Superstructure Formulation and Optimization for Carbon Capture Processes

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OUTLINE

• Motivation
• Carbon capture processes
• Superstructure optimization
• Surrogate models for optimization
• MINLP formulation
• Case study
• Conclusions
MOTIVATION

Backbone of energy supply
- Petroleum
- Coal
- Natural Gas

Huge amount of CO₂ emissions
- One third from power plant

Global warming issues
- Ice melting
- Ocean level rising

CO₂ emissions reduction
- CO₂ capture, Utilization, & Storage (CCUS)

Carbon capture technologies: Key of the CCUS
CO₂ CAPTURE PROCESSES

Most widely investigated capture technology: MEA solvent based postcombustion

- Cost & energy-intensive technology
- Thermal & oxidative degradation

Innovative carbon capture technologies

- High-efficient solvents/sorbents
  - Greater capacity and selectivity
- Cost-effective capture process
  - Reduced energy for regeneration

DOE: Carbon Capture Simulation Initiative (CCSI)

- 5 National Labs and 6 Universities
- Solid sorbent technology: initial demonstration case
- https://www.acceleratecarboncapture.org/drupal/
SOLID SORBENT CAPTURE PROCESS

Solid sorbent reactor

- *Bubbling fluidized bed*
- Fast fluidized bed
- Moving bed
- Fixed bed

Bubbling fluidized bed

- 1D models
- Modeled in Aspen Custom Modeler
- Differential model
- Uses Aspen Properties package

*(A Lee, I&EC Research, 2013)*
General flow sheet for solid sorbent based carbon capture process
SUPERSTRUCTURE OPTIMIZATION

Objectives

• Achieve the set carbon capture rate
• Minimize the cost of electricity \((\text{COE})\)
• Identify & develop the optimized bubbling fluidized bed process designs
  — Optimal topology
  — Optimal design conditions
  — Optimal operating conditions

Hurdles

• Computationally intractable because of the detailed first principle models

Handles

• Generate the set of low complexity algebraic surrogate models
  — Automated Learning of Algebraic Models for Optimization (ALAMO)
  \((http://archimedes.cheme.cmu.edu/?q=alamo)\)
SURROGATE MODEL GENERATION

**Independent variables x**
- Geometry
- Operating conditions
- Inlet flow conditions

**Dependent variables z**
- Geometry required
- Operating condition required
- Outlet flow conditions
- Design constraints

( A. Cozad et al. ALAMO: Automatic learning of algebraic models for optimization. 589b. Thursday, 8:50 AM, AIChE 2013 )
BUBBLING FLUIDIZED BED

Model inputs
- Inlet pressure
- Inlet temperatures
- Inlet mass flow-rates
- Inlet gas mole fractions
- Inlet solid compositions
- Heat exchanger conditions

Model outputs
- Outlet pressure
- Outlet temperatures
- Outlet mass flow-rates
- Outlet gas mole fractions
- Outlet solid compositions

Bubbling fluidized bed reactor diagram
Assumptions for mixed integer nonlinear programming formulation

- Each stage is a single stage operation
- No pressure change for liquid and solid flow
- Each stage of adsorber/regenerator operation requires attached heat exchanger
- Surrogate models for fluidized bed adsorber and regenerator
- First principle models for SolidRich/SolidLean heat exchanger, blower, mixer
OBJECTIVE FUNCTION

Objective function

\[
COE = \frac{(CCF)(TOC_{Sc} + TOC_{Cc}) + OC_{FIX} + (CF)(OC_{VAR})}{(CF)(MWh)} + COE_{TS&M}
\]

Where

- \(TOC_{Cc}\): Capture system capital cost
- \(OC_{FIX}\): Fixed operating & maintenance cost
- \(OC_{VAR}\): Total variable cost
- \(MWh\): Annual net megawatt-hours of power
- \(COE_{TS&M}\): COE increment
- \(TOC_{rhx}\): Cost of Rich solid heat exchanger
- \(TOC_{lhx}\): Cost of Lean solid heat exchanger
- \(TOC_{flx}\): Cost of flue gas heat exchanger
- \(TOC_{Sc}\): Sc plant capital cost
- \(TOC_{Cs}\): Capital cost of reactors
- \(TOC_{ves}\): Cost of vessel
- \(TOC_{blow}\): Cost of blower
- \(TOC_{HX}\): Cost of in-let heat exchanger
- \(TOC_{pla}\): Cost of plate
- \(TOC_{plat}\): Cost of platforms and ladders
- \(TOC_{elem}\): Cost of elevator motor
- \(TOC_{ele}\): Cost of elevator
### MINLP FORMULATION

#### Adsorber series

- **Flue gas flow**
  \[
  x_{a, fc}^{\text{out}} = F(\text{surrogates}) y(a) + x_{a-1, fc}^{\text{out}} (1 - y(a))
  \]
  \[
  F_{a, g}^{\text{out}} = F(\text{surrogates}) y(a) + F_{a-1, g}^{\text{out}} (1 - y(a))
  \]
  \[
  T_{a, g}^{\text{out}} = F(\text{Surrogates}) y(a) + T_{a-1, g}^{\text{out}} (1 - y(a))
  \]

- **Solid sorbent flow**
  \[
  y_{a, A}^{\text{out}} = F(\text{Surrogates}) y(a) + y_{a+1, A}^{\text{out}} (1 - y(a))
  \]
  \[
  x_{a, A}^{\text{out}} = F(\text{Surrogates}) y(a) + x_{a+1, A}^{\text{out}} (1 - y(a))
  \]
  \[
  T_{a, A}^{\text{out}} = F(\text{Surrogates}) y(a) + T_{a+1, A}^{\text{out}} (1 - y(a))
  \]

- **Logical constraints**
  \[
  y(a) \geq y(a + 1), \quad \forall a \in a_{\text{max}}
  \]
  \[
  \sum_a y(a) \geq 1
  \]
MINLP FORMULATION-CONTINUED

Regenerator series

• Clean gas flow

\[ x_{d,fc}^{out} = F(\text{surrogates})y(d) + x_{d-1,fc}^{out}(1 - y(d)) \]

\[ F_{d,g}^{out} = F(\text{surrogates})y(d) + F_{d-1,g}^{out}(1 - y(d)) \]

\[ T_{d,g}^{out} = F(\text{surrogates})y(d) + T_{d-1,g}^{out}(1 - y(d)) \]

• Solid sorbent flow

\[ \gamma_{d,A}^{out} = F(\text{Surrogates})y(d) + \gamma_{d+1,A}^{out}(1 - y(d)) \]

\[ x_{d,A}^{out} = F(\text{Surrogates})y(d) + x_{d+1,A}^{out}(1 - y(d)) \]

\[ T_{d,A}^{out} = F(\text{Surrogates})y(d) + T_{d+1,A}^{out}(1 - y(d)) \]

• Logical constraints

\[ y(d) \geq y(d + 1), \forall d \in d_{\text{max}} \]

\[ \sum_{d} y(d) \geq 1 \]
CASE STUDY

Given conditions
- Conditions of flue gas
- Max number of adsorbers: 4
- Max number of regenerators: 4
- Max number of trains: 16
- Minimum capture rate: 90%

Objectives
- Minimize cost of electricity
- Minimize total capital cost
- Decide the optimal number of trains in parallel
- Decide the optimal number of reactor in series
- Seek optimal operation conditions
- Seek an optimal geometry for each unit

Mixed-integer nonlinear programming model
- Parameters
- Variables
- Equations
  - Economic modules
  - Process modules
    - Material balances
    - Hydrodynamic/Energy balances
    - Reactor surrogate models
  - Link between economic modules and process modules
  - Binary variable constraints
  - Bounds for variables
RESULTS

Optimal topology

Molar composition of flue gas

Outlet sorbent composition (mol/kg)

<table>
<thead>
<tr>
<th>Variables</th>
<th>Lower</th>
<th>Value</th>
<th>Upper</th>
</tr>
</thead>
<tbody>
<tr>
<td>COE($/MWh)*</td>
<td>0</td>
<td>137.3</td>
<td>1000</td>
</tr>
<tr>
<td>CapEX($M)</td>
<td>100</td>
<td>230.1</td>
<td>1000</td>
</tr>
<tr>
<td>steamFlow(kg/s)</td>
<td>~</td>
<td>108</td>
<td>~</td>
</tr>
<tr>
<td>Derate(MW)</td>
<td>0</td>
<td>103.7</td>
<td>650</td>
</tr>
<tr>
<td>sorbentF(kg/hr)</td>
<td>4E5</td>
<td>8.8E5</td>
<td>9E5</td>
</tr>
<tr>
<td>Nu (Number of trains)</td>
<td>12</td>
<td>12</td>
<td>16</td>
</tr>
</tbody>
</table>

- Cost of Electricity based on calculated capture system with base plant. + $48/MWh to account for compression, transport & storage
CONCLUSIONS

• We developed a surrogate model based framework to seek the optimal topology and the relevant optimal design/operating levels for carbon capture processes

• ALAMO provides simple surrogate models of adsorbers and regenerators and thus leads to a low-complexity optimization model

• Next steps:
  — Extend MINLP to select simultaneously the reactor type for each stage
  — Integrate heat integration across the capture and compression system with superstructure formulation