Optimal Design and Operation of Hybrid CO\textsubscript{2} Capture Systems

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Post Combustion Technologies

General issues:
- Costing Methodologies
- Optimization frameworks

Post Combustion CO₂ Capture

Solid Sorbents – adsorption
Issues
- Energy Intensive
- Plant complexity

Solvents - absorption
Issues
- Energy Intensive
- Plant complexity

Membrane-based – gas permeation
Issues
- Flue gas with low CO₂ concentration

Hypothesis
- Hybrid CO₂ capture plants could reduce the capture costs.

Intermediate GOALS
- Establish a consistent framework to optimize the structure and design of capture technologies
  - Superstructure optimization framework
- Robust Mathematical models
Superstructure Optimization Framework

- **Discrete Decisions:**
  - How many units?
  - Parallel trains?
  - What technology used for each reactor?

- **Continuous decisions:**
  - Unit geometries,
  - Operating conditions (temp, pressure, flow rates, compositions)

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Flue Gas
650 MW fired coal power plant

CO₂ rich gas Compression chain

Regeneration beds

**Clean Gas**

- Adsorber beds

**Cold in**

- **aₙ**
- ...

**Warm in**

- **a₁**
- **d₁**
- **d₂**
- ...

**Hot in**

- **Steam + CO₂**

**MINLP**
Problem Statement

Cost of Electricity (COE)

\[
\begin{align*}
\text{min } & \text{COE} \\
\text{s.t. } & \text{Material Balances} \\
& \text{Energy balances} \\
& \text{Equipment design}
\end{align*}
\]

Adsorption model

- Design:
  - # of parallel units,
  - # of adsorbers and # of regenerators,
  - Size of equipment (Heat exchangers, reactors, blowers)
- Operation:
  - Flows (molar and mass flow rates)
  - Temperatures (Coolant, steam, gas, solids)
  - Pressure (gas and solids)
  - Concentrations (gas and solids)

Membrane separation model

- Design:
  - # of membranes to be installed,
  - Size of equipment (Heat exchangers, pumps, expanders, membranes)
- Operation:
  - Flows (permeate, retentate)
  - Temperature (gas, coolant)
  - Pressure (retentate and permeate sides)
  - Concentrations (gas)

\[
\begin{align*}
\text{min } & \text{COE} \\
\text{s.t. } & \text{Material Balances} \\
& \text{Energy balances} \\
& \text{Equipment design}
\end{align*}
\]

- Operating Cost
- Variable Cost
- Fixed annual investment cost
- Net power cost
Solid Sorbent System

Adsorption system
Plant consists on:
- Flue gas (650 MW power plant)
- 90 % capture

Design Decisions:
- # number of parallel units,
- Flue gas heat exchanger,
- Adsorber and Regeneration trains,
- SolidLean and SolidRich Heat exchangers.

Operation
- Flows, temperatures, concentrations
Solid Sorbent System

Adsorption & Regeneration process
- Bubbling fluidized bed reactor
  - Lee and Miller 2013\(^1\)
  - One dimensional model
  - Mass & energy balances
  - Integrated heat exchanger
  - PDEs 10,000 Equations

Mathematical Model
- Mix of \textit{first principle}
- and \textit{Surrogate models} to describe the process.

\(^1\)Lee A, Miller, D.C. I&ECR 2013.
Solid Sorbent System

Algebraic Surrogate Models

First Principle Models

- Heat exchangers, blowers, pumps, etc.
- Nonlinear algebraic equations

Superstructure Optimization

Carbon Capture Process

Optimized Process
Framework for Optimization and Uncertainty Quantification and Surrogates - FOQUS

- Carbon Capture Simulation Initiative tool set
  - Simulation, Statistics, Uncertainty Quantification, Optimization, Surrogate Modeling, Dynamic Models.

ALAMO – Automated Learning of Algebraic Models

“Surrogate models correlate the input and output variables of the process“

\[
\begin{align*}
\mathbf{z}_i &= f(\mathbf{x}_1, \ldots, \mathbf{x}_D) \quad \forall \; i \in K
\end{align*}
\]
Surrogate Model Generation

- **Surrogate models:**
  - Simulation
    - Model 10,000 PDE’s
    - Aspen Custom Modeler
  - Data set
    - 2000 samples
    - Latin Hypercube Sampling method

- **Reactor Design**
  - Dt – unit diameter (m)
  - Heat Exchanger design
  - Solids Fluidization bed

- **Gas Outlet**
- **Solids Outlet**
- **Coolant Outlet**
- **Flue gas**
  - Flow rate
  - Pressure
  - Temperature
  - Concentration
Solid Sorbent System

- **Surrogate models:**
  - **Simulation**
    - Model 10,000 PDE’s
    - Aspen Custom Modeler
  - **Data set**
    - 2000 samples
    - Latin Hypercube Sampling method
  - **Surrogate model generation**
    - Validation and cross-validation

![Fit data](image1)

![Cross-validation](image2)

$R^2 = 0.99$
Optimal Solutions

Optimization:
- Superstructure optimization allows us to explore all the possible plant layouts.
- 90% CO₂ Capture.

<table>
<thead>
<tr>
<th>Fixed layout</th>
<th>Best Case</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>% COE increase</td>
<td>-</td>
<td>3%</td>
<td>4%</td>
<td>5%</td>
</tr>
<tr>
<td>Adsorber beds</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Regeneration beds</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Ads parallel units</td>
<td>6</td>
<td>8</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>Rgn parallel units</td>
<td>4</td>
<td>6</td>
<td>4</td>
<td></td>
</tr>
</tbody>
</table>
Membrane based systems

Membrane separation

Design:
- # of membranes to be installed
- Membrane area
- Size/cost of Heat exchanger, pumps, compressors, expanders

Operation:
- Flows (feed, permeate, retentate)
- Temperature (gas, coolant)
- Pressure
- Concentrations (gas)

T_{mem} = 25 \, \text{C}

Permeance = fixed \, (\text{kgmol/m}^2 \text{s bar})

Operation = co-current flow

Pressure ratio = P_{in} \, \text{(bar) / P_{out} \, \text{bar}}

90% Capture
97 \% \text{CO}_2 \, \text{pure to Storage}
Membrane based systems

- Separation stage

Flue Gas
- 10-15 % CO2
- 1 bar
- 327 K

Stage:
- Compression system
- Heat exchanger
- Membrane
- Vacuum pump
- Expander

Flue Gas
- 3-6 bar
- 298.15 K

Flue Gas
- 3-6 bar
- 400-600 K

T_{mem} = 298.15 K

Retentate
- 3-6 bar
- 298.15 K

Permeate
- 0.01 - 1 bar
- 298.15 K
- 0.25 – 0.8 % CO2

Permeate
- 1 bar
- 298.15 K

\[ \min_{x} f(x) \]

s.t.
\[ g_i(x) \leq 0, \quad i = 1, \ldots, n \]
\[ h_j(x) = 0, \quad j = 1, \ldots, m \]
\[ x \in X \]
Optimal Solutions

Optimization:
• Configuration: 3 membrane stages, flash unit, recirculation R1 and R2 to M3
• 90% CO₂ Capture

Optimization:
• Configuration: 2 membrane stages, flash unit, recirculation R1 and R2 to M3
• 15% COE increase relative to best case
• 70% CO₂ Capture
Conclusions and Future Work

- Configuration of CO\textsubscript{2} systems is extremely **important** for individual technologies.
- Establish a **consistent framework** for evaluating multiple technologies is a critical task.
- Combined technologies could lead to improvements in the separation performance while reducing the energy penalty.

Similar to Superstructure Optimization of Water Networks (Yang & Grossman 2011)

Given is:
- Set of separation stages (U)
  - Adsorber, regenerator, membrane, **others**.
  - Heat exchanger, pump, compressor, expander.
- Minimize Cost of Electricity

MINLP: Mix of First Principle and Surrogate Models
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Thank you for your attention

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