Pressure Swing Adsorption: An Alternate Carbon Capture Process for IGCC Power Plants

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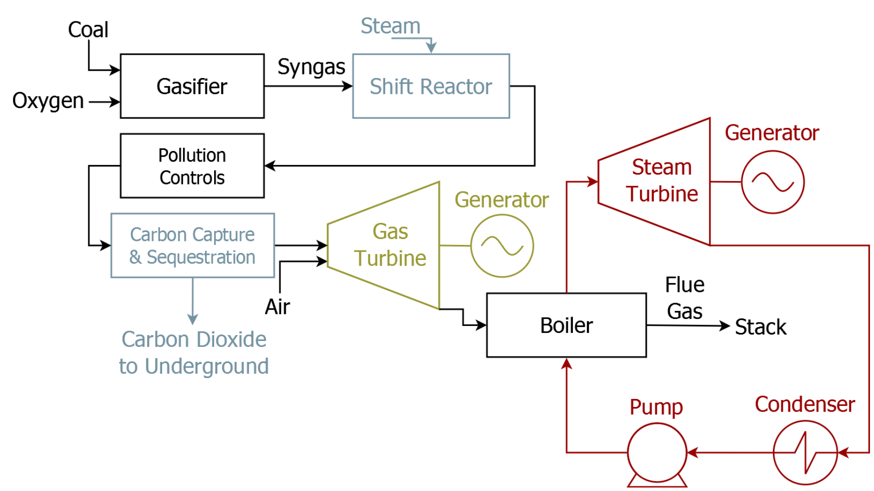
Research Objectives

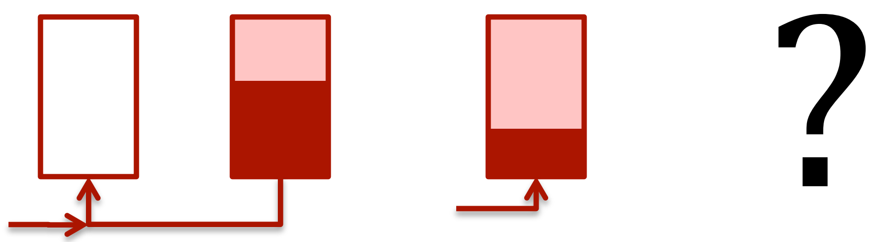
- Demonstrate methods for optimal Pressure Swing Adsorption (PSA) process synthesis

- Design **cost effective** PSA cycle for H_2-CO_2 separation in IGCC power plant

Simplified IGCC Flowsheet



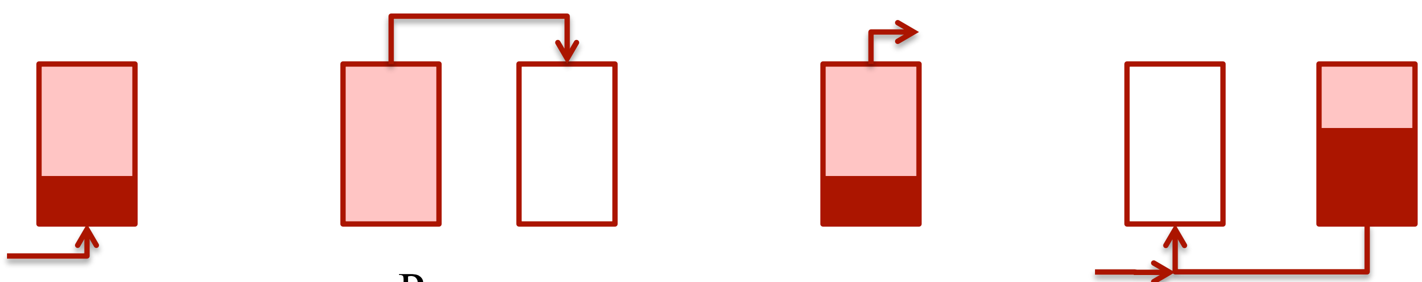
Optimal Cycle Synthesis



Discrete variables make this **too computationally expensive** to solve

Step 1 Step 2 Step 3 Step 4 … Step n

"Parts Box" of Steps



Adsorption

Pressure Equalization

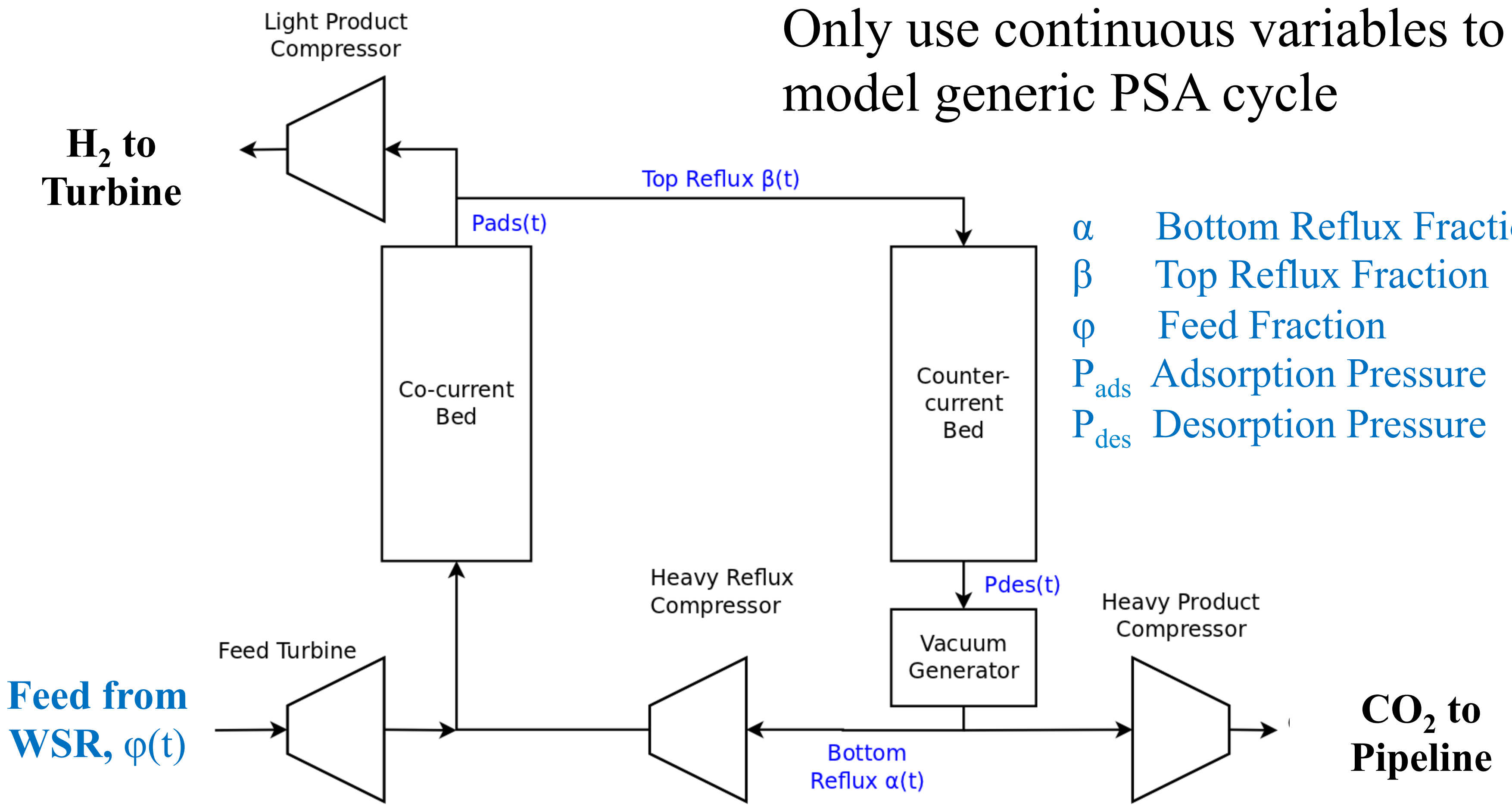
Desorption

Heavy Product Purge

And many more…

PSA "Superstructure"

Only use continuous variables to model generic PSA cycle



α Bottom Reflux Fraction

β Top Reflux Fraction

φ Feed Fraction

P_{ads} Adsorption Pressure

P_{des} Desorption Pressure

PSA Model: Transport Equations

Momentum (Ergun Equation)

$$-\frac{\partial P}{\partial x} = \frac{150\mu(1-\epsilon_b)^2}{d_p^2 \epsilon_b^3} v + \frac{1.75}{d_p}\left(\frac{1-\epsilon_b}{\epsilon_b^3}\right)\left(\sum_i M_w^i C_i\right) v|v|$$

$$v_j(t,x) \leftarrow \begin{cases} \max(0, v_j(t,x)) & \text{if} \quad j = 1 \quad \text{(co-cur. bed)} \\ \min(0, v_j(t,x)) & \text{if} \quad j = 2 \quad \text{(counter-cur. bed)} \end{cases}$$

Energy

$$0 = \left(\epsilon_t \sum_i C_i (C_{pg}^i - R) + \rho_s C_{ps}\right) \frac{\partial T}{\partial t} - \rho_s \sum_i \Delta H_i^{ads} \frac{\partial q_i}{\partial t} + \frac{\partial (vh)}{\partial x} + UA(T - T_w)$$

Material

$$\epsilon_b \frac{\partial C_i}{\partial t} + (1-\epsilon_b)\rho_s \frac{\partial q_i}{\partial t} + \frac{\partial (v C_i)}{\partial x} = \cancel{D_L \frac{\partial^2 C_i}{\partial x^2}} \qquad i = 1 \ldots N_c$$

PSA Model: Adsorption

Linear Driving Force

$$\frac{\partial q_i}{\partial t} = k_i(q_i^\star - q_i) \qquad i = 1...N_c$$

Dual-Site Langmuir Isotherm

$$q_i^\star = \frac{q_1^s b_{1i} P_i}{1 + \sum_j b_{1j} P_j} + \frac{q_2^s b_{2i} P_i}{1 + \sum_j b_{2j} P_j} \qquad i = 1...N_c$$

where $\quad q_{mi}^s = k_{mi}^1 + k_{mi}^2 T \qquad b_{mi} = k_{mi}^3 exp(k_{mi}^4/T) \qquad m = 1, 2$

Thermodynamics: Ideal Gas Law

Optimization Formulation

$$\textbf{min Energy}(u_1, u_2, \ldots, u_{N_{slot}}, L_{bed}, t_{cycle})$$

s.t. Bed Equations

$$u_{low} \le u_j \le u_{high}$$
$$t_{cycle,min} \le t_{cycle}$$
$$L_{bed,min} \le L_{bed}$$
$$\text{Purity } CO_2 \ge 92\%$$
$$\text{Recovery } CO_2 \ge 90\%$$
Cyclic Steady-State

$$i \in \{1, \ldots, N_{comp}\}$$
$$m \in \{1, \ldots, N_{slot}\}$$
$$u_m = [\alpha_m, \beta_m, \phi_m, P_{ads,m}, P_{des,m}]^T$$

$$z = \begin{bmatrix} C_{i,1,1} \\ q_{i,1,1} \\ T_{1,1} \\ \vdots \\ C_{i,N_{grid},N_{bed}} \\ q_{i,N_{grid},N_{bed}} \\ T_{N_{grid},N_{bed}} \end{bmatrix}$$

3 methods for accommodating CSS constraint

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1. Periodic Boundary Conditions

- Add bed initial condition variables and periodic boundary condition constraint to optimization formulation
- Simultaneous optimize cycle and find steady-state state
- Calculate first derivatives from direct sensitivity equations

$$z_0 - z(t_f) = 0$$

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2. Direct Substitution

- Repeat cycle from initial bed until converged to cyclic steady-state
- Suitable for derivative free optimization
- Quadratic penalty function for inequality constraints

$$z^0 \rightarrow z^1 \rightarrow ... \rightarrow z^n \quad \text{until} \quad ||z^n - z^{n-1}||^2 \leq \epsilon$$

$$h_i(\circ) \leq 0 \quad \text{becomes}$$

$$f_{pen}(\circ) = f(\circ) + \rho \sum_i \max(h_i(\circ), 0)^2$$

3. Fixed Horizon

- Simulate bed for a sufficiently large number of fixed cycles to near cyclic-steady state
- Calculate first derivatives from adjoint sensitivity equations
- Suitable for large number of states

$$z^0 \rightarrow z^1 \rightarrow \ldots \rightarrow z^N \text{ where } N \text{ is fixed}$$

Solver Details

- IPOPT for derivative based formulations
  - First derivatives from sensitivity equations
  - Second derivatives approximated with LBFGS

- BOBYQA for direct substitution formulation
  - DFO code based on quadratic approximation to objective function
  - Accommodates variable bounds

Case Study 1

Approach	Obj. Func	CPU Time/Iter	Iter
Derivative Free	146.42	0:04:46	566
Periodic Bnd. Cnd.	89.63	0:03:34	462
Fixed Horizon	98.46	0:04:23	1873

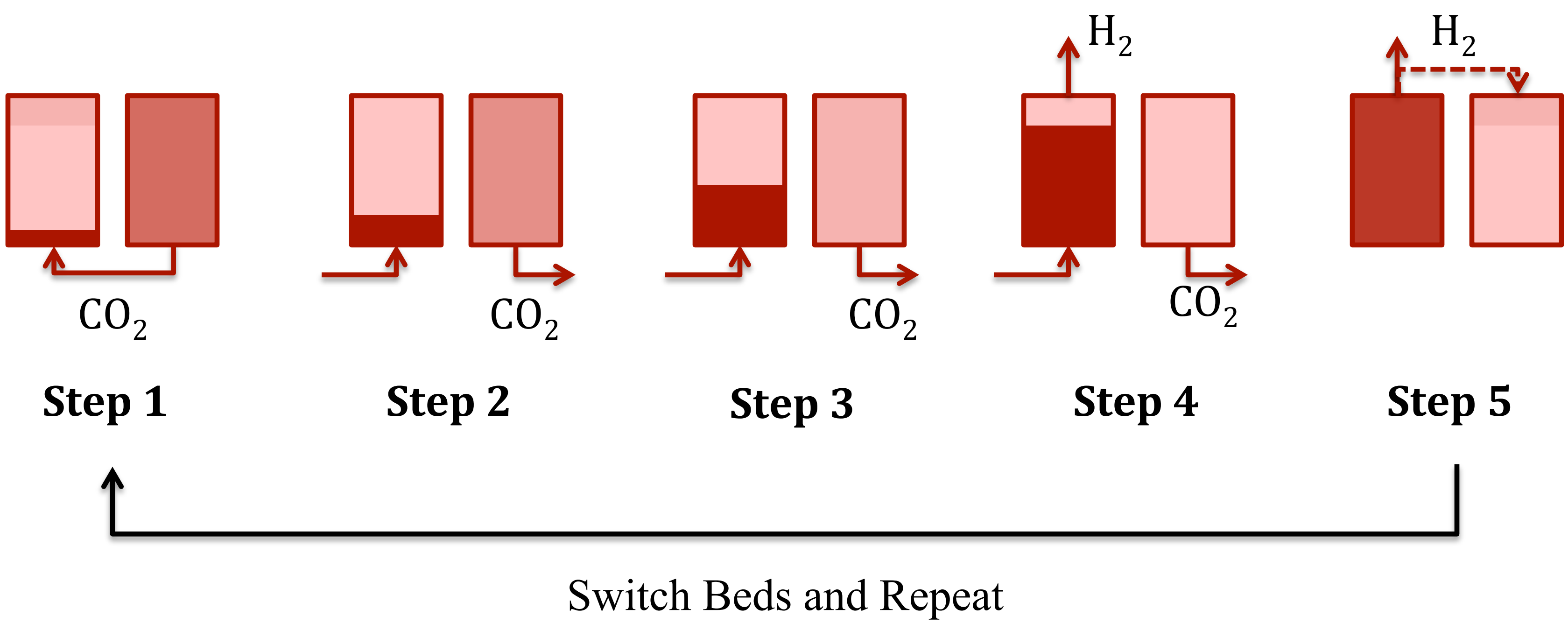
- Common poor starting
- DFO approach terminates at a much poorer solution
  - Local minimia?
- Derivative based approaches don't always converge to satisfied KKT conditions
  - Terminate due to resource limits or integrator failure
  - Noisy first derivatives, approximate second derivatives

Case Study 2

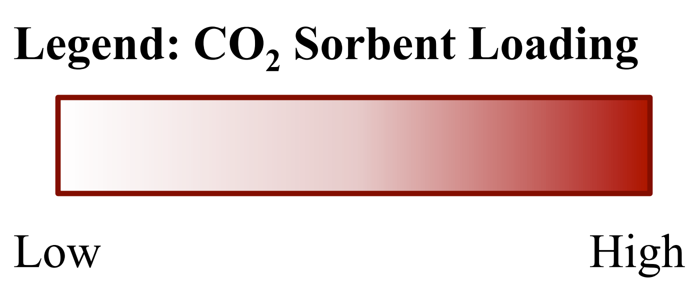
Approach	No. Comp.	Obj. Func	CPU Time/Iter	Iter
Fixed Horizon	Two	86.81	0:04:47	248
Fixed Horizon	Five	86.46	0:20:43	1103
Derivative Free	Five	109.04	0:11:29	2500+

- Common good starting point
- DFO approach terminates at an infeasible solution
- PBC sensitivity equation system too large for 5 component case

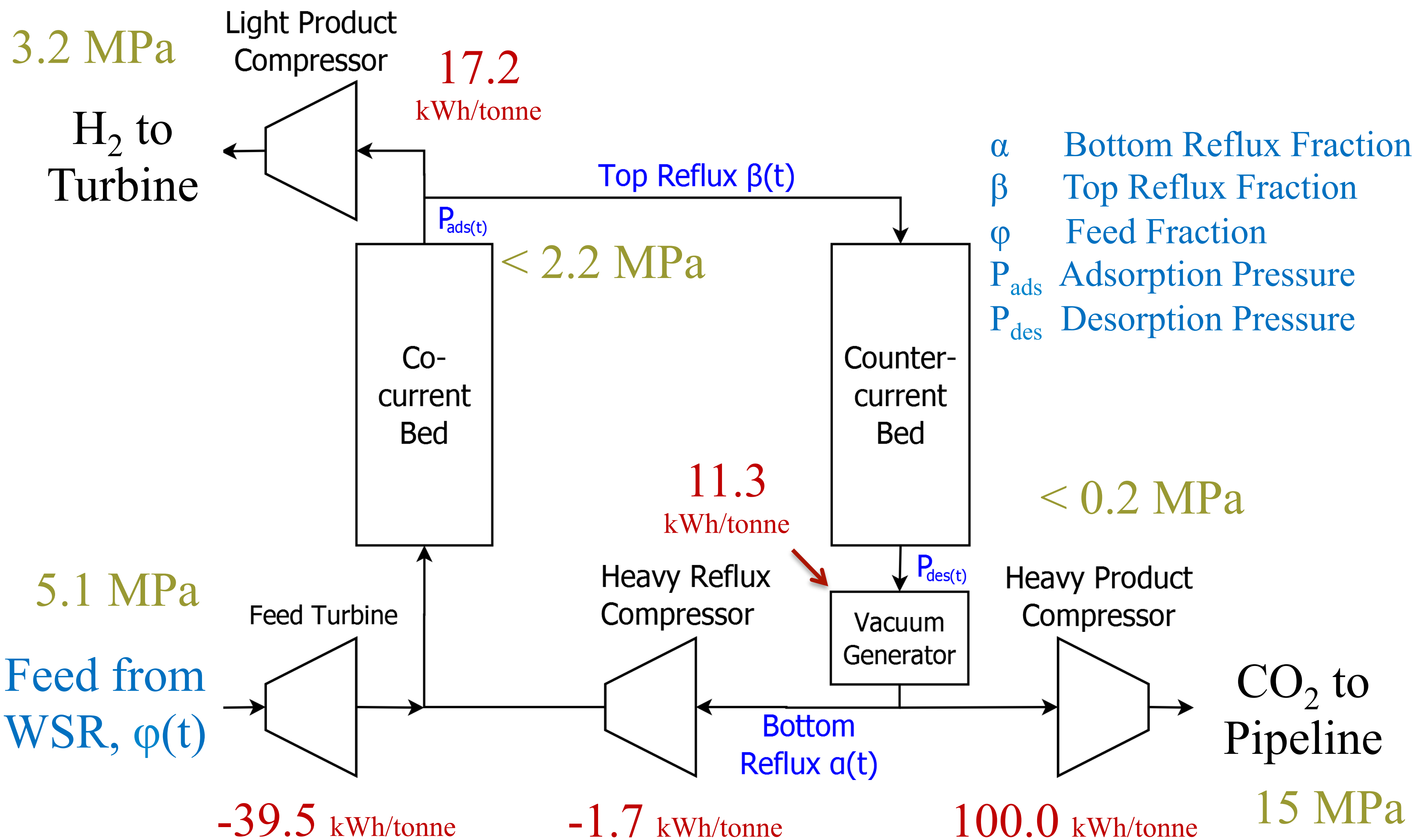
Designed Cycle



Best 5 Component Solution



87.2 kWh/tonne CO_2 captured



Technology Comparison

Economic Metric: Cost of Electricity

IGCC **without** Carbon Capture*	IGCC with **Selexol** Carbon Capture*	IGCC with **PSA** Carbon Capture
$ 76 / MWh	$ 106 / MWh	**$ 103 / MWh**

Goal: $ 83 / MWh

Majority of cost increases due to **Water Gas Shift Reactor**.

**Cost and Performance Baseline for Fossil Energy Plants Vol 1: Bit. Coal and Nat. Gas to Elec.*, NETL

Conclusions

- Compared PSA optimal process synthesis formulations
- Demonstrated novel application of adjoint sensitivity equations to PSA optimization
- Demonstrated cost competitiveness of PSA for H_2-CO_2 separation in IGCC power plant