Advanced Reactor Design for Integrated WGS/ Pre-combustion CO₂ Capture
(Contract No. DE-FE-0012048)

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Project Objective

• The project objective is to demonstrate techno-economic viability of an integrated WGS catalyst/CO₂ removal system for IGCC power plants and CTL plants
  • A high temperature PSA adsorbent is used for CO₂ removal above the dew point of the synthesis gas
  • A commercial low temperature catalyst is used for water-gas-shift

• Critical Need
  • Develop an effective heat management system

• Project Tasks
  • Reactor design aided by CFD modeling to identify the best thermal management option in the integrated WGS/CO₂ removal bed
  • Evaluate the optimum reactor design at bench-scale
  • Demonstrate technical viability of the best design in slipstream tests at the NCCC using real-coal derived syngas
  • Engineering and cost analysis using Aspen Plus™
In the next phase of the project a larger slipstream evaluation will be carried out at 10 SCFM at Wabash River IGCC plant and NCCC (DE- FE-0023684)
TDA’s sorbent is mesoporous carbon modified with surface functional groups that remove CO₂ via strong physical adsorption

- CO₂-surface interaction is strong enough to allow operation at elevated temperatures
- Because CO₂ is not bonded via a covalent bond, the energy input for regeneration is low
- Heat of CO₂ adsorption is 4.9 kcal/mol for TDA sorbent
  - Comparable to that of Selexol
- Net energy loss in sorbent regeneration is similar to Selexol, but a much higher IGCC efficiency can be achieved due to high temperature CO₂ capture

US Pat. Appl. 61787761, Dietz, Alptekin, Jayaraman “High Capacity Carbon Dioxide Sorbent”

US Pat. Appl. 61790193, Alptekin, Jayaraman, Copeland “Pre-combustion Carbon Dioxide Capture System Using a Regenerable Sorbent”
Further Energy Savings

- Conventional IGCC plants use multi-stage WGS reactors with inter-stage cooling
  - WGS is an equilibrium-limited exothermic reaction
- Water is supplied at concentrations well above required by the reaction stoichiometry to completely shift the CO to CO_2

3-stage WGS unit is described in the DOE/NEXTL-2007/1281

- A high temperature CO_2 adsorbent combined with a LT shift catalyst enables high CO conversion at low steam:carbon ratios
Integrated WGS/CO$_2$ Capture System

- Reducing the use of excess steam improves power cycle efficiency
  - Lower energy consumption to raise the steam
- Process intensification reduces the number of hardware components and cost

**Sorbent’s point of view:**
- Less dilution with water increases CO$_2$ partial pressure and in turn improves sorbent’s working capacity
Application to CTL
Prototype system achieved 90+% carbon capture under Steam:CO ratio of 1:1.1 with average CO conversion of 96.4%.

All objectives met (no coking etc.) but observed high reactor T
Technology Status/R&D Needs

• Sorbent is developed under a separate DOE project (DE-FE0000469)
• WGS catalyst is commercially available mature technology
• Early-stage concept demonstration has already been completed (under DE-FE0007966)
  • Integrated sorbent/catalyst operation
  • Pointed out the need to incorporate effective heat management
• Key R&D need is the design/development of a high fidelity prototype to fully demonstrate the concept using actual coal-derived synthesis gas
  • Early-stage prototype demonstration of an integrated system with heat management is also under progress (under DE-FE-00012048)
  • Slipstream test at the NCCC at ~0.2 kg/hr CO₂ removal
• A larger-scale (10 kg/hr CO₂ removal) test will be carried out at the Wabash River IGCC plant (under DE-FE-00012048)
T Profiles - During CO$_2$ Capture Only

- Heat generated during adsorption is removed during regeneration
  - Near isothermal operation
Heat Wave WGS & CO₂ Capture

- Integrated WGS & CO₂ capture results in higher ΔT
- Not ideal for CO₂ capture (the WGS heat accumulates in the beds)
Conventional Heat Management Options

10 kg/hr CO₂ Removal Pilot Test System – 6” reactors
Heat Integrated WGS & CO₂ Capture

- Advanced heat management concept based on direct water injection has proven to achieve much better temperature control
  - Also much better heating efficiency (i.e., kJ heat removed per kg water)
- Objective is more uniform cooling without having hot or cold spots
- We are also optimizing how the WGS catalyst and the sorbent to be distributed in the combined WGS catalyst /CO₂ capture sorbent beds
Bench-Scale Evaluations

- 8L reactors were modified with the heat management options
- Successful proof-of-concept demonstrations have been completed
- $\Delta T <10^\circ\text{C}$ was maintained over extended cycling (much lower than those observed in early field tests)
### IGCC Plant with E-Gas™ Gasifier operating on Bituminous Coal

<table>
<thead>
<tr>
<th>#</th>
<th>CO₂ Capture</th>
<th>Notes</th>
<th>Steam/Water Addition</th>
<th>Overall Steam:CO Ratio</th>
<th>Net Efficiency % HHV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Conventional Technology</td>
<td>Reference IGCC Case with Steam addition to 1&lt;sup&gt;st&lt;/sup&gt; WGS reactor feed</td>
<td>Steam</td>
<td>2.25</td>
<td>31.04</td>
</tr>
<tr>
<td>2</td>
<td>TDA/Advanced Technology</td>
<td>No steam addition to 1&lt;sup&gt;st&lt;/sup&gt; WGS reactor feed; water injection into combined WGS+PSA reactor</td>
<td>Water</td>
<td>1.50</td>
<td>34.30</td>
</tr>
<tr>
<td>2-1</td>
<td>TDA/Advanced Technology</td>
<td>No steam addition to 1&lt;sup&gt;st&lt;/sup&gt; WGS reactor feed; no water injection into combined WGS+PSA reactor</td>
<td>None</td>
<td>1.24</td>
<td>34.55 (87% carbon capture)</td>
</tr>
<tr>
<td>2-3</td>
<td>TDA/Advanced Technology</td>
<td>No 1&lt;sup&gt;st&lt;/sup&gt; WGS reactor &amp; water injection into combined WGS+PSA reactor</td>
<td>Water</td>
<td>2.21</td>
<td>33.73</td>
</tr>
<tr>
<td>2A</td>
<td>TDA/Previous Technology</td>
<td>Steam addition to 1&lt;sup&gt;st&lt;/sup&gt; WGS reactor feed; no water injection into 2&lt;sup&gt;nd&lt;/sup&gt; WGS reactor (not combined with PSA)</td>
<td>Steam</td>
<td>2.25</td>
<td>33.81</td>
</tr>
</tbody>
</table>

- Reducing Steam:CO ratio to 1.50 w/ water addition to Integrated WGS/CO₂ Removal Reactor (2nd stage) provides a net plant efficiency of 34.30%
- 0.5% point improvement over TDA’s previous technology
## IGCC plants with Shell Gasifier

<table>
<thead>
<tr>
<th>Case #</th>
<th>Coal Type</th>
<th>CO₂ Capture</th>
<th>Notes</th>
<th>Overall Steam: CO Ratio</th>
<th>Net Efficiency % HHV</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Bituminous</td>
<td>Conventional Technology</td>
<td>Reference IGCC Case (H₂O/CO in 1ˢᵗ WGS reactor feed = 1.8 mole/mole per corresponding DoE case)</td>
<td>1.8</td>
<td>31.08</td>
</tr>
<tr>
<td>4</td>
<td>Bituminous</td>
<td>TDA/Advanced Technology</td>
<td>No steam addition to 1ˢᵗ WGS reactor feed (H₂O/CO in 1ˢᵗ WGS reactor feed = 1.11 mole/mole); water injection into combined WGS+PSA reactor</td>
<td>1.38</td>
<td>33.71</td>
</tr>
<tr>
<td>5</td>
<td>Lignite</td>
<td>Conventional Technology</td>
<td>Reference IGCC Case (H₂O/CO in 1ˢᵗ WGS reactor feed = 1.8 mole/mole)</td>
<td>1.8</td>
<td>30.89</td>
</tr>
<tr>
<td>6</td>
<td>Lignite</td>
<td>TDA/Advanced Technology</td>
<td>No steam addition to 1ˢᵗ WGS reactor feed (H₂O/CO in 1ˢᵗ WGS reactor feed = 1.60 mole/mole); water injection into combined WGS+PSA reactor</td>
<td>1.78</td>
<td>32.79</td>
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</tbody>
</table>

- Different gasifiers and coal are being evaluated
- Better plant efficiency for all coals and gasifiers

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TDA Research
Slipstream Evaluation at NCCC

- Plan to participate two test campaigns at the NCCC
  - September – October 2015
  - April 2015
Larger Field Evaluation

- Process Design Package (PDP) is complete and being reviewed by the host sites Wabash River IGCC Plant and NCCC
- An additional test with Praxair is also planned
- With DOE’s consent, these skids can be made available for other tests
Vision for Commercialization

- Slipstream to pilot-scale demonstrations to increase technical maturity from TRL = 4 to TRL = 6
- Develop a complete technology package for licensing
  - Intellectual Property
  - Process Design Package
  - Sorbent Manufacturing

- Privately Owned / Began operations in 1987
- Two facilities in Wheat Ridge and Golden, CO
  - 50,000 ft² of office and lab space
- 82 full-time technical staff
  - More than half with advanced degrees (28 PhDs)
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