Dynamic Modeling of Advanced Process Configurations for Post-Combustion Amine Scrubbing

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Challenges for CCS

Energy Penalty
~20-30% reduction in power plant output

Capital Cost
800 MW coal plant: > 3 billion ft$^3$/day flue gas

Tight Integration
High material and energy recycle
Minimization of equipment size and solvent inventory
Heavy Material and Energy Recycle

\[ \frac{RcE_{rec}}{F_{CO2,steam}} \approx 1 \]

\[ Q_{Ex} = \frac{430}{mol \ CO_2} \]

\[ Q_{Steam} = 105 \frac{kJ}{mol \ CO_2} \]

Hierarchical Controller Design

Goal: Develop dynamic model for control strategy design
Process Modeling: Advanced Configuration

Vent to ATM

CO₂ to Compressor

H₂O

Absorber Feedtank

Intercooling

Heat EX

Lean Solvent

High P Flash

Low P Flash
## Process Modeling: Advanced Solvent

### MEA: \( \text{H}_2\text{N}____\text{OH} \)

### PZ: \( \text{H} \)

### Previous Works

<table>
<thead>
<tr>
<th>Property</th>
<th>7 m MEA</th>
<th>8 m PZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_g \times 10^7 ) (mol/Pa·s·m²)</td>
<td>4.3</td>
<td>8.5</td>
</tr>
<tr>
<td>Capacity (mol CO₂/mol PZ + H₂O)</td>
<td>0.67</td>
<td>0.88</td>
</tr>
<tr>
<td>Degradation T (°C)</td>
<td>121</td>
<td>163</td>
</tr>
<tr>
<td>Max stripper P (bar)</td>
<td>4</td>
<td>16</td>
</tr>
<tr>
<td>Degradation rate at 120°C (1/week)</td>
<td>8.1%</td>
<td>0.07%</td>
</tr>
<tr>
<td>( C_{amine} ) in gas at 40°C (ppm)</td>
<td>13</td>
<td>8</td>
</tr>
<tr>
<td>( \Delta H_{abs} ) at lean ldg (kJ/mol CO₂)</td>
<td>-76</td>
<td>-71</td>
</tr>
</tbody>
</table>

### This Research

Equation-oriented process flowsheet

\[ \Delta H_{\text{abs}}, C_p, P^*_\text{CO}_2, \rho, \mu \]
Model Validation: SRP Pilot Plant

Validation Data:
Fall 2011
PZ Solvent
Two-Stage Flash Stripper
Intercooled Absorber
Flash Tank Model

\[ Q_{\text{eff}} = Q_{\text{steam}} - Q_{\text{loss}} \]
\[ Q_{\text{loss}} = UA(T - T_{\text{amb}}) \]

Rich In

\[ T_{\text{in}} \]

Q_{\text{steam}}

\[ \rho = f(T, C_{CO2}, C_{PZ}) \]

\[ \frac{\rho}{\rho_{H2O}} = \left( \frac{\rho}{\rho_{H2O}} \right)_{\text{meas}} + \left( \frac{\rho}{\rho_{H2O}} \right)_{\text{bias}} \]

CO₂/H₂O

Semi-Rich Out

\[ \left( \frac{\rho}{\rho_{H2O}} \right)_{\text{bias}} = 0.0082 \]

\~4\% Increase in experimental loading

Fitted:

\[ UA = 0.075 \text{ kW/K} \]

Experimental (both tanks):

Fitted:

\[ UA = 0.054 \text{ kW/K} \]
Steady State Flash Tank Validation

\[ \leq 1.2^\circ \text{C} \]

- SRP
- gPROMS

Temperature (K) vs Run
Intercooled Absorber Model

• Ideal gas law is valid
• PZ is nonvolatile
• Mass transfer of H₂O is gas film controlled
• Heat transfer is gas film controlled
• Equilibrium at the gas/liquid interface
• No accumulation at the gas/liquid interface
• Constant pressure drop
• Plug flow regime
Absorber Model Development

- Gas/Liq. Interface
  - Gas Mole Balance
  - Gas Energy Balance
- Bulk Gas
  - Gas Film
    - $N_{CO2}$
- Liq. Film
  - $N_{H2O}$
  - $N_H$
  - Gas/Liq. Interface
- Bulk Liquid
  - Liquid Mole Balance
  - Liquid Energy Balance
Absorber Mass Transfer

Liquid film:

\[ k_g' = f(\alpha) \]

Overall Mass Transfer Coefficient:

\[ \frac{1}{K_{tot}} = \frac{1}{k_g} + \frac{1}{k_g'} \]

Rate-Based Flux:

\[ N_{CO2} = K_{tot}(P_{CO2} - P_{CO2}^*) \]
Wetted Wall Column Validation

\[ \frac{\partial E}{\partial t} = 0 \]

\[ \alpha_{in} \approx \alpha_{out} \]

\[ \ln[P_{CO2}^*] = f(\alpha, T) \]

Given loading

Predict Flux
Wetted Wall Column Validation Results

\[ N_{CO2} = K_{tot}(P_{CO2} - P_{CO2}^*) \]

\[ \ln[P_{CO2}^*] = f(\alpha, T) \]
Steady State Absorber Validation

Vent to ATM
Lean Solvent (40°C)
$\alpha_{\text{lean}} = 0.26$ 
Input

(kg)'
$ae$ Factor
0.74
Consistent with Schade (2012)

12% CO2
~1% H2O
~87% Air
Ambient T

Rich Solvent
$\alpha_{\text{rich}} = 0.36$ 
Match within 7%

$K_g'a_e$
Mass Transfer Coefficient Uncertainty

Empirical Correlation Uncertainty

\[ k'_g = -2.0 \times 10^{-5} \alpha + 8.2X \times 10^{-6} \pm 20\% \]

\[ \frac{a_e}{a_p} = 1.34 \left( \frac{(We) (Fr)^{-\frac{1}{3}}}{3} \right)^{0.116} \pm 13\% \]

Liquid film mass transfer coefficient:

\[ \frac{1}{k'_g} = \frac{m_{CO2}}{k_l} + \frac{1}{k''_g} \]

\( k''_g \) - Pseudo 1st order mass transfer coefficient
Steady State Absorber Validation

Run 8

- SRP
- Liquid T
- Gas T

Normalized Distance vs. Temperature (°C)

Temperature (°C):
20 30 40 50 60
Steady State Absorber Validation

Run 8

Normalized Distance

- SRP
- Liquid T
- Gas T

Temperature (°C)

Normalized Distance

20 30 40 50 60
Conclusions

• Heavy energy and material recycle lead to multiple time scale behavior in the amine scrubbing system
• Flash tank temperature predicted within 1.2°C after adjusting loading by 4% heat loss by 40%
• Absorber with $k_g' = f(\alpha)$ predicts experimental $\ln[P_{CO2}]$ for wetted wall column with average error of 2.2%
• Absorber loading matched within 7% with 26% decrease in $a_e k_g'$
• Behavior of absorber temperature profile consistent with pilot plant measurements
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