Plantwide Control of Chemical Looping Combustion

T. McFarland and B. Erik Ydstie

Carnegie Mellon University
Pittsburgh, PA 15213
Objectives

- Develop theory for plantwide control that guarantees stability
  - Input-Output Stability
  - Lyapunov Stability

- Develop procedure for determining control variables
  - Guarantee stability
  - Based on minimal process information

- Apply procedure to Chemical Looping Combustion process
Chemical Process Networks

- Follow a set of principal rules
  - Conservation Laws (Mass, Energy, Stoichiometry)
  - Second Law of Thermodynamics (Entropy Production)

- State of a Chemical Process Network (CPN)

  \[ TS = U + PV + \mu_i N_i \]

  \[ S = \left( \frac{1}{T} \right) U + \left( \frac{P}{T} \right) V - \left( \frac{\mu_i}{T} \right) N_i \]

  \[ S(Z) = \omega^T Z \]

\[
\begin{align*}
Z &= \begin{pmatrix} U \\ V \\ N_i \end{pmatrix} \\
\omega &= \begin{pmatrix} \left( \frac{1}{T} \right) \\ \left( \frac{P}{T} \right) \\ -\left( \frac{\mu_i}{T} \right) \end{pmatrix}
\end{align*}
\]
Topological properties of CPNs

- State Space System

\[ \frac{dZ}{dt} = p(Z) + \phi(Z, u) \]

- CPNs as directed graphs

- Extensive Variables, $Z_{\text{group}}$, act as inventories

\[ Z_{\text{group}} = Z_1 + Z_2 \]
Passive Systems

• Passivity defined by Storage Function, $W$

$$\int_0^t u^T y d\tau + W(0) \geq W(t) \geq 0 \quad W(0) \geq 0$$

• Advantageous Stability Properties
  – $L_2$ norm input-output stable
  – Lyapunov stability

• A Network of Passive Nodes is Passive
  – Apply decentralized control to achieve passivity
  – Stability properties apply network wide
A Thermodynamic Storage Function

- Entropy is concave
- Availability – “useful work of a system”

\[ A(\omega - \omega^*) = Z^T(\omega - \omega^*) \]

- \( \omega \) converges, \( Z \) does not converge

\[ A(\omega - \omega^*) \geq 0 \quad A(0) \geq 0 \quad \dot{A}(\omega - \omega^*) \leq 0 \]

- Must control some extensive variables, \( Z_c \)

\[ W = \dot{A}(\omega - \omega^*) + \frac{1}{2}(Z_c - Z_c^*)^2 \]

- Minimal control for passivity: 1 extensive variable per independent phase
Control Structure Design

- General Control Law, $\Gamma(Z - Z^*)$
  - Locally Lipschitz continuous
  - $(Z - Z^*)\Gamma > 0$
  
  \[
  \frac{dZ}{dt} = p(Z) + \phi(Z, u) \quad \Rightarrow \quad -\Gamma(Z - Z^*) = p(Z) + \phi(Z, u)
  \]

- Develop a procedure for the control system based on minimal control
  - Draw digraph of process
  - Determine control degrees of freedom
  - Control Total Mass Inventories
  - Control Phase Inventories
  - Additional degrees of freedom
    - Meet physical constraints
    - Optimization
Chemical Looping Combustion Process

• Oxidation-Reduction
• > 90 % CO2 effluent
• Low NOx emissions
• No oxygen-nitrogen separation
• Iron Oxide used for simulations

\[ M_e + O_2 \rightarrow M_e O_x \]

\[ M_e O_x + C \rightarrow CO + CO_2 + M_e \]
Determining Control Degrees of Freedom

\[ F_{\text{cont}} = s - f - \gamma \]

- \( s \): number of streams
- \( f \): number of non-terminal feeds
- \( \gamma \): number of non-controllable phases

### Table 1: CLC Control Degrees of Freedom

<table>
<thead>
<tr>
<th>Node</th>
<th>Unit</th>
<th>( s )</th>
<th>( f )</th>
<th>( \gamma )</th>
<th>( F_{\text{cont}} )</th>
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<tr>
<td>1</td>
<td>Compressor</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Mixer</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>0</td>
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<td>3</td>
<td>Oxidation Rxr</td>
<td>2</td>
<td>4</td>
<td>0</td>
<td>2</td>
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<tr>
<td>4</td>
<td>HEX (steam)</td>
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<td>2</td>
<td>1</td>
<td>0</td>
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<tr>
<td>5</td>
<td>Splitter</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
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<td>Compressor</td>
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<td>2</td>
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<td>0</td>
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<tr>
<td>7</td>
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<td>1</td>
<td>2</td>
<td>1</td>
<td>0</td>
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<tr>
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<td>Reduction Rxr</td>
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<td>4</td>
<td>0</td>
<td>2</td>
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<tr>
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<td>2</td>
<td>1</td>
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</tr>
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</table>

Control Degrees of Freedom: 9
Assigning Control Variables

1) Total Mass Inventory
2) Phase Mass Inventory
3) Additional DOF
   3a) Physical Constraints
   3b) Terminal Flows
   3c) Optimization

CDOF
Properties of Extensive Variable Control

- Extensive state variables are deg. 1 homogeneous functions
  \[ [U, V, N_1...N_n]^T_1 = \alpha[U, V, N_1...N_n]^T_2 \]

- State 1 varies from State 2 only in quantity, intensive variables same value

- By setting extensive state, we have a one to one transformation \( Z_1 \rightarrow \omega_1 \)
  \[ \omega_1 \rightarrow \alpha Z_1 \]

- Control of extensive variables gives a much more constrained system

- If the plant is highly constrained and a specific objective drives the change in plant state
  - Driving Setpoints (Energy, Oxygen Inventory)
  - Tracking Setpoints (Methane Flow, Reduction Energy)
State Control : A Feasible Trajectory

• State Control : move the plant from one state to another
  – Feasible, Stable trajectory \[ Z_1' = \alpha Z_2' \]

• Define an augmented state vector : terminal flows and objective function
  \[ Z' = [Z, m, q]^T \]

• Find a relationship of augmented vectors, \( \alpha \) diagonal matrix

• Relationships ( ) defined by
  – Active constraints (T, P)
  – Kinetic Relationships \[ \frac{U_1}{M_1} = \frac{U_2}{M_2} \rightarrow \alpha U = \alpha M \]
  – Balance Equations
  – Ex : Move along constant temperature trajectory \( q \)
Results of State Control

- Random demand swings applied

- Demand change
  - Compare to previous and calculate $\alpha_{demand}$
  - Based on predetermined relationships among $Z$ variables, entire state determined
Gas Phase Inventory

Oxidation Reactor Gas Phase Mass Inventory

Reduction Reactor Gas Phase Mass Inventory

- Blue line: Oxi Mass
- Red line: Oxi SP
- Green line: Man Mole Flow

- Blue line: Red Mass
- Red line: Red SP
- Green line: Man Mole Flow
Total Mass/Solid Phase Inventory
Controlling Energy, Not Temperature

- Achieve temperature control without explicit control law
- Gas Temp fluctuates slightly
  - Heat capacity varies
- Solid Temp held constant

![Oxidation Reactor Temperatures Graph](image-url)
Summary

• Developed a plantwide control procedure (stability driven)
  – Establish local passivity first
  – Remaining degrees of freedom reduce operating space based on economics/safety
  – independent of choice of controller

• Inventory controllers stabilize CLC process

• State Control
  – Deterministic model for setpoints
  – Feasible trajectories
  – Plants with Constrained Extensive State