Transformational Sorbent System for Post-Combustion Carbon Capture (DE-FE0031734)

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Capture from Power Generation Lab/Bench-Scale Research

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Project Objective and Team

- Objective is to develop a transformational sorbent based on a metal-organic framework (MOF)
  - 90+% capture efficiency of CO$_2$
  - 95% purity recovered CO$_2$ purity
  - 30% lower costs than amine based systems with <$30 per tonne of CO$_2$

- Main Project Tasks
  **BP1**
  - Demonstrate sorbent performance at the bench scale
  - Assess impact of flue gas contaminants (SO$_2$, NOx)
  - Develop cycle sequence
  - Preliminary TEA

  **BP2**
  - Scale-up sorbent production
  - Complete Life/Durability Tests
  - Optimize adsorption cycles and update TEA

  **BP3**
  - Slipstream field tests (6 months)
  - High Fidelity TEA and EH&S

Overall Project Duration
- Start Date = June 1, 2019
- End Date = May 31, 2024

Budget
- Project Cost = $3,750,000
- DOE Share = $3,000,000
- TDA and its partners = $750,000
- Sorbent operates between 30-50°C under vacuum (0.2-0.3 atm)
  - Commercially available vacuum equipment
- Capability to achieve 99% CO₂ removal efficiency
- High CO₂ selectivity results greater than 95% CO₂ product purity
- A new reactor design to ensure low pressure drop and reduced parasitic load
- Similar technology can also be applied to NGCC applications, with higher steam purge/energy penalty
CO$_2$/N$_2$ Adsorption Isotherms

- **High CO$_2$ uptake**
  - >2 mmol/g at 0.15 bar
  - ~3 mmol/g for the modified version

- **Very high selectivity towards CO$_2$ over N$_2$, which ensures a very high product purity**
  - Over 95% without any downstream purification needs

- **Heat of adsorption of CO$_2$ is measured as 11 kcal/mol at low surface coverage and 8 kcal/mol at higher coverages**

- **Improvements in linker synthesis results in very high CO$_2$ uptake**
Low pressure water isotherms are linear indicating that water easily desorbs from the sorbent surface.

No change in low pressure isotherm before and after water isotherm measurements.
Pelletization of the MOF Sorbent

- MOFs are difficult to pelletize or granulate
- Conventional powder compaction techniques could potentially damage the MOF structure
- TDA developed a pill-pressing method that results in pelletized sorbent to retain >95% of their capacity when normalized based on active MOF weight
Scale-up of MOF Production

- Scale-up from 1L to 22L flask and to 180L Hastelloy reactor in BP2
- BP1 evaluations have focused on improving synthesis parameters and space-time yields while conserving raw materials (via recycle)
  - Space yield improvements of 10-15X
  - Time yield improvements of 5-8X
- MOF synthesis, Filtration/Rinsing, Drying/Devolatilization are all sequentially carried out in the same reactor
- A classified area is designed and built to handle the equipment and solvents required for MOF processing
Optimization of Space Time Yield

- Space Yield was increased from <10 g/L to 75-80 g/L
- Synthesis time was reduced from 7 days to 1 day (24 h)
- We were able to increase the space time yield from <0.1 g/L/hr to >3.0 g/L/hr
Reduced Preparation time of 24 hours was still able to provide a high yield while retaining the CO$_2$ adsorption capacity (Sorbent performance)
Performance in Flow Experiments

A working capacity of 5+% wt. CO₂ at ~15% vol. CO₂ was demonstrated
  • ~2.5% wt. CO₂ at 4% vol. CO₂

Temperature and humidity have limited impact on working capacity
  • Higher temperatures lowered the working capacity
  • No significant impact of humidity up to 65%
Evaluation of Sorbent Life

5/15/20% CO₂ in N₂ at T = 30°C, GHSV = 2,400 h⁻¹, 30/50/65% RH
Regen Purge gas: N₂, Counter flows

- A stable working capacity of 5.5% wt. CO₂ was demonstrated in counter flow desorption under simulated coal flue gas conditions
Life Tests in Presence of Contaminants

- Stable working capacity in the presence of flue gas contaminants such as humidity, NOx and SOx
- High stability up to 65% RH, 500 ppm NOx, 50 ppm SOx
- Maximum ~20% drop in capacity under high SOx and NOx concentrations

15% CO$_2$ in N$_2$ at T = 30/45/60°C, GHSV = 1,000 h$^{-1}$, 0-6% H$_2$O - Regen Purge gas: N$_2$, Counter flows
Impact of Contaminants

- Only <5% drop in working capacity was observed at 100 ppm NOx and 10 ppm SOx.
- At 500 ppm NOx and 50 ppm SOx the working capacity dropped by 10%.
- After saturating the sorbent with 500 ppm NOx or 50 ppm SOx the sorbent working capacity dropped by ~ 20%.
Adsorption Cycle Modeling

- Initial modeling results from University of Alberta shows simple cycle schemes without addition of steam purge can get close to DOE targets.
- More advanced cycle schemes with steam assisted VSA results in 95% CO₂ purity with a CO₂ levels in flue gas as low as 4% (NGCC simulation).
### Capture Technology

<table>
<thead>
<tr>
<th>Capture Technology</th>
<th>Sorbent Only</th>
<th>Amine</th>
<th>No Capture</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Case Studies</strong></td>
<td>Case 1</td>
<td>B12B</td>
<td>B12A</td>
</tr>
<tr>
<td><strong>Gross Power, kWe</strong></td>
<td>795,063</td>
<td>770,000</td>
<td>685,000</td>
</tr>
<tr>
<td><strong>CO₂ Capture/Removal, kWe</strong></td>
<td>47,679</td>
<td>29,530</td>
<td>-</td>
</tr>
<tr>
<td><strong>CO₂ Purification, kWe</strong></td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>CO₂ Compression, kWe</strong></td>
<td>58,141</td>
<td>44,380</td>
<td>-</td>
</tr>
<tr>
<td><strong>Balance of Plant, kWe</strong></td>
<td>39,243</td>
<td>46,050</td>
<td>35,040</td>
</tr>
<tr>
<td><strong>Total Auxiliaries, kWe</strong></td>
<td>145,063</td>
<td>119,960</td>
<td>35,040</td>
</tr>
<tr>
<td><strong>Net Power, kWe</strong></td>
<td>650,000</td>
<td>650,040</td>
<td>649,960</td>
</tr>
<tr>
<td><strong>Net Plant Efficiency, % HHV</strong></td>
<td>33.4</td>
<td>31.5</td>
<td>40.3</td>
</tr>
<tr>
<td><strong>Carbon Capture, %</strong></td>
<td>90</td>
<td>90</td>
<td>0</td>
</tr>
<tr>
<td><strong>Coal Feed Rate, kg/h</strong></td>
<td>258,208</td>
<td>273,628</td>
<td>214,112</td>
</tr>
</tbody>
</table>

- Energy for CO₂ capture is 26% lower compared to amine scrubbing
Reactor Vessel Design and Costing

- Four radial beds per train (total of 16 beds)
- SA516-70 carbon steel, 0.5” thickness
- 120 in OD x 872 in T/T

<table>
<thead>
<tr>
<th>Total ΔP (across the entire system)</th>
<th>=105 mbar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Module Size:</td>
<td>137.5 MW</td>
</tr>
<tr>
<td>No. of Trains:</td>
<td>4</td>
</tr>
<tr>
<td>Beds/Train:</td>
<td>4</td>
</tr>
<tr>
<td>Total Beds:</td>
<td>16</td>
</tr>
<tr>
<td>Flue Gas Flow:</td>
<td>116.5 m³/s</td>
</tr>
<tr>
<td>CO₂ Flow:</td>
<td>1.96 tonne/min</td>
</tr>
<tr>
<td>Capacity:</td>
<td>3.6% Wt%</td>
</tr>
<tr>
<td>Cycle Time:</td>
<td>1 min</td>
</tr>
<tr>
<td>Sorbent Inventory:</td>
<td>54.5 tonne/m³</td>
</tr>
<tr>
<td>Sorbent Density:</td>
<td>0.55 tonne/m³</td>
</tr>
<tr>
<td>Bed Volume:</td>
<td>99.5 m³</td>
</tr>
<tr>
<td>Bed Area:</td>
<td>7.3 m²</td>
</tr>
</tbody>
</table>
Rapidly actuating valves are identified to change the bed position in a few seconds.

60 in NPS, 0.375 in thickness (standard schedule) process piping for flue gas and air regeneration lines.
3-D Layout of the Sorbent System

37.0 m (121.5')

35.1 m (115')

67.1 m (220')
## Cost of Capture Summary (Rev. 4 basis)

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<td>B12B</td>
<td>B12A</td>
</tr>
<tr>
<td>Basis for Cost Estimates (Year)</td>
<td>2018</td>
<td>2018</td>
<td>2018</td>
</tr>
<tr>
<td>Net power, MW</td>
<td>650</td>
<td>650</td>
<td>650</td>
</tr>
<tr>
<td>Capacity factor (CF), %</td>
<td>85</td>
<td>85</td>
<td>85</td>
</tr>
<tr>
<td>Total plant cost (TPC), $</td>
<td>2,053,929,454</td>
<td>2,468,373,000</td>
<td>1,364,033,000</td>
</tr>
<tr>
<td>Total overnight cost (TOC), $</td>
<td>2,553,134,556</td>
<td>3,023,049,325</td>
<td>1,678,411,825</td>
</tr>
<tr>
<td>Total as spent capital (TASC), $</td>
<td>2,946,317,278</td>
<td>3,488,598,921</td>
<td>1,937,578,752</td>
</tr>
<tr>
<td>LCOE $/MWh</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Capital Charge (0.0707 X TASC)</td>
<td>43.04</td>
<td>50.96</td>
<td>28.30</td>
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<tr>
<td>Fixed Charges</td>
<td>13.73</td>
<td>16.13</td>
<td>9.48</td>
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<tr>
<td>Variable Costs</td>
<td>12.15</td>
<td>14.00</td>
<td>7.72</td>
</tr>
<tr>
<td>Fuel Costs</td>
<td>22.75</td>
<td>24.08</td>
<td>18.87</td>
</tr>
<tr>
<td>Byproducts (Credit)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Total (Excluding T&amp;S)</td>
<td>91.67</td>
<td>105.18</td>
<td>64.37</td>
</tr>
<tr>
<td>CO2 T&amp;S Costs</td>
<td>8.45</td>
<td>8.96</td>
<td>0.00</td>
</tr>
<tr>
<td>Total (Including T&amp;S)</td>
<td>100.12</td>
<td>114.14</td>
<td>64.37</td>
</tr>
<tr>
<td>Cost of Capture $/tonne</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Breakeven CO2 Sales Price (compared to SCPC W/O capture)</td>
<td>32.25</td>
<td>45.52</td>
<td>-</td>
</tr>
<tr>
<td>Breakeven CO2 emissions penalty (compared to SCPC W/O capture)</td>
<td>52.29</td>
<td>73.40</td>
<td>-</td>
</tr>
</tbody>
</table>

- Cost of CO₂ capture with VLP steam purge is ~$32.25/tonne
- Cost of CO₂ captured is considerably lower for TDA’s CO₂ capture system about 29.2% lower the reference Amine Case
Sensitivity Analysis – CAPEX (Rev. 4 basis)

- Total cost of CO₂ Capture System including flue gas treatment and compression is $368 MM
  - Cost of CO₂ capture ~$32.25/tonne
- CAPEX for CO₂ capture needs to go below $274 MM to meet transformational CO₂ capture targets (<$30/tonne)
Acknowledgments

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• Wyoming Integrated Test Center - Dr. Will Morris

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