Design and Operations Optimization of Membrane Separation for Flexible Carbon Capture

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Flexibility will be required for carbon capture in the energy transition

- Increasing integration of intermittent renewable energy
- Natural gas as a bridge fuel providing flexible generation
  - Natural gas combined cycles have ramp times on order of minutes
- Flexible carbon capture may have economic advantage

Membrane separation as a competitive technology for flexible carbon capture

- Flexible operations by changing pressures
  - Fast response times compatible with natural gas power generation
Membrane separation as a competitive technology for flexible carbon capture

- Flexible operations by changing pressures
  - Fast response times compatible with natural gas power generation

- Pilot membrane capture plant developed by Membrane Technology & Research, Inc.
- 1 ton/day capacity
- 15 mins cold start

Membrane separation as a competitive technology for flexible carbon capture

- Flexible operations by changing pressures
  - Fast response times compatible with natural gas power generation
- Other advantages of membrane separation
  - Competitive energy use
  - Smaller footprint
  - Environmentally benign

- Pilot membrane capture plant developed by Membrane Technology & Research, Inc.
  - 1 ton/day capacity
  - 15 mins cold start

Project goal

- Demonstrate methodology for joint design and operations optimization of membrane-based flexible carbon capture from natural gas combined cycle
System overview

400 MW

natural gas combined cycle (NGCC)

400 MW

partload

electricity to grid

electricity price profile + carbon tax

flue gas (flowrate, composition, temperature)

membrane capture unit

CO₂ to storage / utilization

System overview

- Natural gas combined cycle modeled in the Hybrid Power Plant Optimization (HyPPO) model
  - Developed at Stanford University for modeling and optimization of flexible and renewable-integrated power systems

Membrane modeling

- Membrane mass balance and area: crossflow model
- Compression and expansion: adiabatic processes

Membrane modeling

- Membrane mass balance and area: crossflow model
- Compression and expansion: adiabatic processes

\[
\frac{(1 - \theta^*)(1 - x)}{(1 - x_f)} = \left( \frac{u_f - E/D}{u - E/D} \right)^R \left( \frac{u_f - \alpha + F}{u - \alpha + F} \right)^S \left( \frac{u_f - F}{u - F} \right)^T
\]

\[
A_m = \frac{L_f}{p_h P_B} \int_{i_r}^{i_f} \frac{(1 - \theta^*)(1 - x)di}{(f_i - i) \left[ \frac{1}{1 + i} - \frac{1}{r(1 + f_i)} \right]}
\]

\[
\theta^* = 1 - \frac{L}{L_f}
\]

\[
i = \frac{x}{1 - x}
\]

\[
u = -Di + (D^2i^2 + 2Ei + F^2)^{0.5}
\]

\[
D = 0.5 \left[ \frac{1 - \alpha}{r} + \alpha \right]
\]

\[
E = \frac{\alpha}{2 - DF}
\]

\[
F = -0.5 \left[ \frac{1 - \alpha}{r} - 1 \right]
\]

\[
R = \frac{1}{2D - 1}
\]

\[
S = \frac{\alpha(D - 1) + F}{(2D - 1)(\alpha/2 - F)}
\]

\[
T = \frac{1}{1 - D - E/F}
\]

\[
f_i = (Di - F) + (D^2i^2 + 2Ei + F^2)^{0.5}
\]

Membrane modeling

- Membrane mass balance and area: crossflow model
- Compression and expansion: adiabatic processes

\[
(1 - \theta^*)(1 - x) \frac{(1 - \theta^*)}{(1 - x_f)} = \left( \frac{u_f - E/D}{u - E/D} \right)^R \left( \frac{u_f - \alpha + F}{u - \alpha + F} \right)^S \left( \frac{u_f - F}{u - F} \right)^T
\]

\[
A_m = \frac{L_f}{p_h \overline{P}_B} \int_{i_r}^{i_f} \left( \frac{1}{1 + i} - \frac{1}{r(1 + f_i)} \right) dt
\]


\[
\theta^* = 1 - \frac{L}{L_f}
\]

\[
i = \frac{x}{1 - x}
\]

\[
u = -Di + (D^2i^2 + 2Ei + F^2)^{0.5}
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\[
D = 0.5 \left[ \frac{1 - \alpha}{r} + \alpha \right]
\]

\[
E = \frac{\alpha}{2 - DF}
\]

\[
F = -0.5 \left[ \frac{1 - \alpha}{r} - 1 \right]
\]

\[
R = \frac{1}{2D - 1}
\]

\[
S = \frac{\alpha(D - 1) + F}{(2D - 1)(\alpha/2 - F)}
\]

\[
T = \frac{1}{1 - D - E/F}
\]

\[
f_i = (Di - F) + (D^2i^2 + 2Ei + F^2)^{0.5}
\]

Highly nonlinear equations \(\rightarrow\) challenge for optimization
Two-stage membrane cascade overview

\[ x_{\text{CO}_2} \approx 3.9\% \]

\[ x_{\text{CO}_2} \approx 36\% \text{ (example)} \]

\[ x_{\text{CO}_2} = 95\% \]

NGCC

Electricity

Flue gas

\( p_{\text{high}}(p_1) \)

\( p_{\text{low}} \)

To stack

\( p_1 = p_2 \)

To storage / utilization

Multistage compression
Overview of operational decision variables

- Design decision variables
- Operational decision variables
Overview of possible design decision variables

- Design decision variables
- Operational decision variables

Diagram:
- NGCC
- Flue gas
- Electricity
- To storage/utilization
- To stack
- Multistage compression
- Design decision variables: x_{duty}, x_{power}
- Operational decision variables: x_{sel}, x_{size}, x_{perm}, p_1 = p_2
Overview of possible design decision variables

- Design decision variables
- Operational decision variables

Computation time increases with number of decision variables
Focus on most important design decision variables
Decision variables evaluated

- **NGCC**
  - $u_{\text{partload}}$
  - electricity

- flue gas
  - $x_{\text{power}}$
  - $u_{\text{pres}}$

- to stack
  - $x_{\text{size}}$

- to storage / utilization
  - $u_{\text{capture}}$

- multistage compression
  - $u_{\text{pres}}$

- $p_1 = p_2$

- **design decision variables**
- **operational decision variables**

Feed compressor sizes and membrane areas dominate capital cost
Objective function

- Maximize net present value (NPV)

\[
\max_{x \in X, u \in U} \text{NPV}(x, u)
\]

\[
\text{NPV} = -C(x) + \sum_{t=1}^{n_{\text{years}}} \frac{P(x, u)}{(1 + r)^t}
\]

- Subject to design and operational constraints

\[
h_{\text{des}}(x, u) \leq 0, \ h_{\text{op}}(x, u) \leq 0
\]

- \( x \) = design decision variables
- \( u \) = operational decision variables
Objective function

- Maximize net present value (NPV)

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\]

\[
\text{NPV} = -C(x) + \sum_{t=1}^{n\text{years}} \frac{P(x, u)}{(1 + r)^t}
\]

- Subject to design and operational constraints

\[h_{\text{des}}(x, u) \leq 0, h_{\text{op}}(x, u) \leq 0\]

\[x = \text{design decision variables}\]
\[u = \text{operational decision variables}\]
Optimization framework

Design Optimization

\[ \max_{x \in X} \text{NPV}^*(x) \]

Subject to
\[ h_{\text{op}} \leq 0 \text{ and } h_{\text{des}} \leq 0 \]

Calculate
\[ \text{NPV}^*(C(x^k), P(x^k, u^*)) \]
and
\[ h_{\text{des}}(x^k, u^*) \]

Operations Optimization

\[ u^* = \arg\max_{u \in U} P(x^k, u) \]

Subject to
\[ h_{\text{op}}(x^k, u) \leq 0 \]

Assign \( x^k \)
for Design \( k \)

Framework adapted from Brodrick et al., *Energy*, 2015
Timesteps and electricity prices

- Timesteps are characterized by different electricity prices and can be evaluated independently

Electricity prices: California ISO. "Open Access Same-time Information System (OASIS)."
Timesteps and electricity prices

- Timesteps are characterized by different electricity prices and can be evaluated independently.
- Synthetic electricity price profile
  - 2015 hourly prices from California ISO “Stanford node”
  - K-means clustering to generate 6 representative electricity prices (timesteps) and associated weights (# hours in a year)

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Multistart operations optimization

- Multistart optimization to ensure repeatability
  - 10–50 starting points for each given partload and design
  - Stop when same solution found 5 times or 50 runs completed

```
multistart optimization
# starting points = 10

# optimal solutions ≥ 5?

terminate loop
save results
```

```
total # iterations = 50?
```

yes

no
Operational decision variables and computation time

- Computation time (single core)
  - \((15–20\ \text{seconds/starting point}) \times (10–50\ \text{starting points/partload}) \times (8\ \text{partloads/timestep}) = 0.3–2\ \text{hours/timestep})\)
  - \((0.3–2\ \text{hours/timestep}) \times (6\ \text{timesteps/design}) = 2–8\ \text{hours/design})\)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Lower bound</th>
<th>Upper bound</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combined cycle partload</td>
<td>-</td>
<td>0 (shutdown)</td>
<td>1 (full load)</td>
<td>Discrete</td>
</tr>
<tr>
<td>Feed-side pressure for each stage</td>
<td>bar</td>
<td>1.013</td>
<td>10</td>
<td>Continuous</td>
</tr>
<tr>
<td>1st-stage permeate-side pressure</td>
<td>bar</td>
<td>0.2</td>
<td>1.013</td>
<td>Continuous</td>
</tr>
<tr>
<td>2nd-stage permeate-side pressure</td>
<td>bar</td>
<td>0.2</td>
<td>1.013</td>
<td>Continuous</td>
</tr>
<tr>
<td>Capture rate</td>
<td>%</td>
<td>0</td>
<td>95</td>
<td>Continuous</td>
</tr>
</tbody>
</table>
Design decision variables

- **Fixed membrane properties**
  - Selectivity = 50
  - Permeance = 1000 GPU

<table>
<thead>
<tr>
<th>#</th>
<th>Variable</th>
<th>Unit</th>
<th>Values</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>1st-stage membrane area</td>
<td>m²</td>
<td>$0.25 \times 10^6$, $0.5 \times 10^6$, $1 \times 10^6$</td>
</tr>
<tr>
<td>2</td>
<td>2nd-stage membrane area</td>
<td>m²</td>
<td>$0.5 \times 10^4$, $1 \times 10^4$, $2 \times 10^4$</td>
</tr>
<tr>
<td>3</td>
<td>1st-stage feed compressor size</td>
<td>MW</td>
<td>100, 150, 200</td>
</tr>
<tr>
<td>4</td>
<td>2nd-stage feed compressor size</td>
<td>MW</td>
<td>10, 25, 50</td>
</tr>
</tbody>
</table>
Design decision variables

- Fixed membrane properties
  - Selectivity = 50
  - Permeance = 1000 GPU
- 81 design combinations, can be easily expanded

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<td>m²</td>
<td>$0.5 \times 10^4$</td>
</tr>
<tr>
<td>3</td>
<td>1st-stage feed compressor size</td>
<td>MW</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>2nd-stage feed compressor size</td>
<td>MW</td>
<td>10</td>
</tr>
</tbody>
</table>
Results: Optimized NPVs

Breakeven carbon price close to ~$100/tonne
Results: Optimized design decision variables

![Diagram showing optimized design decision variables for different costs: $0/tonne, $50/tonne, $100/tonne, $200/tonne.](image)
Results: Optimized partload and capture rate, carbon price = $0/tonne
Results: Optimized partload and capture rate, carbon price = $0/tonne

Maximize electricity generation

Minimize carbon capture
Results: Optimized partload and capture rate, carbon price = $50/tonne
Results: Optimized partload and capture rate, carbon price = $100/tonne
Results: Optimized partload and capture rate, carbon price = $200/tonne
Summary and proposed future work

- Developed methodology for joint design and operations optimization of membrane-based flexible carbon capture
  - Optimal system design should balance capital cost and operating cost
  - Optimal operating schedule depends on relative prices of electricity and carbon
Summary and proposed future work

- Developed methodology for joint design and operations optimization of membrane-based flexible carbon capture
  - Optimal system design should balance capital cost and operating cost
  - Optimal operating schedule depends on relative prices of electricity and carbon
- Methodology developed in this study is robust and can be used to explore different scenarios
  - New materials and designs to further decrease CO$_2$ separation cost
  - Guide performance and cost targets for membranes
  - Identify proper emissions regulations (tax or cap)
Thank you!
Questions?

myuan@carnegiescience.edu
References


Backup slides
MEMBRANE 101

- Permeability
- Permeance
- Selectivity
- Driving force = $\Delta$ (partial pressure)

feed stream

feed/retentate side

permeate side

retentate stream

selectivity

$\alpha_{A/B} = \frac{P_A}{P_B}$

flux

$J_A = \frac{P_A}{\delta} \left( p_{A,\text{feed}}^n - p_{A,\text{permeate}}^n \right)$

Gas A, e.g., CO$_2$

Gas B, e.g., N$_2$
Decision variables evaluated in advanced membranes case

- Varying membrane selectivity and permeance
- Focus on membrane areas

NGCC

$u_{\text{partload}}$

electricity

flue gas

$u_{\text{pres}}$

$x_{\text{sel}}$

$x_{\text{size}}$

$x_{\text{perm}}$

to stack

$p_1 = p_2$

to storage / utilization

$u_{\text{capture}}$

multistage compression

$u_{\text{pres}}$

$\star$ design decision variables

$\star$ operational decision variables
## List of design decision variables, base case

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st-stage membrane selectivity</td>
<td>-</td>
<td>50</td>
</tr>
<tr>
<td>2nd-stage membrane selectivity</td>
<td>-</td>
<td>50</td>
</tr>
<tr>
<td>1st-stage membrane permeance</td>
<td>GPU*</td>
<td>1000</td>
</tr>
<tr>
<td>2nd-stage membrane permeance</td>
<td>GPU</td>
<td>1000</td>
</tr>
<tr>
<td>1st-stage membrane area</td>
<td>m²</td>
<td>2.5 × 10⁵</td>
</tr>
<tr>
<td>2nd-stage membrane area</td>
<td>m²</td>
<td>5 × 10³</td>
</tr>
<tr>
<td>1st-stage feed compressor size</td>
<td>MW</td>
<td>100</td>
</tr>
<tr>
<td>2nd-stage feed compressor size</td>
<td>MW</td>
<td>10</td>
</tr>
<tr>
<td>1st-stage vacuum pump size</td>
<td>MW</td>
<td>20</td>
</tr>
<tr>
<td>2nd-stage vacuum pump size</td>
<td>MW</td>
<td>5</td>
</tr>
<tr>
<td>Expander size (power recovery)</td>
<td>MW</td>
<td>−150</td>
</tr>
<tr>
<td>Product compressor size (each stage)</td>
<td>MW</td>
<td>2.5</td>
</tr>
<tr>
<td>Heat exchanger duty after 1st-stage compressor</td>
<td>MW</td>
<td>250</td>
</tr>
<tr>
<td>Heat exchanger duty after 2nd-stage compressor</td>
<td>MW</td>
<td>50</td>
</tr>
<tr>
<td>Product compression interstage heat exchanger duty (each stage)</td>
<td>MW</td>
<td>5</td>
</tr>
</tbody>
</table>
List of design decision variables, adv. membranes case

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st-stage membrane selectivity</td>
<td>-</td>
<td>50</td>
</tr>
<tr>
<td>2nd-stage membrane selectivity</td>
<td>-</td>
<td>50</td>
</tr>
<tr>
<td>1st-stage membrane permeance</td>
<td>GPU</td>
<td>1000</td>
</tr>
<tr>
<td>2nd-stage membrane permeance</td>
<td>GPU</td>
<td>1000</td>
</tr>
<tr>
<td>1st-stage membrane area</td>
<td>m²</td>
<td>1.5 \times 10^5</td>
</tr>
<tr>
<td>2nd-stage membrane area</td>
<td>m²</td>
<td>2.5 \times 10^3</td>
</tr>
<tr>
<td>1st-stage feed compressor size</td>
<td>MW</td>
<td>150</td>
</tr>
<tr>
<td>2nd-stage feed compressor size</td>
<td>MW</td>
<td>25</td>
</tr>
</tbody>
</table>
Design decision variables, advanced membranes case

- Varying membrane properties
  - $\alpha$: selectivity
  - $P$: permeance
- Focus on membrane area
  - $A_m$: membrane area
- 64 design combinations, can be easily expanded

<table>
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<tbody>
<tr>
<td>1</td>
<td>1st-stage membrane selectivity</td>
<td>-</td>
<td>50, 200</td>
</tr>
<tr>
<td>2</td>
<td>2nd-stage membrane selectivity</td>
<td>-</td>
<td>50, 200</td>
</tr>
<tr>
<td>3</td>
<td>1st-stage membrane permeance</td>
<td>GPU</td>
<td>1000, 3500</td>
</tr>
<tr>
<td>4</td>
<td>2nd-stage membrane permeance</td>
<td>GPU</td>
<td>1000, 3500</td>
</tr>
<tr>
<td>5</td>
<td>1st-stage membrane area</td>
<td>m²</td>
<td>$1.5 \times 10^5$, $5 \times 10^5$</td>
</tr>
<tr>
<td>6</td>
<td>2nd-stage membrane area</td>
<td>m²</td>
<td>$0.25 \times 10^4$, $1 \times 10^4$</td>
</tr>
<tr>
<td>7</td>
<td>1st-stage feed compressor size</td>
<td>MW</td>
<td>150</td>
</tr>
<tr>
<td>8</td>
<td>2nd-stage feed compressor size</td>
<td>MW</td>
<td>25</td>
</tr>
</tbody>
</table>
Results: Optimized NPVs, base case vs. advanced membranes case

NPV [M$]

$50/tonne  $200/tonne

NGCC
NGCC + capture, base case
NGCC + capture, adv. membr.
Results: Optimized design decision variables, advanced membranes case

$50/\text{tonne}$

<table>
<thead>
<tr>
<th>#1</th>
<th>#2</th>
<th>#3</th>
<th>#4</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>H</td>
<td>XS</td>
<td>M</td>
</tr>
</tbody>
</table>

$200/\text{tonne}$

<table>
<thead>
<tr>
<th>#1</th>
<th>#2</th>
<th>#3</th>
<th>#4</th>
</tr>
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<td>L</td>
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<td>XS</td>
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$\alpha$: selectivity
$\overline{P}$: permeance
$A_m$: membrane area

compare: base case
Results: Optimized partload and capture rate, carbon price = $50/tonne, advanced membranes case
Results: Optimized partload and capture rate, carbon price = $200/tonne, advanced membranes case
Results: Optimized operating pressures, base case
Results: Optimized operating pressures, advanced membranes case

![Graph showing pressure variations over time with different labels for feed, perm1, and perm2.]

- **Pressure (bar)**
  - $50/tonne
  - $200/tonne

- Hour in year:
  - 4326, 4332, 4338, 4344, 4350, 4356, 4362, 4368