Dynamic Modeling and Control of a Solid-Sorbent CO₂ Capture Process with Two-stage Bubbling Fluidized Bed Adsorber-Reactor

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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 CO₂ emissions, it is required that power plants have to satisfy certain amount of CO₂ capture over a period of time.

- Under Carbon Capture Simulation Initiative (CCSI), the US DOE is working on various post-combustion CO₂ capture technologies, e.g. solid-sorbent based CO₂ capture.

- As part of this project, our current focus is on the development of dynamic models and control systems for solid-sorbent CO₂ capture.
DYNAMIC MODEL DEVELOPMENT

• 1-D two-phase pressure-driven non-isothermal dynamic model of a solid-sorbent CO₂ 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.

MODEL DEVELOPMENT

- **Gaseous species**: CO₂, N₂, H₂O
- **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.**

CONSERVATION EQUATIONS

**Bubble Region:**

**Gaseous Components**

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

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

**Cloud-wake Region:**

**Gaseous Components**

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

\[
\frac{\partial (C_{P,g} C_{ct} V \delta f_{cw} \varepsilon_d (T_{g,c} - T_{ref}))}{\partial t} - A \delta H_{b,c} (T_{g,b} - T_{g,c}) + A \delta H_{c,e} (T_{g,c} - T_{g,e}) + A f_{cw} \delta (1 - \varepsilon_d) \rho_s a_p h_p (T_{g,c} - T_{s,c})
\]

\[- f_{cw} \delta (1 - \varepsilon_d) A \sum_j r_{g,c,i} C_{p,g,c,i} (T_{g,c} - T_{ref}) = 0
\]

**Adsorbed Species**

\[
\frac{\partial (V f_{cw} \delta (1 - \varepsilon_d) n_{c,i})}{\partial t} - \frac{V}{\rho_s} \frac{\partial (n_{c,j} \varepsilon_d)}{\partial x} + K_{s,bulk} + V \delta K_{c,e,b} (n_{c,i} - n_{e,j}) - V f_{cw} \delta (1 - \varepsilon_d) r_{s,c} = 0
\]

\[
\frac{\partial \left( A A \delta f_{cw} \delta \rho_s C_{p,s} \delta (1 - \varepsilon_d) (T_{s,c} - T_{ref}) \right)}{\partial t} + A \frac{\partial (f_{cw} C_{p,s} (T_{s,c} - T_{ref}) + h_{ads,c})}{\partial x} + A \frac{\partial \delta \rho_s C_{c,e,b} (T_{s,c} - T_{ref}) + h_{ads,c} - C_{p,s} (T_{s,e} - T_{ref}) + h_{ads,e}}{\partial x}
\]

\[+ f_{cw} \delta (1 - \varepsilon_d) A \sum_j r_{g,c,i} C_{p,g,c,i} (T_{g,c} - T_{ref}) - A f_{cw} \delta (1 - \varepsilon_d) \rho_s a_p h_p (T_{g,c} - T_{s,c}) = 0
\]
CONSERVATION EQUATIONS CONT'D.

Emulsion Region:

Gaseous Components

\[
\frac{\partial}{\partial t} \left( V(1 - f_{cw}\delta - \delta)\epsilon_d C_{e,i} \right) - \delta A K_{ce,i}(C_{c,i} - C_{e,i}) - K_{g,bulk} + (1 - f_{cw}\delta - \delta)A(1 - \epsilon_d)r_{g,e} = 0 \\
\frac{\partial}{\partial t} \left( C_{p,g}C_{el}V(1 - f_{cw}\delta - \delta)\epsilon_d(T_{g,e} - T_{ref}) \right) - A\delta H_{ce}(T_{g,c} - T_{g,e}) + H_{g,bulk} + (1 - f_{cw}\delta - \delta)(1 - \epsilon_d)A\rho_s a_p h_p(T_{g,e} - T_{s,e}) \\
- (1 - f_{cw}\delta - \delta)(1 - \epsilon_d)A \sum_j r_{g,e,i} C_{p,g,e,i}(T_{g,e} - T_{ref}) = 0
\]

Adsorbed Species

\[
\frac{\partial}{\partial t} \left( V(1 - f_{cw}\delta - \delta)(1 - \epsilon_d)n_{e,j} \right) + \frac{V}{\rho_s} \frac{\partial (n_{e,j}J_e)}{\partial x} - K_{s,bulk,j} - \nabla \delta K_{cebs}(n_{c,j} - n_{e,j}) - V(1 - f_{cw}\delta - \delta)(1 - \epsilon_d)r_{s,e} = 0
\]

\[
\frac{\partial}{\partial t} \left( C_{p,s}\rho_s A(1 - f_{cw}\delta - \delta)(1 - \epsilon_d)(T_{s,e} - T_{ref}) \right) + A \frac{\partial (J_e C_{p,s}(T_{s,e} - T_{ref}) + h_{ads,e})}{\partial x} - H_{s,bulk} \\
- A\delta \rho_s K_{cebs}(C_{p,s}(T_{s,c} - T_{ref}) + h_{ads,c} - C_{p,s}(T_{s,e} - T_{ref}) + h_{ads,e}) \\
+ (1 - f_{cw}\delta - \delta)(1 - \epsilon_d)A \sum_j r_{g,e,i} C_{p,g,e,i}(T_{g,e} - T_{ref}) - (1 - f_{cw}\delta - \delta)(1 - \epsilon_d)A\rho_s a_p h_p(T_{g,e} - T_{s,e}) \\
- \pi d_{Hx}h_{t,x}\Delta T_{Hx}N_{Hx}C_r = 0
\]
HYDRODYNAMIC MODEL

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

where \( \gamma_1 = \frac{2.56 \times 10^{-2}}{v_{mf}} \sqrt{\frac{D_t}{g}} \) and \( \gamma_{3,x} = \sqrt{\gamma_1^2 + 4 \frac{d_{b,m,x}}{D_t}} \)

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

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

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

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

\[
K_{bc,j,x} = 1.32 \times 4.5 \frac{v_{mf}}{d_{b,x}} + 5.85 \frac{D_{j,x}^{0.5} \, g^{0.25}}{d_{b,x}^{5/4}}
\]

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

Sit and Grace (1981)

Mori and Wen (1975)
REACTION KINETICS

\[ \text{H}_2\text{O}_{(g)} \leftrightarrow \text{H}_2\text{O}_{(phys)} \]

\[ 2\text{R}_2\text{NH} + \text{CO}_2,(g) \leftrightarrow \text{R}_2\text{NH}_2^+ + 2\text{R}_2\text{NCO}_2^- \]

\[ \text{R}_2\text{NH} + \text{CO}_2,(g) + \text{H}_2\text{O}_{(phys)} \leftrightarrow \text{R}_2\text{NH}_2^+ + \text{HCO}_3^- \]

\[ r_{1,r,i} = k_{1,r,i} \left( \frac{P_{C_{r,H_2O,i}}}{C_{r,H_2O,i}} - \frac{n_{r,H_2O,i}}{K_{1,r,i}} \right) \]

\[ r_{2,r,i} = k_{2,r,i} \left[ 1 \right. - \left. 2 \frac{n_{r,\text{carb},i}}{n_v} - \frac{n_{r,\text{bicarb},i}}{n_v} \right] n_{r,H_2O,i} \left[ \frac{P_{C_{r,\text{CO}_2,i}}}{C_{r,\text{CO}_2,i}} \right] - \left[ \left\{ \frac{n_{r,\text{carb},i}}{n_v} + \frac{n_{r,\text{bicarb},i}}{n_v} \right\} n_{r,\text{bicarb},i} \right] \]

\[ r_{3,r,i} = k_{3,r,i} \left[ 1 \right. - \left. 2 \frac{n_{r,\text{carb},i}}{n_v} - \frac{n_{r,\text{bicarb},i}}{n_v} \right]^2 \left[ \frac{P_{C_{r,\text{CO}_2,i}}}{C_{r,\text{CO}_2,i}} \right] - \left[ \left\{ \frac{n_{r,\text{carb},i}}{n_v} + \frac{n_{r,\text{bicarb},i}}{n_v} \right\} n_{r,\text{carb},i} \right] \]
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

\[ \Delta P_d = (0.2-0.3) \Delta P_{bed} \]

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 in CO₂ capture due to a 20% step increase in the flue gas flowrate

Transient in CO₂ capture due to an increase of 10 °C in the flue gas inlet temperature

Transient in CO₂ 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 CO₂ capture by manipulating the solid sorbent flowrate.

• Note the large undershoot and long settling time.
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®

![Graph showing deviation from the steady state CO₂ capture (%) over time in blue and green lines. The graph includes a blue line representing measured data and a green line representing simulated data. The graph's x-axis is labeled "Time (s)" and the y-axis is labeled "Deviation from the steady state CO₂ capture (%)".]

**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 CONT'D.

Linear Model Predictive controller (LMPC)

Measured and simulated model output

Deviation from the steady state CO₂ capture (%)

Time (s)

Estimated using ARX on data set t

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

\[
A(q) = 1 - 1.473 q^{-1} + 0.2636 q^{-2} + 0.2923 q^{-3} - 0.08314 q^{-4}
\]

\[
B_1(q) = -0.03877 q^{-1} + 0.1641 q^{-2} + 0.05974 q^{-3} - 0.1471 q^{-4}
\]

\[
B_2(q) = -4.348 q^{-1} + 0.03616 q^{-2} - 21.36 q^{-3} + 20.11 q^{-4}
\]

ARX model for the disturbance rejection using MATLAB® System identification tool box
CONTROLLER DESIGN CONT'D.

Linear Model Predictive controller (LMPC)

Servo Problem
CONTROLLER DESIGN CONTD.

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

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

Configuration of LPC with Additional Integrator
CONTROLLER DESIGN CONT'D.

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

- 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.

Configuration and performance of LMPC with estimation of unmeasured disturbance
CONTROLLER PERFORMANCE COMPARISON

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

Control Performance Table

<table>
<thead>
<tr>
<th>CONTROLLER</th>
<th>IAE</th>
<th>ISE</th>
<th>ITAE</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) PID</td>
<td>0.8111</td>
<td>1.7551</td>
<td>1.12E-04</td>
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<td>(2) FBAUGFF</td>
<td>0.4751</td>
<td>0.5502</td>
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<td>(3) LMPC-I</td>
<td>0.3913</td>
<td>0.6138</td>
<td>5.57E-05</td>
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<tr>
<td>(4) LMPC-II</td>
<td>0.4007</td>
<td>0.6386</td>
<td>6.30E-05</td>
</tr>
</tbody>
</table>
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.
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