CCSI

Carbon Capture Simulation Initiative

Post-Combustion Gas Permeation Carbon Capture System Models

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Los Alamos National Laboratory EST. 1943
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Outline

- Carbon Capture Simulation Initiative (CCSI)
  - Membrane Device Model
- Gas Permeation Carbon Capture with Boiler Air Sweep
  - Compression/Vacuum Process Configuration
  - All Compression Process Configuration
  - Process Decision Variables
  - Process Constraints
- Example
- Conclusions

Carbon Capture Simulation Initiative

Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

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AIR PRODUCTS

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SOUTHERN CALIFORNIA EDISON An EDISON INTERNATIONAL Company San Onofre Nuclear Generating Station

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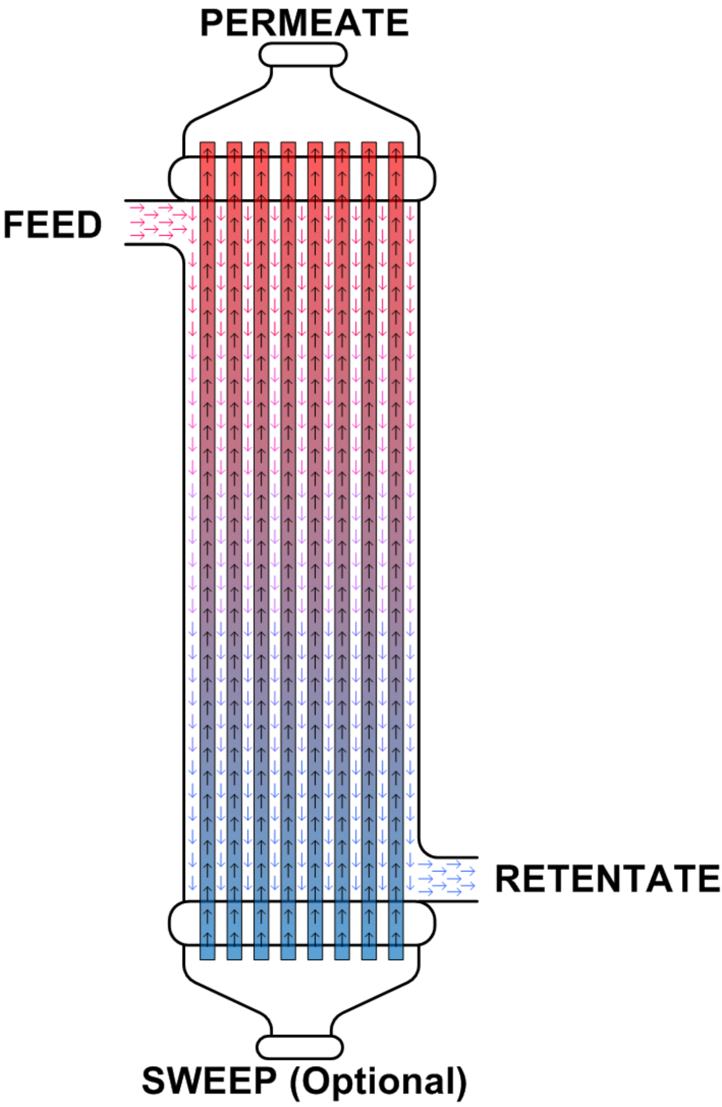
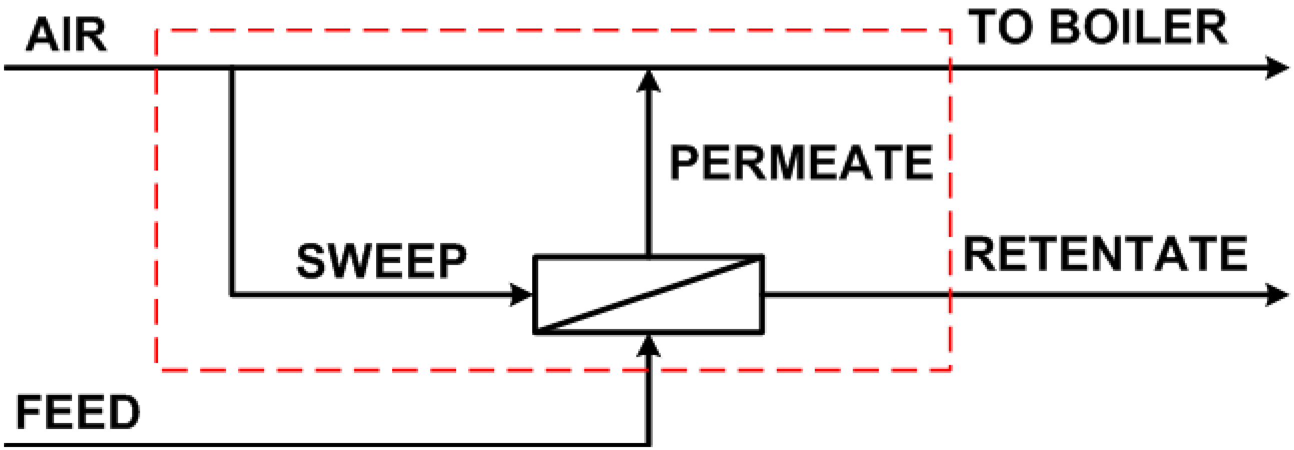
EASTMAN

Membrane Device Scale Model

- Hollow Fiber 1D steady state distributed model
- Optional sweep stream
- Counter-current flow
- Hollow fiber dimensions specified at average values
- Neglects pressure drop in feed side
- CO_2 Permeance: 1000 - 5000 GPU
- Selectivity: 50 - 200
- Implemented in ACM® and gPROMS®

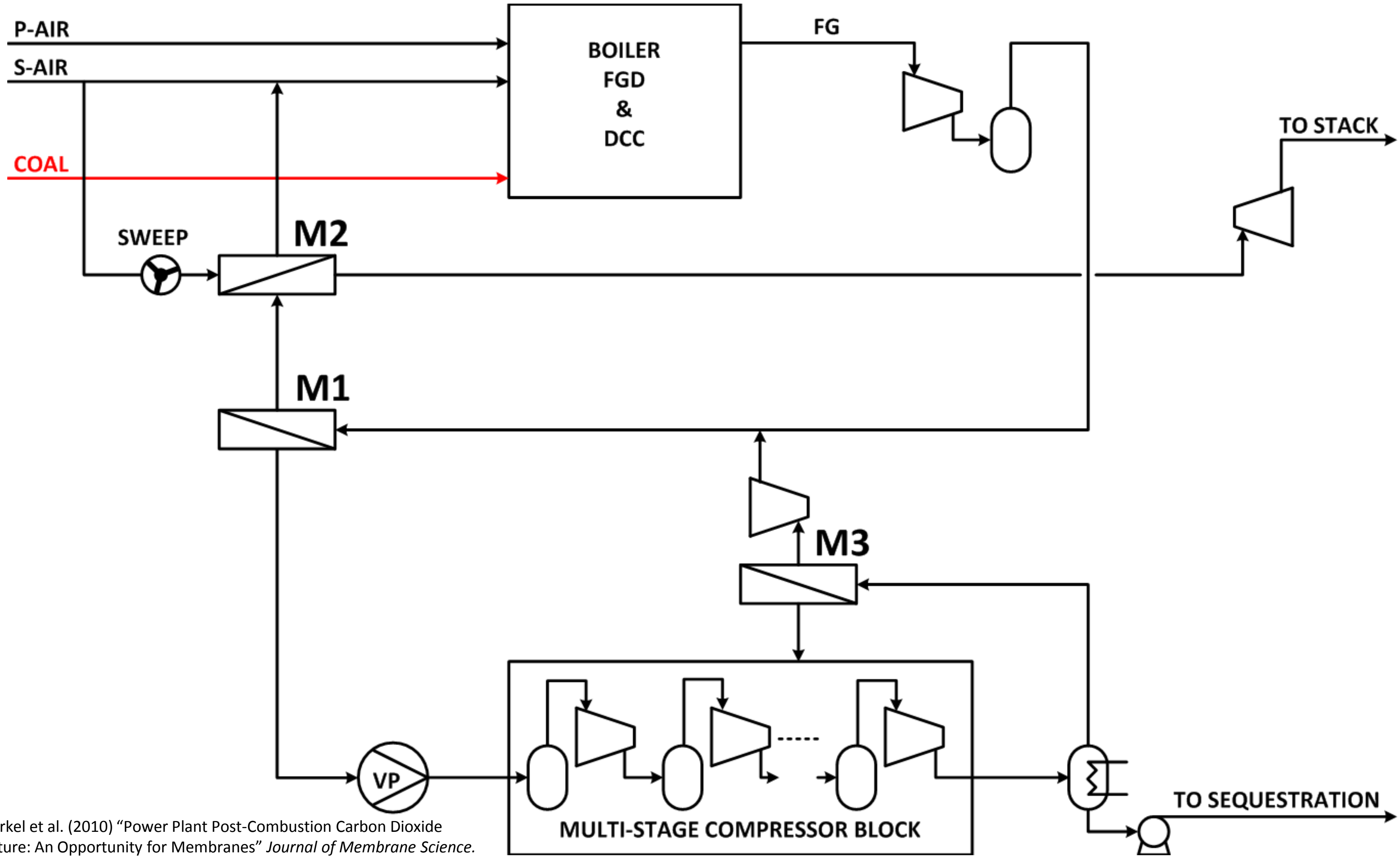


Multi-Stage Processes with Air Sweep



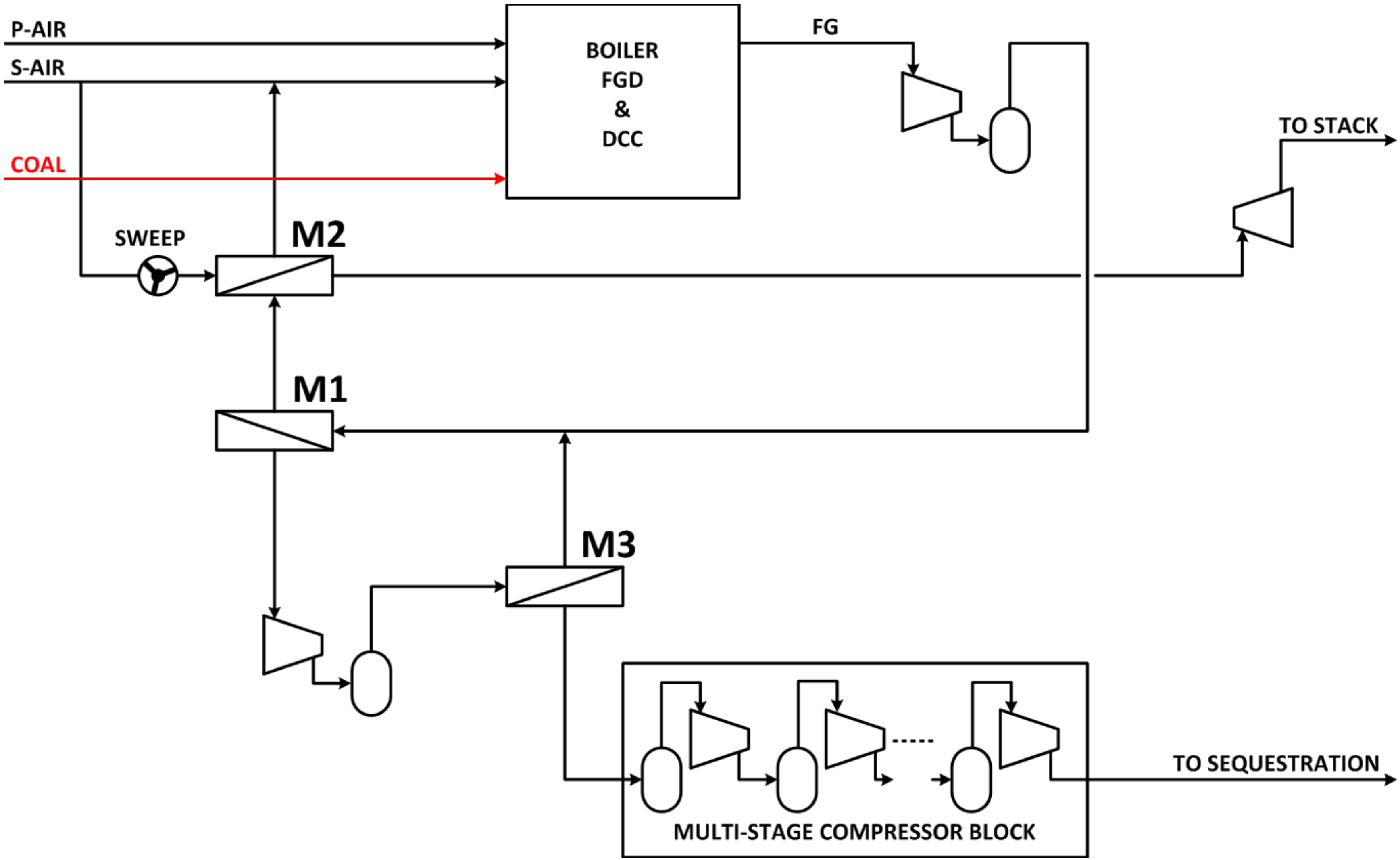
- Multi-stage processes are required due to characteristics of flue gas stream to be treated and 90% capture rate
- Sweep stream reduces membrane area and/or required compression power
- Integrated process: Must be analyzed with interacting parts of the power generation system

Compression/Vacuum Process*

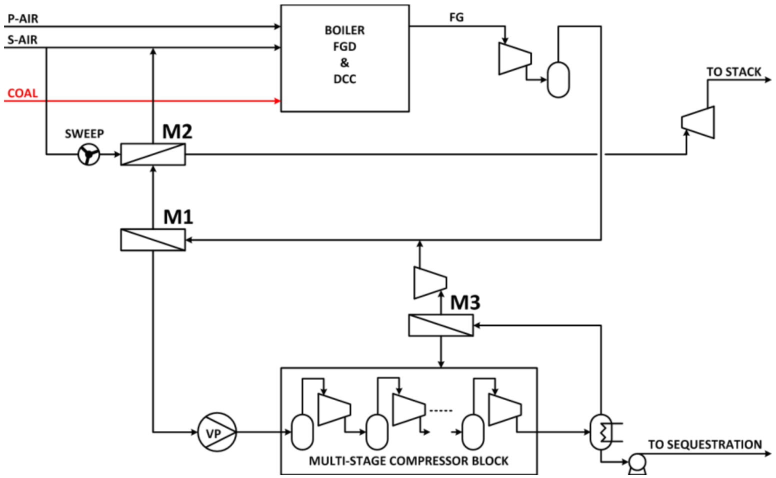


[*] Merkel et al. (2010) "Power Plant Post-Combustion Carbon Dioxide Capture: An Opportunity for Membranes" *Journal of Membrane Science.* 359, p. 126-139

All Compression Process

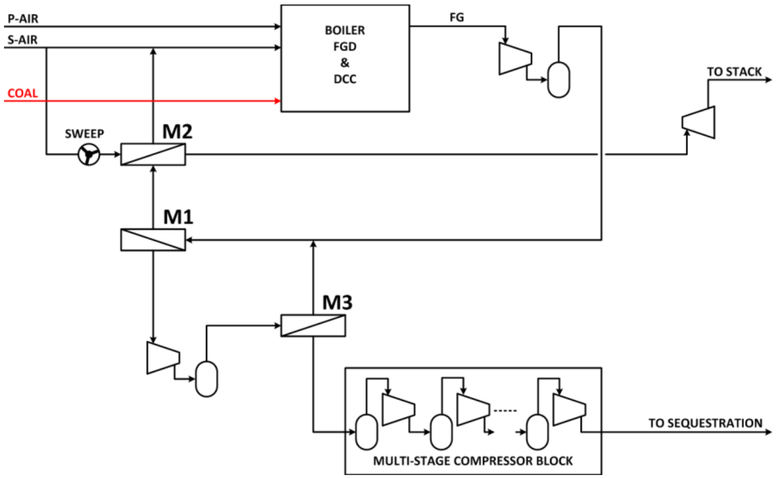


Process Decision Variables



Compression/Vacuum

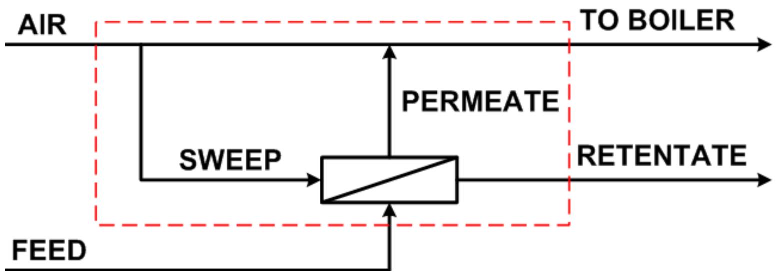
- M1 Feed Inlet Pressure
- M1 Permeate Outlet Pressure
- Liquefaction Pressure
- Liquefaction Temperature
- Air Sweep Flow Rate
- M1 CO_2 Stage Cut
- M2 CO_2 Stage Cut
- M3 CO_2 Stage Cut



All Compression

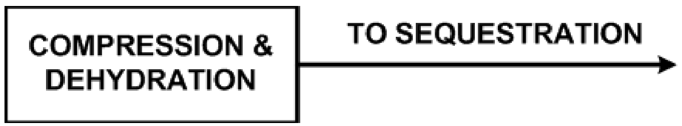
- M1 Feed Inlet Pressure
- Air Sweep Flow Rate
- M1 CO_2 Stage Cut
- M2 CO_2 Stage Cut
- M3 CO_2 Stage Cut

Process Constraints


AIR
TO BOILER
PERMEATE
SWEEP
RETENTATE
FEED

Increased Flue Gas Flow

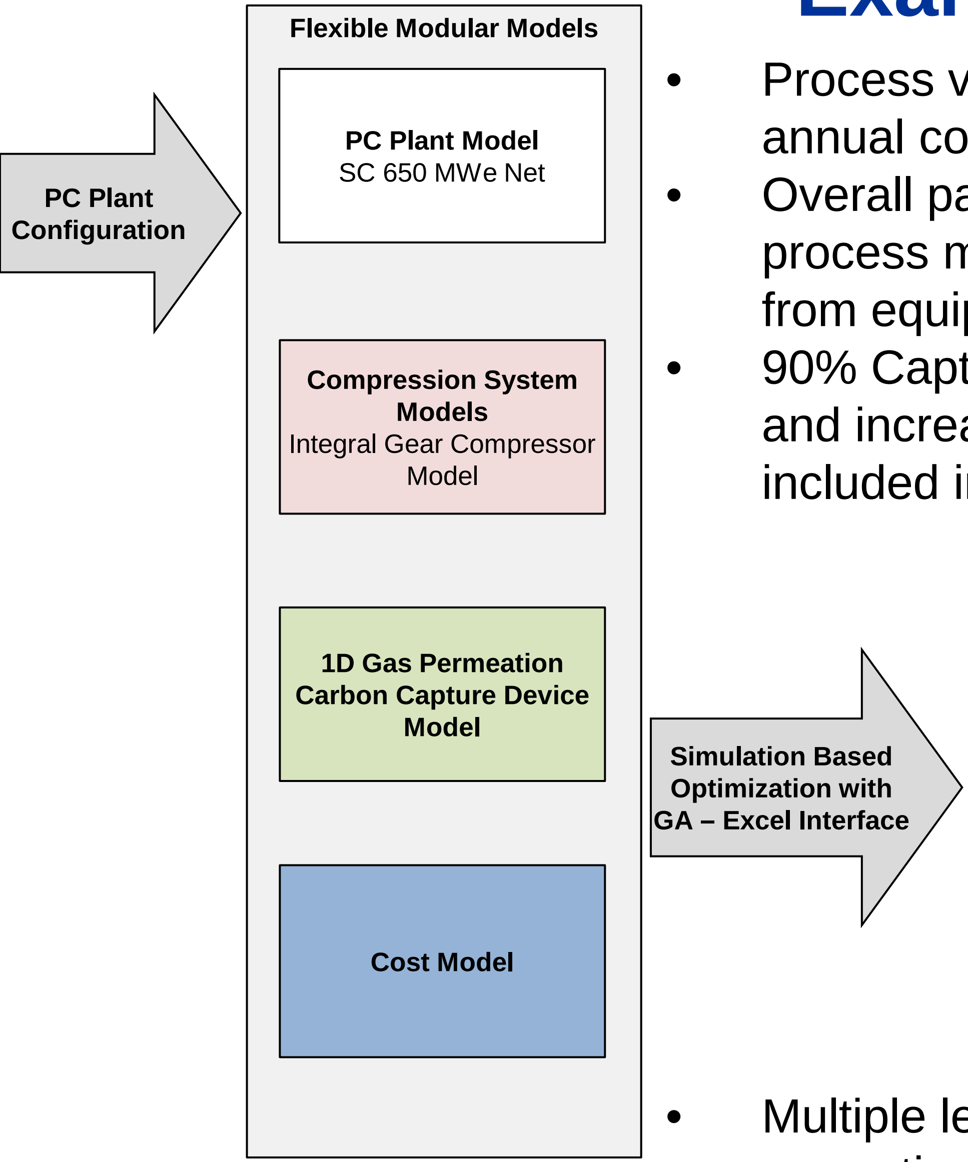
- The effect of feeding CO_2-enriched air to the boiler is uncertain
- Increased flow due to recirculation of gases could have significant impact in boiler and auxiliary equipment
- Constraint: ≤15mol%


COMPRESSION & DEHYDRATION
TO SEQUESTRATION

Sequestration Stream Purity

- Presence of impurities in the sequestration stream have significant downstream consequences
- Determines decision variables related to polishing section affecting entire process
- Constraint: ≥95mol% (CO_2)

Example



PC Plant Configuration

Flexible Modular Models

PC Plant Model
SC 650 MWe Net

Compression System Models
Integral Gear Compressor Model

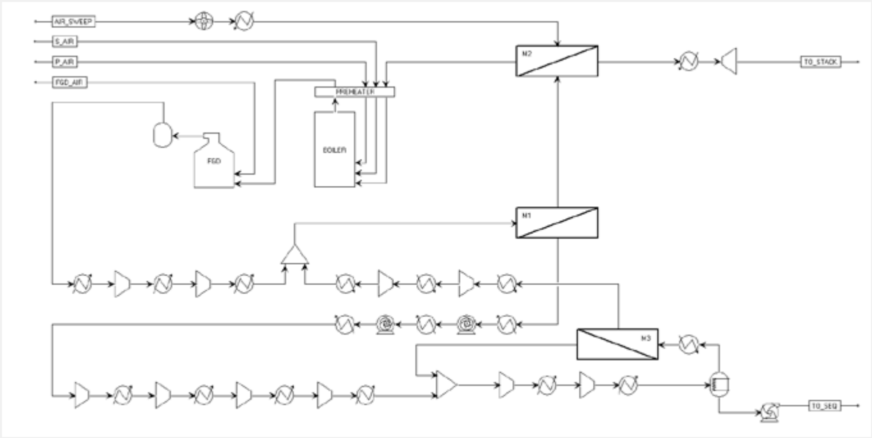
1D Gas Permeation Carbon Capture Device Model

Cost Model

Simulation Based Optimization with GA – Excel Interface

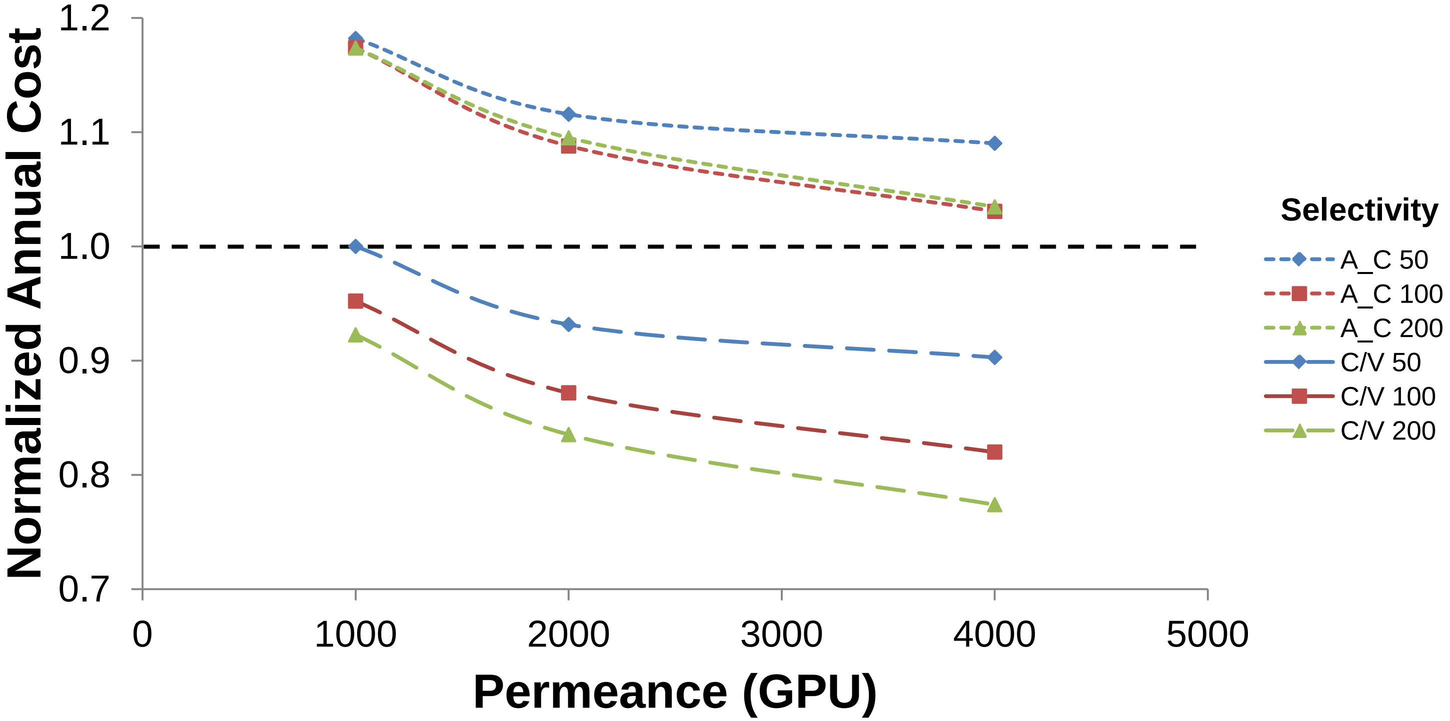
- Process variables are optimized with respect to annual cost function
- Overall parasitic power demand is calculated from process model output, capital cost is obtained from equipment cost correlations
- 90% Capture Rate, sequestration stream purity, and increased volumetric flow constraints are included in optimization

Multi-Stage Gas Permeation Carbon Capture Model



- Multiple levels of improvement for membrane properties were analyzed

Potential System Improvements with Advanced Membranes



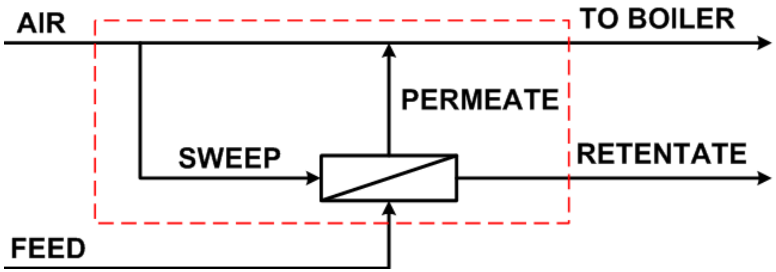
- All compression performance is comparatively limited even for most advanced membrane
- Improvements in permeance are not linear with improvement in annual cost

Optimized Variables for C/V Design

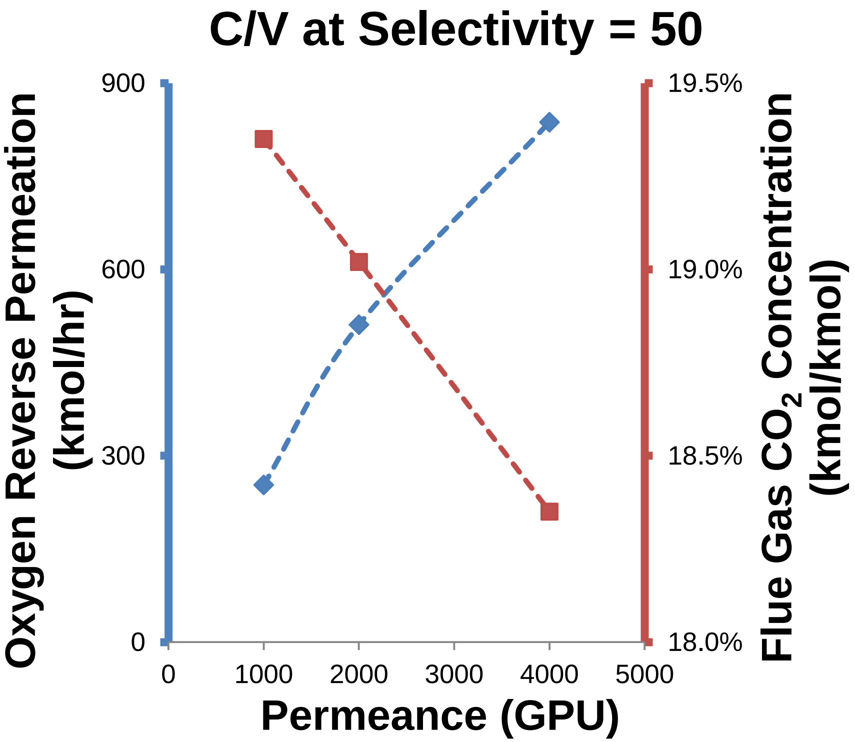
Permeance (GPU)	**1000**	**4000**	**1000**	**4000**
	Selectivity 50		**Selectivity 200**	
M1 Feed P (bar)	2.08	1.46	2.11	1.32
Liq. P (bar)	26.8	30.7	22.3	22.3
Sweep F (kmol/hr)	64300	68800	62400	66700
M1 CO_2 Stage Cut	0.512	0.536	0.488	0.451

- High permeance membrane reduces optimized compression but results in lower recirculation of CO_2
- High selectivity membrane allows higher recirculation of CO_2 and reduces the optimized liquefaction pressure

Effects of Membrane Sweep with Boiler Constraints



- O_2 reverse permeation results in additional air to the boiler reducing flue gas CO_2 partial pressure
- This effect is greater with higher permeance



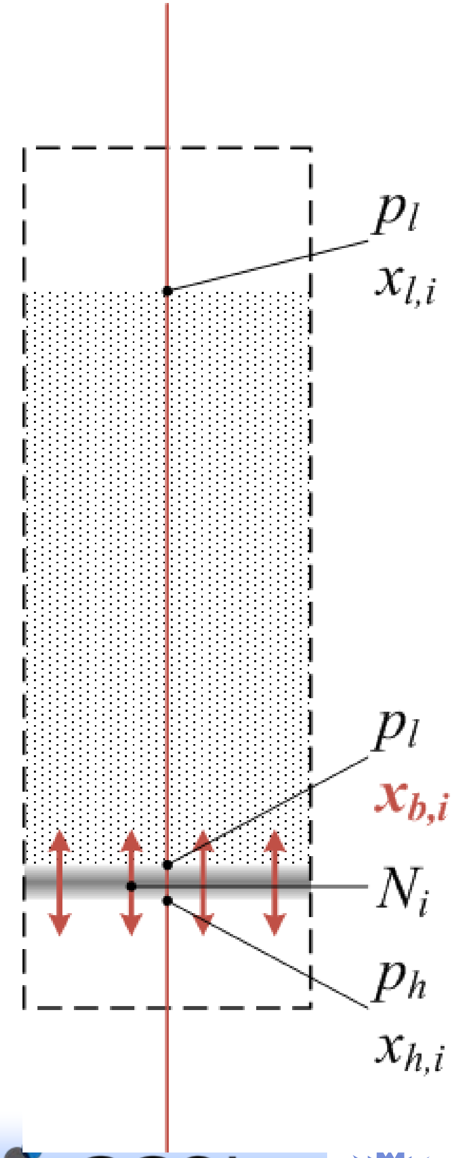
Summary

- Flexible system-level models were developed in order to evaluate the performance of gas permeation membranes for post-combustion carbon capture
- Optimal designs were generated using CCSI's Simulation Based Optimization Framework under different scenarios
  - Improvements to membrane properties
  - Scale and type of power generation system
  - Improvements to auxiliary equipment cost or performance
- Boiler constraints and oxygen depletion in the air sweep limit the performance of the membrane capture system

Questions?

Disclaimer

Extra - Asymmetric Membrane Model



- Fluids on either side of the selective layer are in equilibrium at the interface
- Pressure across the selective layer is constant at the highest value

$$P_i = K_i^G \cdot D_i$$

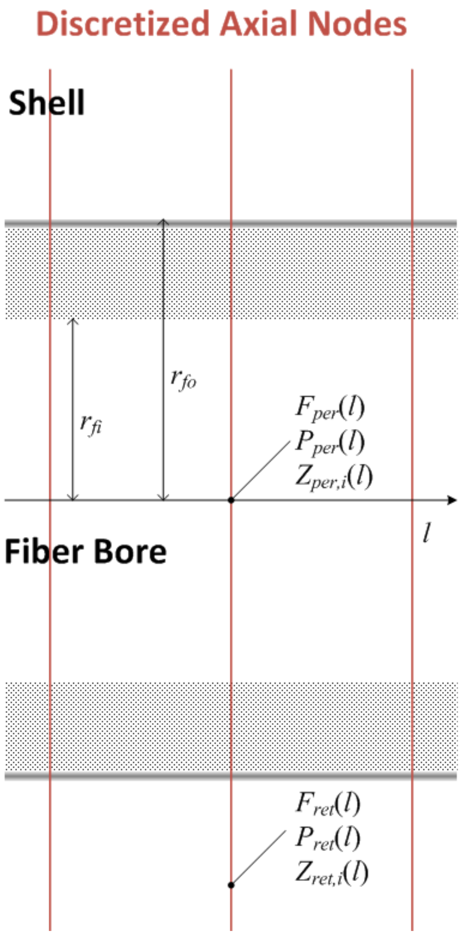
$$Q_i = \frac{P_i}{\delta_m}$$

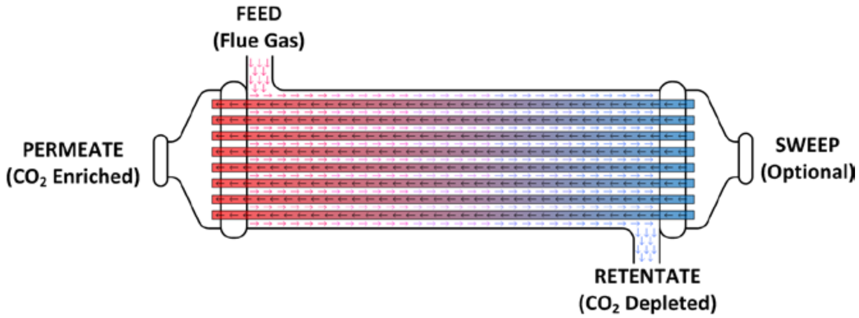
$$\alpha_i = \frac{Q_{CO_2}}{Q_i}$$

$$N_i = \frac{Q_{CO_2}}{\alpha_i}\left(p_h x_{h,i} - p_l x_{b,i}\right)$$

$$N_t = \sum_j^n N_j$$

Extra - 1D Hollow Fiber Model





Variable	Typical	This Model
Inner fiber Diameter (µm)	100-700*	400
Outer fiber diameter (µm)	200-800*	600
Effective fiber length (m)	0.15-1.50*	1.00

- Isothermal
- Shell Feed
- Perfectly cylindrical fibers
- Shell flow evenly distributed
- Counter-current flow
- Dense skin layer faces the shell side

$$J_i = 2\pi r_{fo} n_f N_i$$

$$J_t = \sum_{j}^{n} J_j$$

$$\frac{dF_{per}}{dl} = -J_t$$

$$\frac{dP_{per}^{\ 2}}{dl} = \frac{16RT\mu F_{per}}{\pi r_{fi}^{\ 4} n_f}$$

$$F_{per}\frac{dZ_{per,i}}{dl} = J_t Z_{per,i} - J_i$$

$$\frac{dF_{ret}}{dl} = -J_t$$

$$\frac{dP_{per}}{dl} = 0$$

$$F_{ret}\frac{dZ_{ret,i}}{dl} = J_t Z_{ret,i} - J_i$$

*Chowdhury et al. (2005) “A New Numerical Approach for a Detailed Multicomponent Gas Separation Membrane Model and Aspen Plus Simulation” *Chemical Engineering and Technology.* 28, p. 773-782.