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

National Labs
- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University

Academia
- Fluor
- ADA
- B&W
- GE
- Alstom
- SOUTHERN COMPANY
- Duke Energy
- Boeing
- Dupont
- Worley Parsons
- ExxonMobil
- Eastman
- U.S. Department of Energy

Industry
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\textsubscript{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
Process Decision Variables

**Compression/Vacuum**
- M1 Feed Inlet Pressure
- M1 Permeate Outlet Pressure
- Liquefaction Pressure
- Liquefaction Temperature
- Air Sweep Flow Rate
- M1 CO₂ Stage Cut
- M2 CO₂ Stage Cut
- M3 CO₂ Stage Cut

**All Compression**
- M1 Feed Inlet Pressure
- Air Sweep Flow Rate
- M1 CO₂ Stage Cut
- M2 CO₂ Stage Cut
- M3 CO₂ Stage Cut
**Process Constraints**

**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: $\leq 15\text{mol}\%$

**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: $\geq 95\text{mol}\%$ (CO$_2$)
• 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

• 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

<table>
<thead>
<tr>
<th>Permeance (GPU)</th>
<th>1000</th>
<th>4000</th>
<th>1000</th>
<th>4000</th>
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<tbody>
<tr>
<td></td>
<td>Selectivity 50</td>
<td></td>
<td>Selectivity 200</td>
<td></td>
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<tr>
<td>M1 Feed P (bar)</td>
<td>2.08</td>
<td>1.46</td>
<td>2.11</td>
<td>1.32</td>
</tr>
<tr>
<td>Liq. P (bar)</td>
<td>26.8</td>
<td>30.7</td>
<td>22.3</td>
<td>22.3</td>
</tr>
<tr>
<td>Sweep F (kmol/hr)</td>
<td>64300</td>
<td>68800</td>
<td>62400</td>
<td>66700</td>
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<tr>
<td>M1 CO₂ Stage Cut</td>
<td>0.512</td>
<td>0.536</td>
<td>0.488</td>
<td>0.451</td>
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</tbody>
</table>

- High permeance membrane reduces optimized compression but results in lower recirculation of CO₂
- High selectivity membrane allows higher recirculation of CO₂ and reduces the optimized liquefaction pressure
Effects of Membrane Sweep with Boiler Constraints

- O₂ reverse permeation results in additional air to the boiler reducing flue gas CO₂ 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?

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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**

![Discretized Axial Nodes](image1)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Typical</th>
<th>This Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner fiber Diameter (μm)</td>
<td>100-700*</td>
<td>400</td>
</tr>
<tr>
<td>Outer fiber diameter (μm)</td>
<td>200-800*</td>
<td>600</td>
</tr>
<tr>
<td>Effective fiber length (m)</td>
<td>0.15-1.50*</td>
<td>1.00</td>
</tr>
</tbody>
</table>

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

\[ J_i = 2\pi r_{fi} n_f N_i \]
\[ J_t = \sum_{j=1}^{n} J_j \]
\[ \frac{dF_{per}}{dl} = -J_t \]
\[ \frac{dP_{per}}{dl} = 0 \]
\[ F_{per} \frac{dZ_{per,i}}{dl} = J_t Z_{per,i} - J_i \]