FE0026334: ADVANCED CONTROL ARCHITECTURE AND SENSOR INFORMATION DEVELOPMENT FOR PROCESS AUTOMATION, OPTIMIZATION, AND IMAGING OF CHEMICAL LOOPING SYSTEMS

Tien-Lin Hsieh
Andrew Tong (PI), Umit Ozgunner (Co-PI), Arda Kurt (Co-PI)
Department of Chemical and Biomolecular Engineering
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Chemical Looping: Fossil Fuel Conversion with Carbon Capture

Cost Reduction Benefit

- Post-combustion (existing, new PC)
- Pre-combustion (IGCC)
- Oxy-combustion (new PC)
- CO₂ compression (all)

- Amine solvents
- Physical solvents
- Cryogenic oxygen
- Advanced physical solvents
- Advanced chemical solvents
- Ammonia CO₂ compression
- PBI membranes
- Solid sorbents
- Membrane systems
- ITMs
- Biomass co-firing
- Ionic liquids
- Metal organic frameworks
- Enzymatic membranes

CO₂ Capture Targets:
- 90% CO₂ Capture
- <10% increase in COE (IGCC)
- <35% increase in COE (PC)

José D. Figueroa, National Energy Technology Laboratory (NETL), U.S. DOE
Applying chemical looping to coal-based hydrogen production

Conventional coal-based hydrogen production w/ carbon capture

Chemical looping hydrogen production w/ carbon capture

Syngas Chemical Looping (SCL) Process for H₂ Production

Main reactions:

Reducer: \( C_x H_y O_z + Fe_2 O_3 \rightarrow CO_2 + H_2O + Fe \)

Oxidizer: \( Fe + H_2O \rightarrow Fe_3 O_4 + H_2 + Q \)

Combustor: \( Fe_3 O_4 + O_2 \rightarrow Fe_2 O_3 + Q \)

Total: \( C_x H_y O_z + H_2O + O_2 \rightarrow CO_2 + H_2 + Q \)

>99% H₂ Purity
Evolution of The Ohio State Syngas Chemical Looping

Reducer: \[ C_xH_yO_z + Q + Fe_2O_3 \rightarrow CO_2 + H_2O + Fe \]

Oxidizer: \[ Fe + H_2O \rightarrow Fe_3O_4 + H_2 + Q \]

Combustor: \[ Fe_3O_4 + O_2 \rightarrow Fe_2O_3 + Q \]

Net: \[ C_xH_yO_z + H_2O + O_2 \rightarrow CO_2 + H_2O + H_2 \]
• Objective: develop an advanced process automation control architecture and imaging and optimization sensor information for the OSU chemical looping process
  • Develop HLC-SMC control scheme for process automation (OSU ECE)
  • Establish sensor algorithm for high temperature ECVT (Tech4Imaging)
  • Integrate process performance parameters with FocalPoint Optimization System (B&W)
  • Prepare and test process control and optimization concepts in 25 kW_{th} sub-pilot test unit (OSU CBE)
Sliding Mode Controller (SMC)

- Advantage: State trajectory control, robustness
- Controller changes behavior as the state trajectory crosses the surface
- Exemplary mathematical form:
  \[ \ddot{x} + a_2 \dot{x} + a_1 x = u, \]
  \[ u = -M \text{sign}(s), \quad s = cx + \dot{x}, \quad a_1, a_2, M, c - \text{const} \]
- Two stages:
  - Reaching mode: to get to the sliding surface
  - Sliding mode: reduced order motion on the surface
- Disadvantage: chattering ➔
  - actuator wear-and-tear
  - potential plant excitement

Design of adaptive M

Modified sigmoid function:

\[ M = \left( b + \frac{a}{1 + e^{c-d|s|}} \right) k \]

Goal:
- Reduce chattering
- Enhance disturbance rejection

- Dead band
- Transitional zone
- \( M_{\text{max}} \): upper limit of designed actuator action
- \( M_{\text{min}} \): minimum control effort to maintain steady state
Adaptive $M$

$N_2$ Flow rate

$M = 0.4$

$M = 0.8$

$X_2$

$DP$ Ratio
Implementation of automatic start-up algorithm

- Pre-set operation goals
- HLC-SMC structure
- 1-click startup for fluidization, entrainment and maintaining circulation during heat-up
- Fuel injection upon reaching reaction temperatures and operation 1-click acknowledgement
Achieved automatic startup with zero operator intervention

Maintained oxygen carrier circulation at minimal solid flow rate using self-regulating aeration and entrainment gases
Circulation rate control

- SMCs attempt to minimize attrition by controlling circulation rate

High-potential circulation stoppage indicator

Aggressive control action

Process responded, circulation resumed
• Simultaneous control actions correctly executed by all SMCs with no operator intervention
• Achieved ~99% syngas conversion
• No gas breakthrough was observed in either reactor
SCL Pilot Unit Pressurization/Depressurization

Ramp surface:
\[ u = M_2 \cdot \text{sign}(S_2) \]
\[ S_2 = \frac{dP}{dt} - RR \]
RR: Ramp rate

SS surface:
\[ u = M_3 \cdot \text{sign}(S_3) \]
\[ S_2 = \frac{dP}{dt} + (P - P_{sp}) \cdot K \]
\[ P_{sp} = \text{setpoint}, K = \text{const} \]
\[ u = \frac{dx}{dt} \]
Electrical Capacitance Volume Tomography (ECVT)

Sensor Assembly

Capacitance Probe Arrangement

Ceramic Lining

Capacitance Probe

24 channel Sensor

The Ohio State University
ECVT on OSU Chemical Looping System

Moving Bed

Fluidized Bed
Fluidized Bed Combustor - Slug Flow 800˚C

Operating Conditions

\[ T = 800^\circ C \]
\[ Q_{\text{Air}} = 283 \text{ slpm} \]
\[ U_{mf} = 0.84 \text{ m/s} \]
\[ U = 4.07 \text{ m/s} \]
\[ U/U_{mf} = 4.82 \]
\[ d_p = 1.5 \text{ mm} \]
\[ \rho_p = 2500 \text{ kg/m}^3 \]

Raw Capacitance Measurement

Vertical Cross-Sectional Image

3-Dimensional Image

Normal Plane Image
Temperature Variation of Slugging Fluidized Bed

Image Reconstruction:

- 23 C, 600 slpm
  \( U_g - U_{mf} = 1.49 \)

- 335 C, 300 slpm
  \( U_g - U_{mf} = 1.5 \)

- 640 C, 220 slpm
  \( U_g - U_{mf} = 1.80 \)

- 720 C, 176 slpm
  \( U_g - U_{mf} = 1.47 \)

Image reconstruction frame rate: 80 Hz ~ 260 Hz
Fluidized Bed Characterization

- Separate fluidization regimes identified
  - Bubbling, Slugging, and Transition Regimes
  - Bubbling – irregular gas bubbles
  - Transition – bubble coalescence and partial gas slugs
  - Slugging – fully developed gas slugs
Moving Bed Velocity - ECVT

- Parallel pairs of plates at different vertical locations chosen
- Irregularities in solid holdup detected as bed moves through sensor
- Capacitance signals cross-correlated to find frame ‘lag’
- Using sensor dimensions and data framerate, linear velocity can be extracted
Moving Bed Velocity – Cross Correlation

- Before cross correlation, capacitance data for each pair is normalized
- Commonly referred to as Normalized Cross Correlation
- Two signals are shifted to find the maximum cross correlation
- From the magnitude of the shift, data capture frequency, and solid density, linear velocity and mass flow can be extracted

\[
\hat{C}_1 = \frac{C_1 - \bar{C}_1}{\sqrt{\frac{1}{N-1} \sum |C_{1i} - \bar{C}_1|}}
\]
Moving Bed Velocity – Image Reconstruction

Raw Image  Enhanced Color Contrast  Processed
Moving Bed Velocity – Frequency Effect & Results

- High frequency generally generates noisier signals, which leads to non-matching capacitances patterns in half of the trials (*).
- Low frequency signals generally show clear patterns, which consistently allow accurate calculation of solid linear velocities by cross correlation.

<table>
<thead>
<tr>
<th>Framerate</th>
<th>Measured (Scale + Timer)</th>
<th>Calculated (ECVT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>81.16 Hz</td>
<td>1.62 cm/s</td>
<td>1.66 cm/s</td>
</tr>
<tr>
<td>184.81 Hz</td>
<td>1.62 cm/s</td>
<td>1.62 cm/s*</td>
</tr>
</tbody>
</table>
# Moving Bed Velocity - Plate Pairing Effect

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<thead>
<tr>
<th>Plates</th>
<th>Velocity (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,4 – 13,16</td>
<td>1.66</td>
</tr>
<tr>
<td>2,5 – 14,17</td>
<td>1.65</td>
</tr>
<tr>
<td>3,6 – 15,18</td>
<td>1.65</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>Plates</th>
<th>Velocity (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7,10 – 19,22</td>
<td>1.72</td>
</tr>
<tr>
<td>8,11 – 20,23</td>
<td>1.73</td>
</tr>
<tr>
<td>9,12 – 21,24</td>
<td>1.72</td>
</tr>
</tbody>
</table>

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<th>Velocity (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,9 – 13,21</td>
<td>1.72</td>
</tr>
<tr>
<td>2,10 – 14,22</td>
<td>1.89</td>
</tr>
<tr>
<td>3,11 – 15,23</td>
<td>1.75</td>
</tr>
</tbody>
</table>
Project Achievements

- Autonomous startup, steady-state operation and shutdown
  - Implemented hybrid HLC-SMC structure
  - Designed system successfully carried out complete operation sequence with minimal human intervention
- ECVT Solid flow control development
  - Developed two different applications of ECVT to non-intrusively monitor different gas-solid flow patterns at high temperatures

Remaining Task

- Optimization Software
  - Designed optimization problem: minimizing aeration/entrainment gas while maximizing gas conversion
  - Preliminary data obtained. Analyzing data and revising program
Acknowledgements

• DOE/NETL
• Ohio Development Service Agency: Gregory Payne
Dynamic Modeling

- **Ergun Equation**
  \[
  \frac{DP_{360}}{d_p^2} = \frac{150 \mu N_2 L_{361} (1 - \epsilon)^2}{\epsilon^3} u_{361} + 1.75 \rho_{360} L_{361} (1 - \epsilon) \frac{u_{361}}{d_p^2} u_{361}\]

- **Valve Equation**
  \[
  F_{490} = 3.455 \times 10^{-5} \left( \text{mol} \cdot s^{-1} \cdot Tg_{490} \right) \cdot P_{a^{-1}} \cdot x_{490} \cdot \sqrt{\frac{p_{490}^2 - p_0^2}{Tg_{490} S_g}} \quad \text{when} \quad \frac{p_{490}}{p_0} < 1.89
  \]
  \[
  F_{490} = 2.934 \times 10^{-5} \left( \text{mol} \cdot s^{-1} \cdot Tg_{490} \right) \cdot P_{a^{-1}} \cdot x_{490} \cdot P_{490} \cdot \sqrt{\frac{1}{Tg_{490} S_g}} \quad \text{when} \quad \frac{p_{490}}{p_0} > 1.89
  \]

- **Gas Mass Balance**
  \[
  \frac{dP_0}{dt} = \frac{R \cdot Tg_{490} \cdot (F_{420} + F_{371} + F_{362} - F_{490})}{V} + \frac{P_0}{Tg_{490}} \cdot \frac{dTg_{490}}{dt}
  \]

- **Combustor/Riser Correlation**
  \[
  DP_c = \begin{cases} 
  H_c \times \rho_c \times \alpha_c \times g & \text{if} \quad u_{gc} > u_{mf} \\
  L \times \left( 150 \left( \frac{1}{\epsilon^2} \frac{\mu_{air} u_{gc}}{d_p^2} + 1.75 \left( 1 - \epsilon \frac{\rho_c u_{gc}^2}{\epsilon^2} \frac{d_p^2}{d_p} \right) \right) \right) & \text{if} \quad u_{gc} \leq u_{mf}
  \end{cases}
  \]
  \[
  \alpha_c = 0.63 \left( 1 + \frac{21.4 (u_g - u_{mf})^{0.738}}{d_p^{0.006} \rho_{1.376}} \right)^{-1}
  \]
  \[
  u_{mf} = \left( \frac{M_p P_{11}^{0.126}}{P_a} \right)
  \]
  \[
  \]
Phase Plane

Arrows represent the direction of system state as time progresses:
1, 2: Pressurization
4, 5: Controller action in response to the disturbance

Sliding surface S2
\[ \frac{dP}{dt} - 1 = 0 \]

Sliding surface S3
\[ \frac{dP}{dt} + \frac{P - 30}{3} = 0 \]
Matlab simulation of a sliding mode controller design for pressure control

• Control law: rate of valve opening change
  • $u = \frac{dx}{dt}$

• S2 Controller:
  • $u = M_2 \cdot \text{sign}(S_2)$
  • $S_2 = \frac{dP}{dt} - RR$
  • $RR = 1 \text{ psi/min}$

• S3 Controller:
  • $u = M_3 \cdot \text{sign}(S_3)$
  • $S_3 = \frac{dP}{dt} + (P - P_{sp}) \cdot K$
  • $P_{sp} = 30 \text{ psig}, K = \frac{1}{3} \text{ min}^{-1}$
Goal:
• Reduce chattering
• Enhance disturbance rejection

Design of adaptive M

Modified sigmoid function:

\[ M = \left( b + \frac{a}{1 + e^{c-d|s|}} \right) k \]

- \( M_{\text{min}} \): minimum control effort to maintain steady state
- Dead band
- Transitional zone

\( b \)
\( d \)
\( k \)
Sliding Mode Controller for Pilot Unit System Pressure Control

• Vessel model:
  • Consider the reactor as a single tank with one inlet and one outlet
  • Isothermal
  • \( \frac{dP}{dt} = \frac{RT}{V} \times (F_{210} - x \cdot f(P_{204})) \)
  • \( x \) is valve opening ZYT-700, \( x \cdot f(P_{204}) \) is the valve flow equation:
    
    \[
    f(P) = \begin{cases} 
    C_v \cdot Y \cdot N \cdot P \cdot \frac{P-P_0}{P_{M_w}T} & \text{if } \frac{P-P_0}{P} < 0.64 \\
    C_v \cdot Y \cdot N \cdot P \cdot \frac{0.64}{M_wT} & \text{if } \frac{P-P_0}{P} \geq 0.64 
    \end{cases}
    \]

• Initial condition: \( P_{204} = 0 \) psig, \( T = 300K \), ZYT-700 = 0
• \( F_{210} \) increase from 0 to 1000 lb/hr at 1 lb/hr/s
• \( F_{210} \) sudden increase from 1000 to 1300 at t=45min
• Pressurization in three stages:
  • S1: outlet closed, start gas flow, till \( dP/dt > 1 \) psi/min
  • S2: pressurize at \( dP/dt = 1 \) psi/min, until
  • S3: gradually slow down pressurization, and maintain pressure at 30 psig
• Nitrogen injection to verify behaviors for individual SMCs

• Extreme capacity change to test disturbance rejection performance
SMC Response to Capacity Change

Gauge Pressure (in H₂O)

- P_Gas seal, top
- P_Red, out
- P_Red, in
- P_Gas seal, bottom

Capacity (kW)

- Capacity

Time

08:09 08:24 08:38 08:52 09:07 09:21

-2 0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36 38 40