Plantwide Control of Chemical Looping Combustion

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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)

$$TS = U + PV + \mu_i N_i$$

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

$$S(Z) = \omega^T Z$$

Extensive

$$Z = \begin{pmatrix} U \\ V \\ N_i \end{pmatrix}$$

Intensive

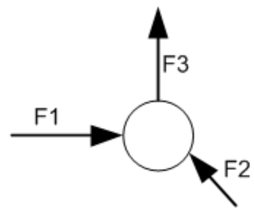
$$\omega = \begin{pmatrix} \left(\frac{1}{T}\right) \\ \left(\frac{P}{T}\right) \\ \left(\frac{-\mu_i}{T}\right) \end{pmatrix}$$

Topological properties of CPNs

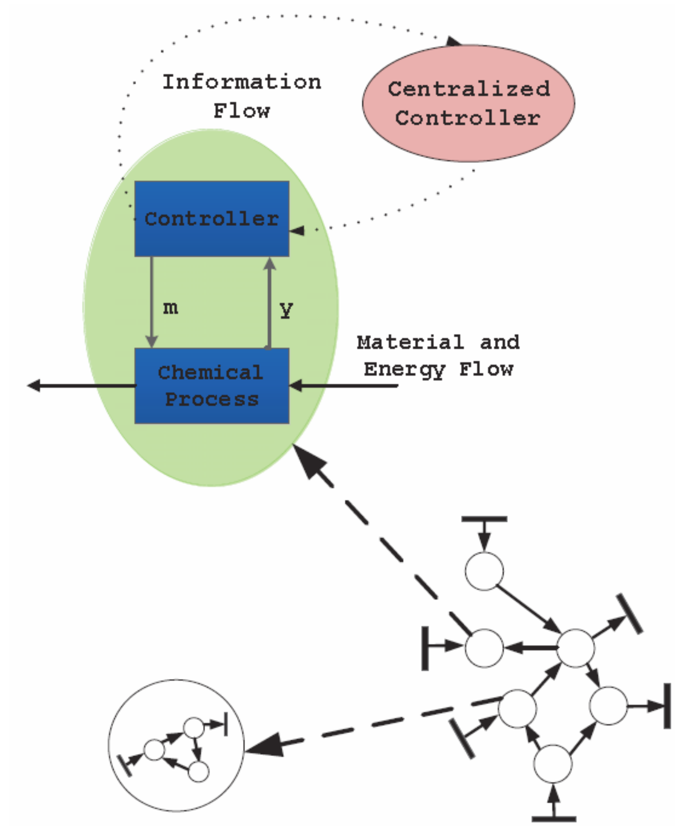
- State Space System

$$\phi = F_1 - F_2 - F_3$$

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



- CPNs as directed graphs



- Extensive Variables, Z , act as inventories

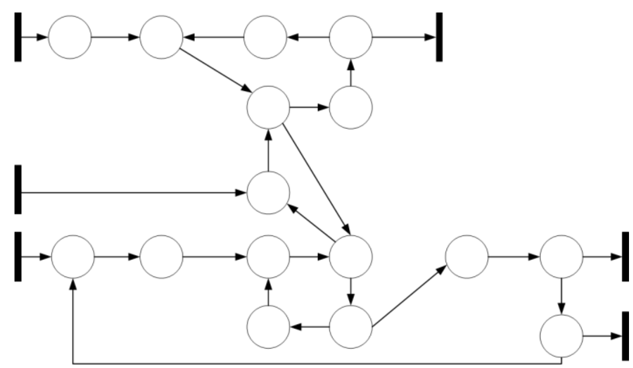
$$Z_{group} = Z_1 + Z_2$$

Passive Systems

- Passivity defined by Storage Function, W

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

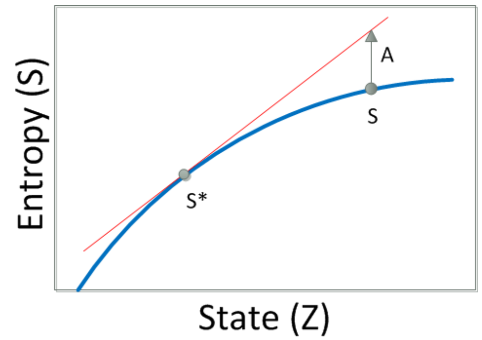
- Advantageous Stability Properties
  - L_2 norm input-output stable
  - Lyapunov stability
- A Network of Passive Nodes is Passive
  - Apply decentralized control to achieve passivity
  - Stability properties apply network wide



A Thermodynamic Storage Function

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

$$A(\omega - \omega^*) = Z^T(\omega - \omega^*)$$



- ω 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
  - $(Z - Z^*)\Gamma > 0$

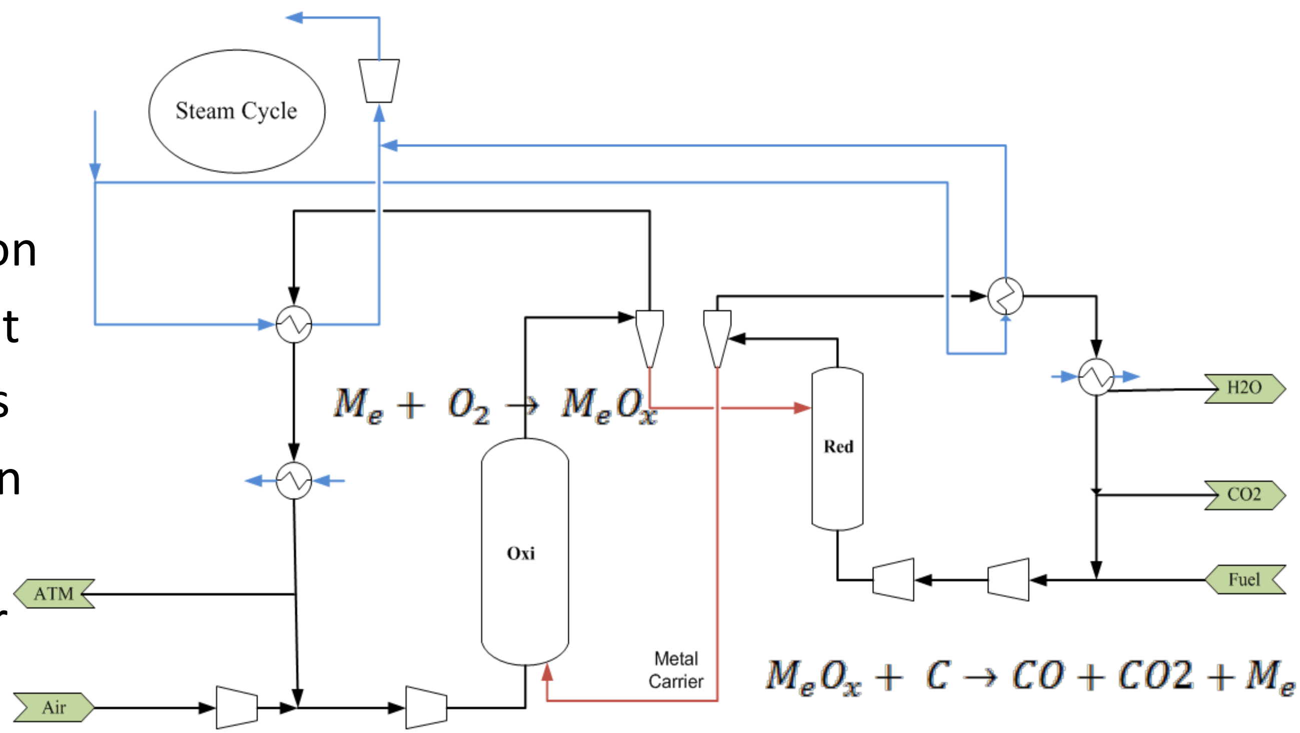
$$\frac{dZ}{dt} = p(Z) + \phi(Z, u) \quad \Longrightarrow \quad -\Gamma(Z - Z^*) = p(Z) + \phi(Z, u)$$

- 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

Power Generation for Carbon Sequestration

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



Determining Control Degrees of Freedom

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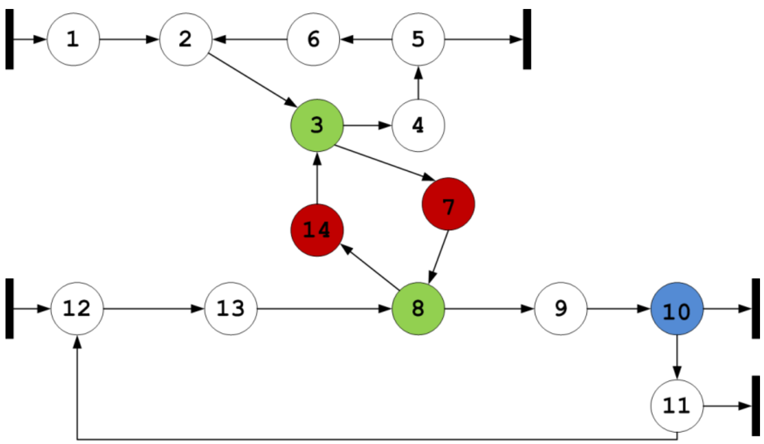


$$F_{cont} = s - f - \gamma$$

s # of streams

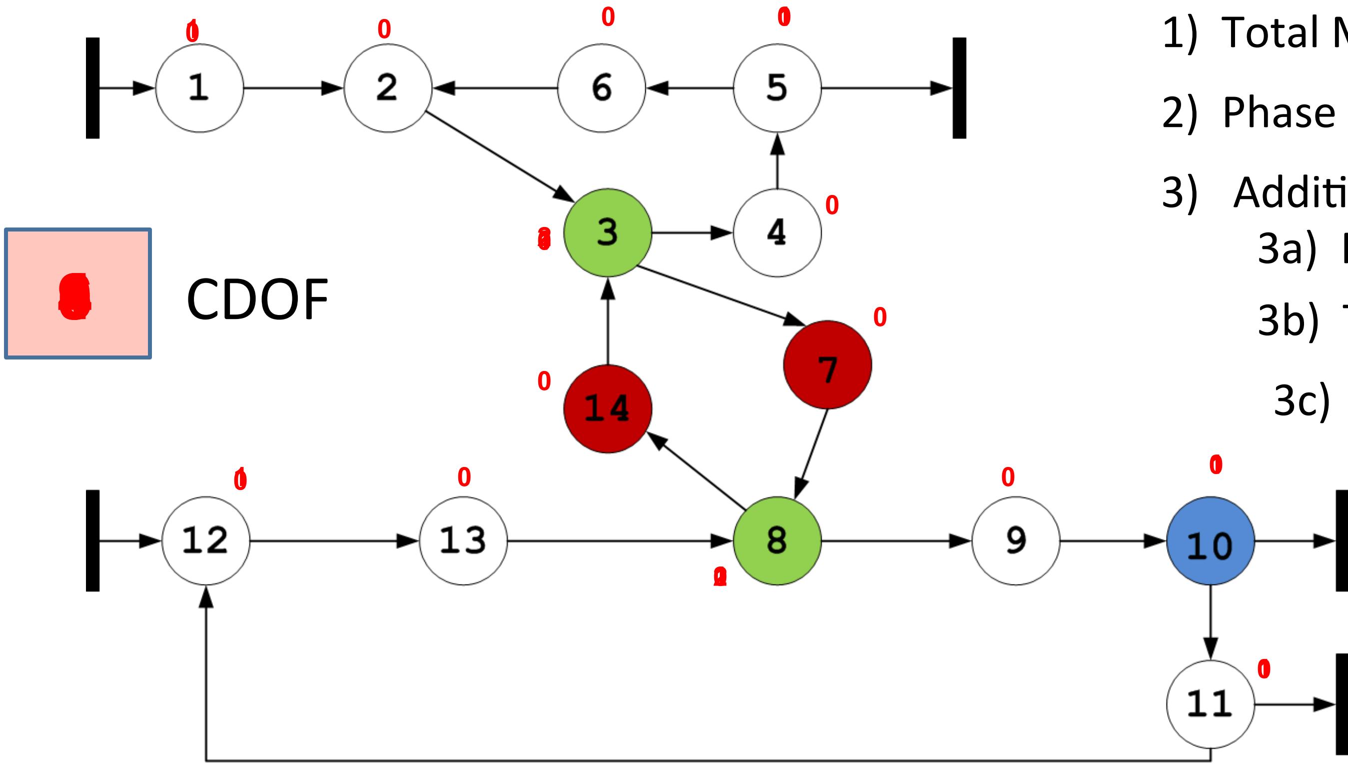
f # of non-terminal feeds

γ # of non-controllable phases

Table 1: CLC Control Degrees of Freedom

Node	Unit	¼	s	f	°	F_{cont}
1	Compressor	1	2	0	1	1
2	Mixer	1	3	2	1	0
3	Oxidation Rxr	2	4	2	0	2
4	HEX (steam)	1	2	1	1	0
5	Splitter	1	3	1	1	1
6	Compressor	1	2	1	1	0
7	Solids Storage	1	2	1	1	0
8	Reduction Rxr	2	4	2	0	2
9	HEX Steam	1	2	1	1	0
10	Condenser	2	3	1	1	1
11	Splitter	1	3	1	1	1
12	Mixer	1	3	1	1	1
13	Compressor	1	2	1	1	0
14	Solids Storage	1	2	1	1	0
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

Properties of Extensive Variable Control

- Extensive state variables are deg. 1 homogeneous functions

$$[U, V, N_1 ... N_n]_1^T = \alpha [U, V, N_1 ... N_n]_2^T$$

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

- By setting extensive state, we have a one to one transformation $Z_1 \rightarrow \omega_1$

$$\omega_1 \rightarrow \alpha Z_1$$

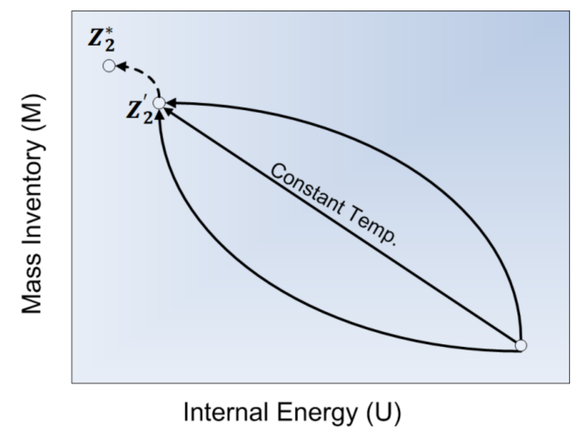
- Control of extensive variables gives a much more constrained system
- If the plant is highly constrained and a specific objective drives the change in plant state
  - Driving Setpoints (Energy, Oxygen Inventory)
  - Tracking Setpoints (Methane Flow, Reduction Energy)

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

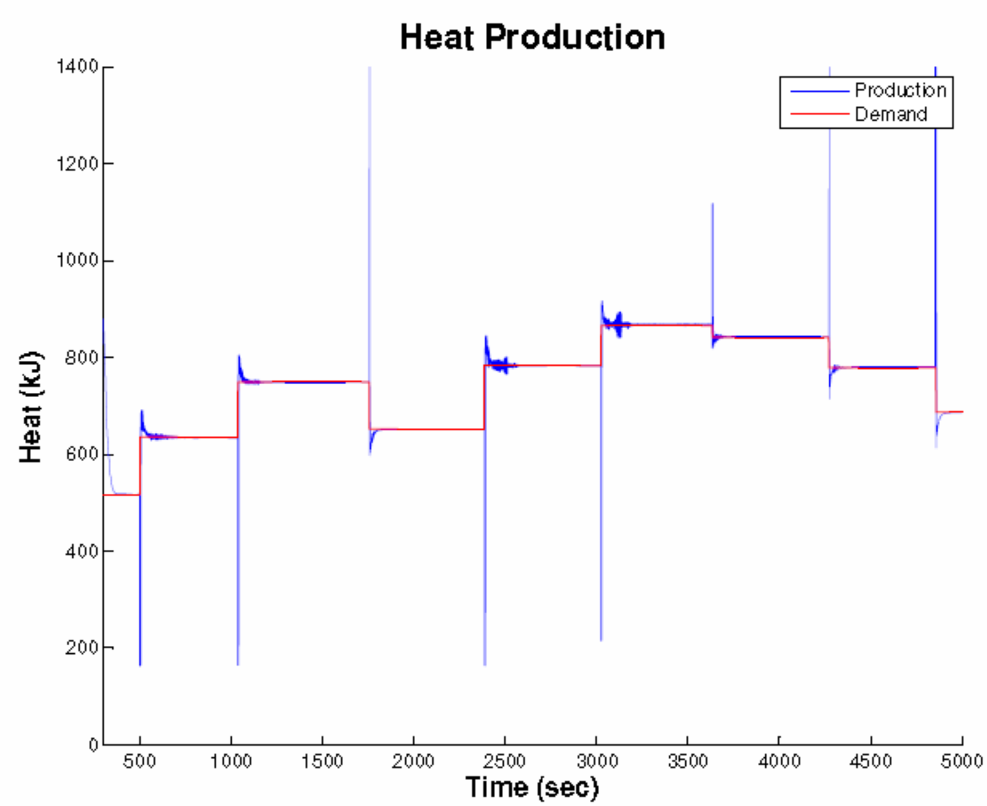
$$Z^{'} = [Z, m, q]^T$$

- Find a relationship of augmented vectors, α 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 trajecto q

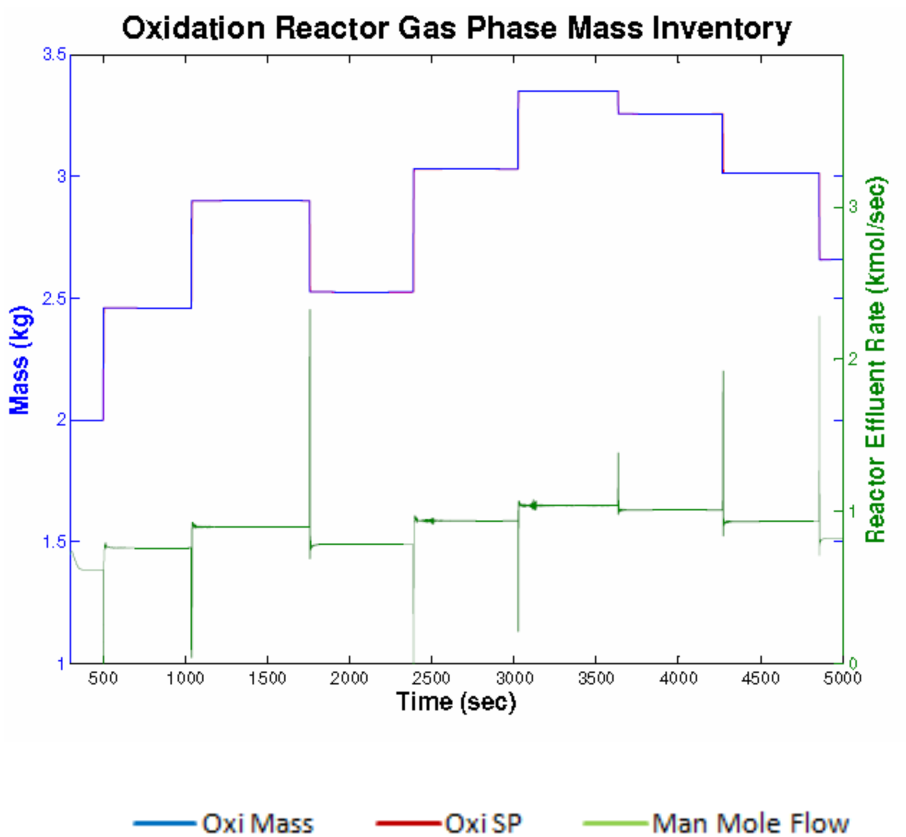


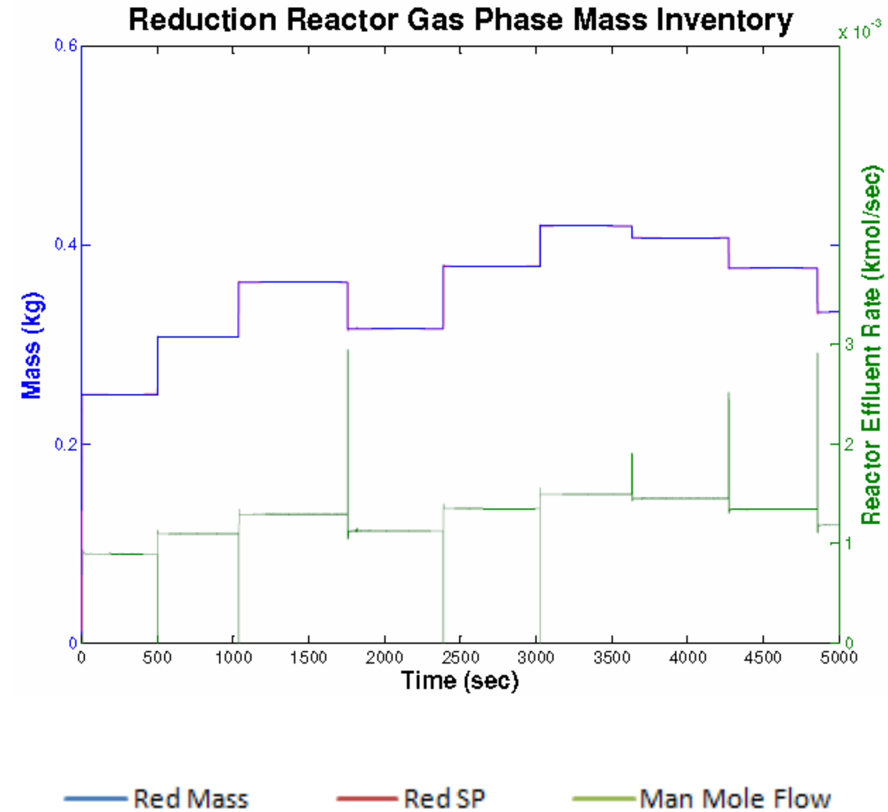
Results of State Control

- Random demand swings applied
- Demand change
  - Compare to previous and calculate α_{demand}
  - Based on predetermined relationships among Z variables, entire state determined

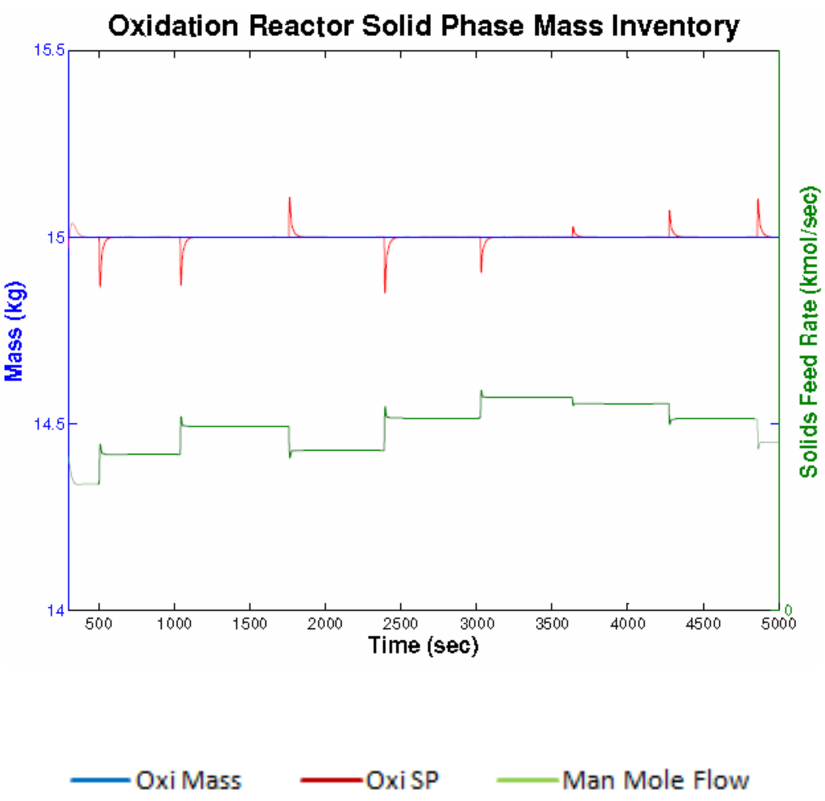


Gas Phase Inventory



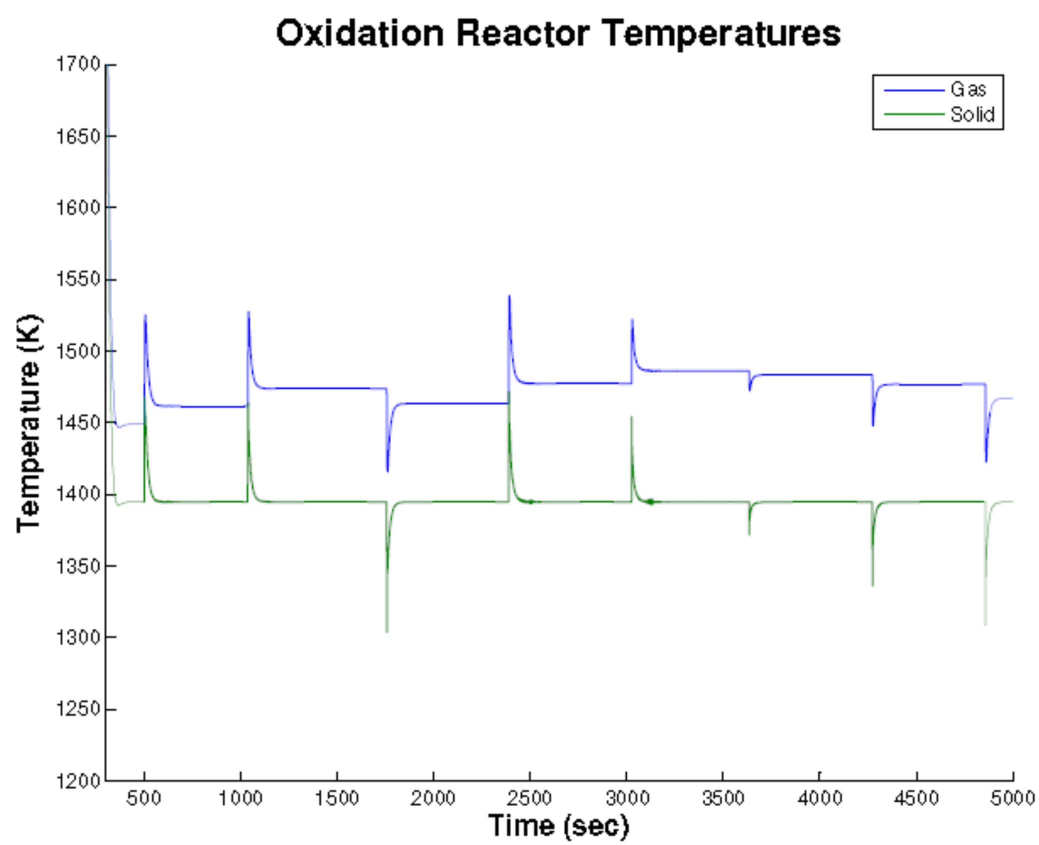


Total Mass/Solid Phase Inventory



Controlling Energy, Not Temperature

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



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