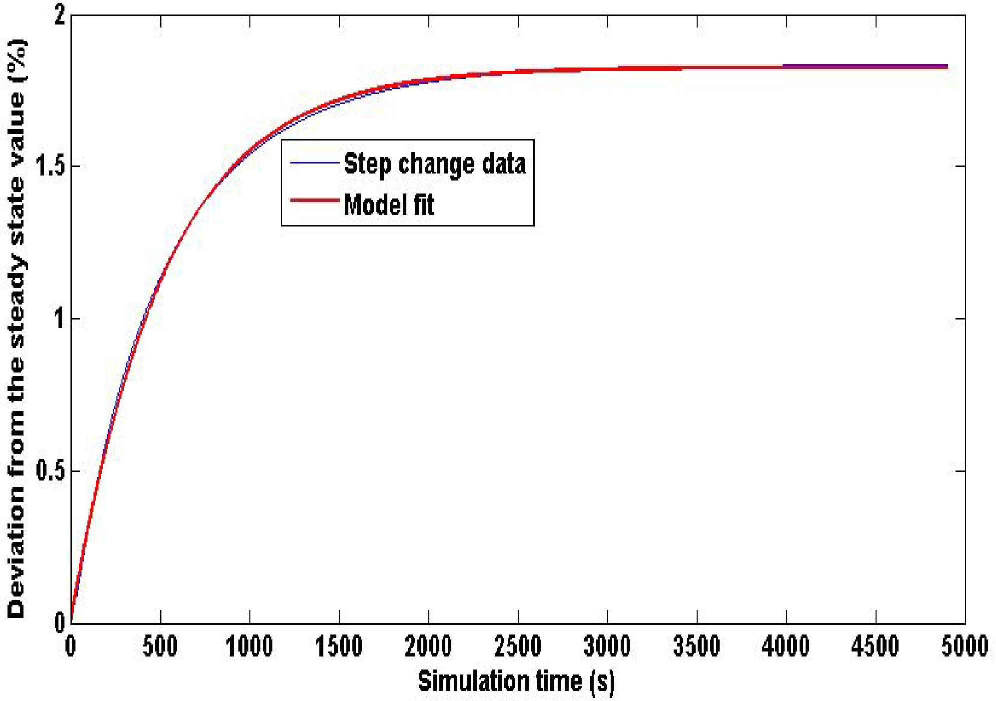


Configuration and Performance of the PID Controller

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.**

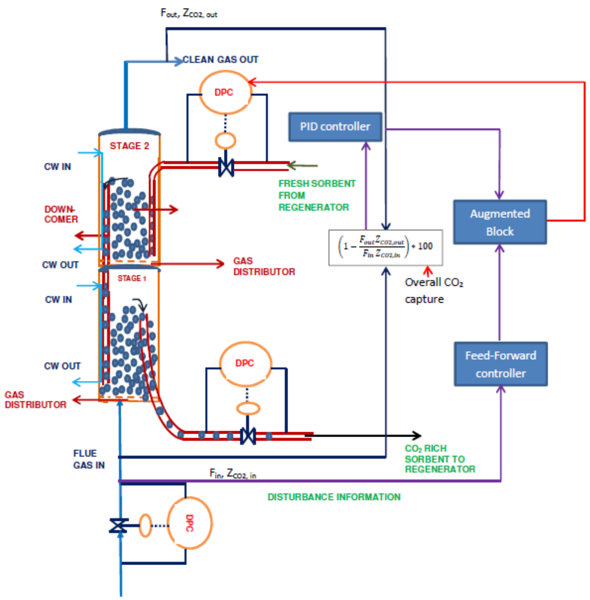


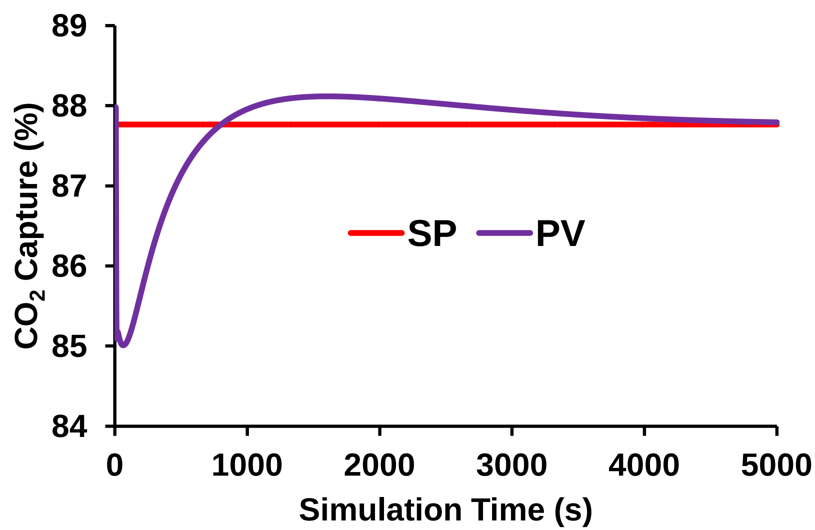
Comparison of the process model to the data from ACM®

CONTROLLER DESIGN CONTD.

FEEDBACK-AUGMENTED FEEDFORWARD CONTROLLER

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



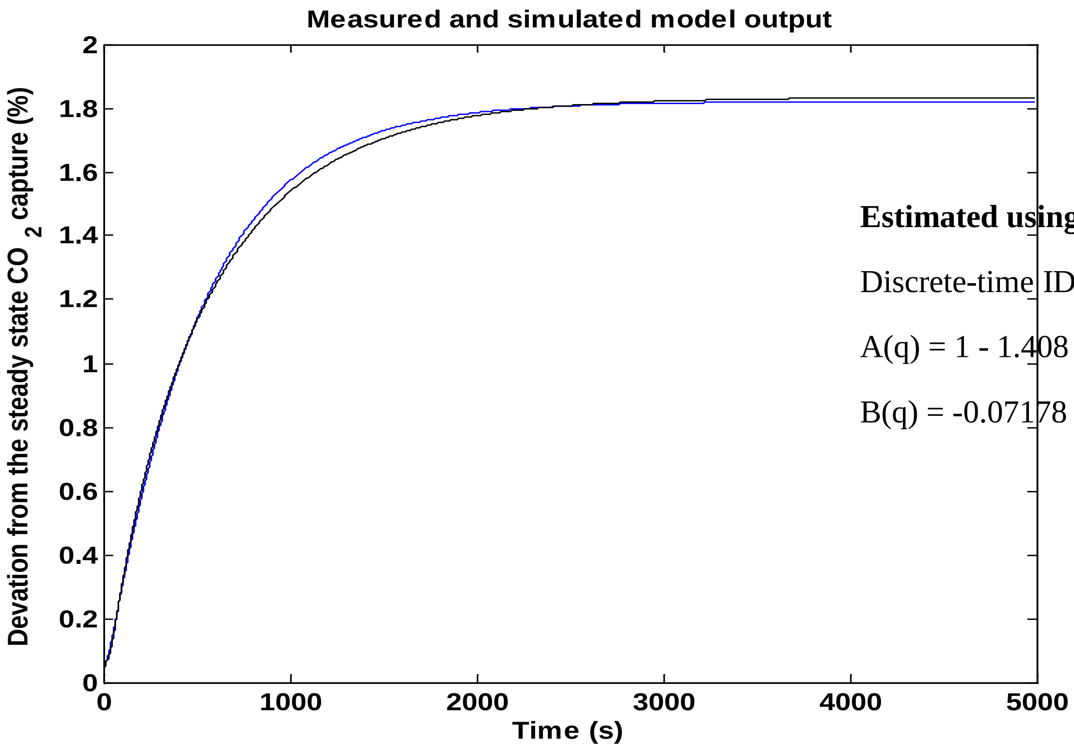


Configuration and Performance of the Feedback-Augmented Feedforward Controller

CONTROLLER DESIGN CONTD.

3. Linear Model Predictive Controller (LMPC)

- **Identification of a multiple-input-single-output (MISO) auto-regressive with exogenous inputs (ARX) model using MATLAB®**



Estimated using ARX on data set t

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

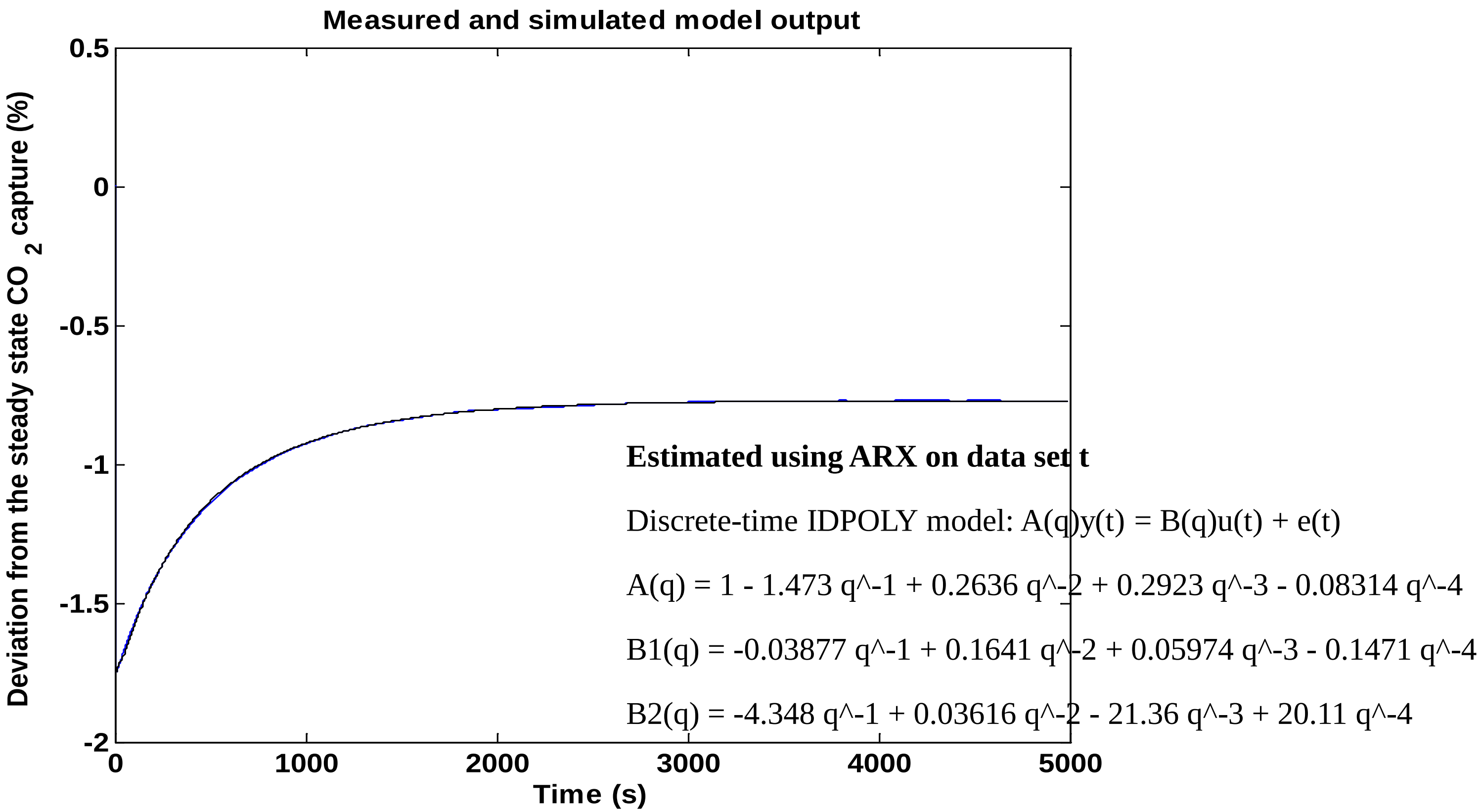
A(q) = 1 - 1.408 q^-1 - 0.1453 q^-2 + 0.5946 q^-3 - 0.04143 q^-4

B(q) = -0.07178 q^-1 - 0.01151 q^-2 + 0.01254 q^-3 + 0.07076 q^-4

ARX model for the process using MATLAB® System identification tool box

CONTROLLER DESIGN CONTD.

Linear Model Predictive controller (LMPC)

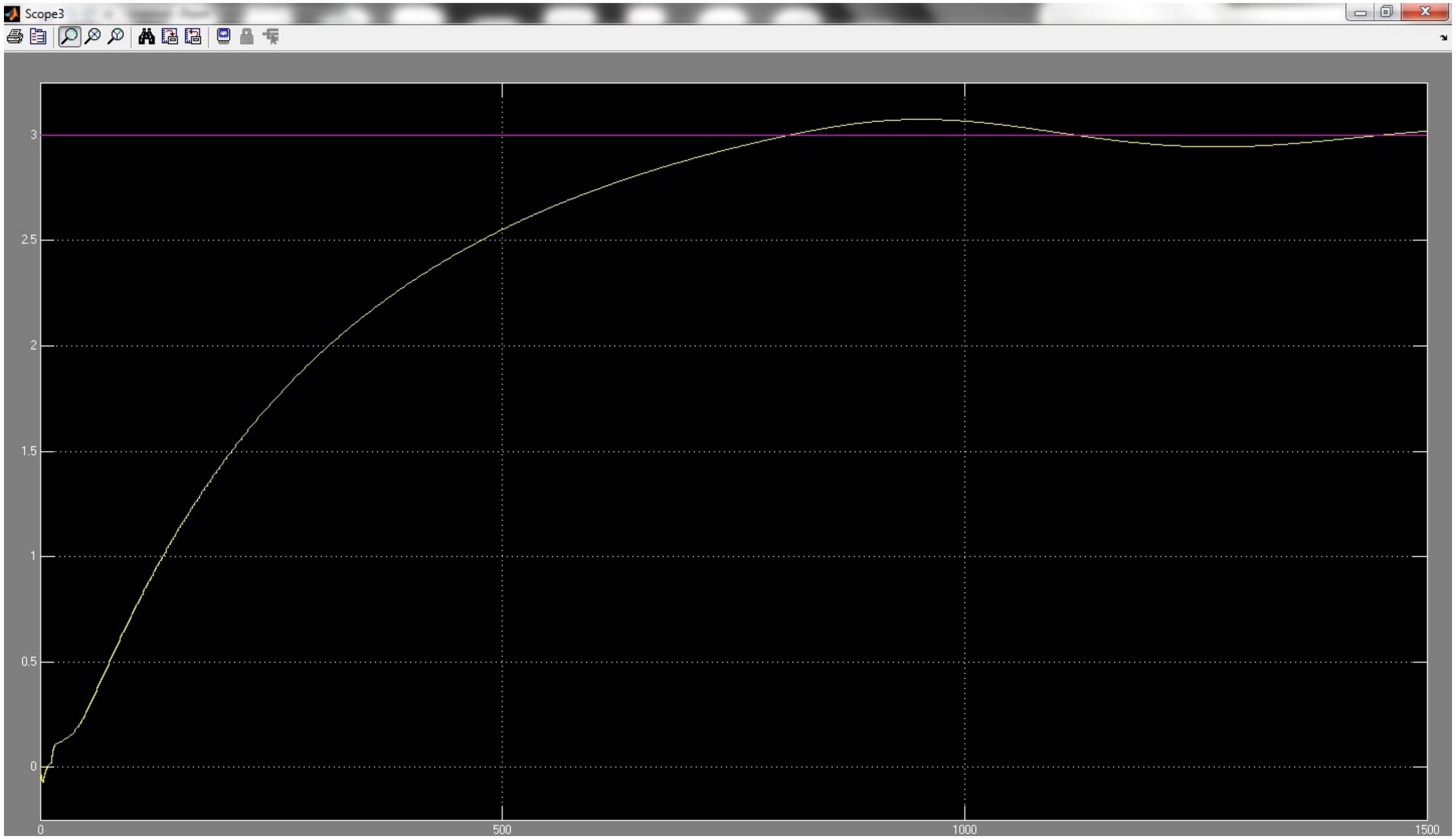


ARX model for the disturbance rejection using MATLAB® System identification tool box

CONTROLLER DESIGN CONTD.

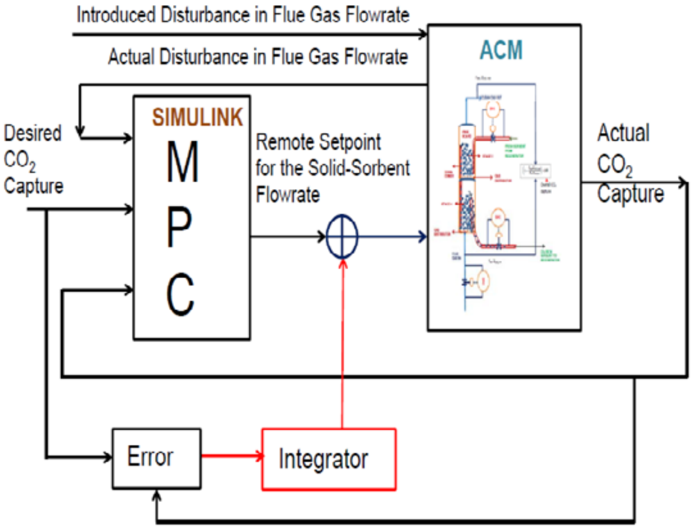
Linear Model Predictive controller (LMPC)

Servo Problem



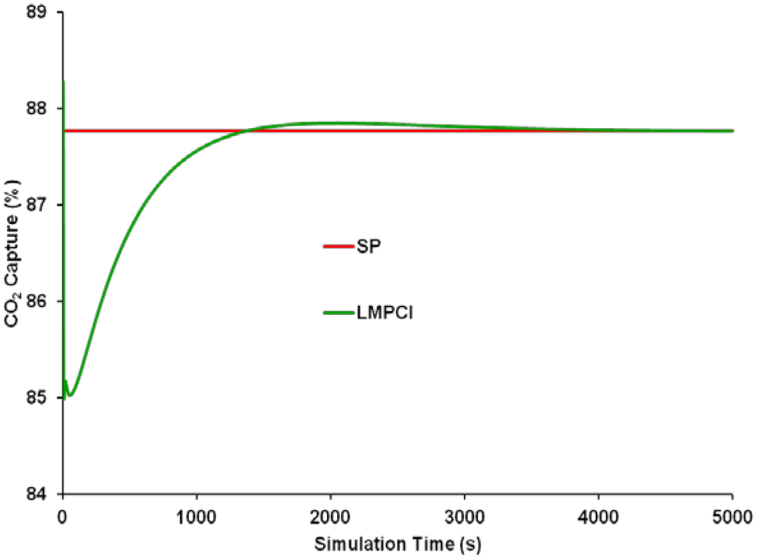
CONTROLLER DESIGN CONTD.

3.1. Offset-free LMPC Using an Integrator (LMPC-I)



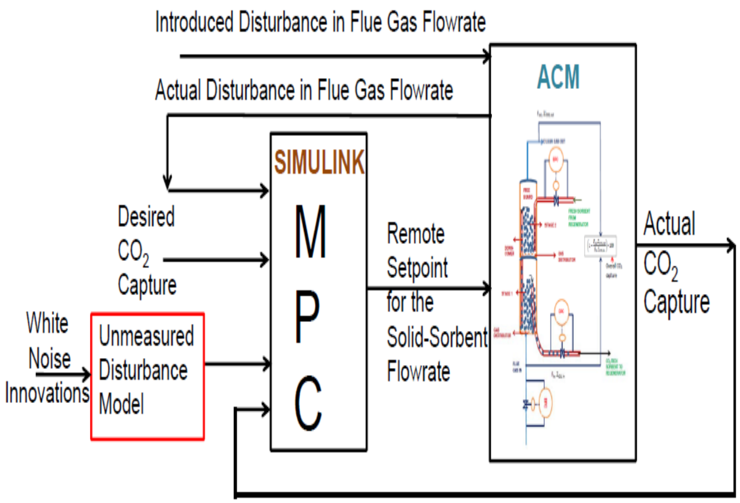
Configuration of LPC with Additional Integrator

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



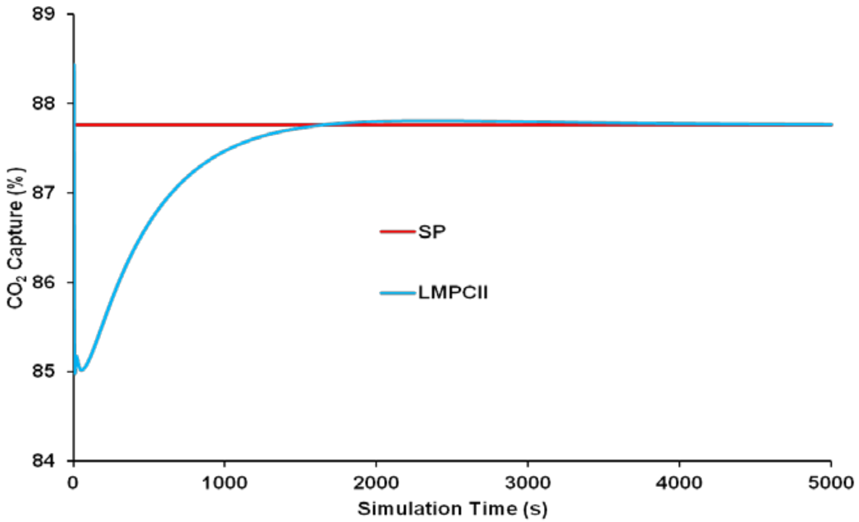
CONTROLLER DESIGN CONTD.

3. 2. Offset-free LMPC Using Estimation of Unmeasured Disturbance (LMPC-II)

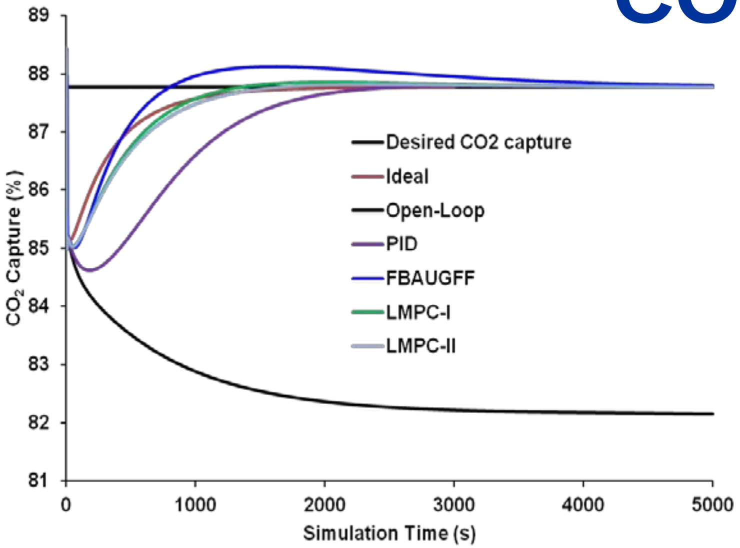


Configuration and performance of LMPC with estimation of unmeasured disturbance

- *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

CONCLUSIONS

1. A one-dimensional, non-isothermal, pressure-driven dynamic model of a two-stage BFB adsorber-reactor has been developed for solid-sorbent CO_2 capture in ACM.

2. The dynamics of CO_2 capture have been studied for step changes in flue gas inlet flowrate, temperature and composition.

3. Different control strategies have been considered for disturbance rejection.

4. Among all the designs, the performances of both LMPC strategies are superior to others.

• 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 DE-FE0004000.
- We acknowledge Drs. Lee and Miller, NETL, for the steady-state model which is the basis of this work and also for the fruitful discussions.

• Disclaimer:

Thank you