Evaluation of Life Support Candidate Technology for 100% Oxygen Recovery

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• Current life support onboard the International Space Station (ISS) utilizes a Sabatier based oxygen recovery system which results in approximately 50% O\textsubscript{2} recovery from CO\textsubscript{2}.

• Resulting water is stored for future use and CH\textsubscript{4} is vented out of the vessel, resulting in a net loss of hydrogen needed to react with CO\textsubscript{2}.

• The Bosch process is of interest as there is the potential for zero net H\textsubscript{2} loss and therefore 100% O\textsubscript{2} recovery.

\begin{table}[h]
\begin{tabular}{|c|c|}
\hline
\textbf{Sabatier Reaction} & \\
\hline
CO\textsubscript{2} +4H\textsubscript{2} &  \rightleftharpoons  \text{CH}_4 +2H\textsubscript{2}O \\
\hline
\end{tabular}
\caption{The Sabatier reaction.}
\end{table}
Background

- There are two steps in the Bosch Process: Reverse Water-Gas Shift (RWGS) and carbon formation.
- Carbon formation may occur by the Boudouard or CO Hydrogenation reaction.

Table 2. Reactions Involved in the Bosch Process.

<table>
<thead>
<tr>
<th>Step 1 (RWGSr):</th>
<th>RWGS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{CO}_2 + \text{H}_2 \leftrightarrow \text{CO} + \text{H}_2\text{O}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Step 2 (CFR):</th>
<th>Boudouard</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$2\text{CO} \leftrightarrow \text{C}(s) + \text{CO}_2$</td>
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</table>

<table>
<thead>
<tr>
<th></th>
<th>CO Hydrogenation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{CO} + \text{H}_2 \leftrightarrow \text{C}(s) + \text{H}_2\text{O}$</td>
</tr>
</tbody>
</table>

| Overall Bosch Process: | CO$_2$ + H$_2$ $\leftrightarrow$ C$_{(s)}$ + 2H$_2$O |
Objectives

PCI RWGS Reactor Modification and Testing (RWGSR):  
• Eliminate the internal temperature gradient to improve reactor performance over previous testing and increase resistance to fouling

Steel Bead Kinetic Analysis (CFR):  
• Characterize reactions over steel beads to support sizing calculations for next generation reactor design

CFR Modification (CFR):  
• Improve fluid flow distribution and catalyst flow within the reactor to maximize carbon formation  
• Prepare for future CFR testing
Materials and Methods

PCI RWGSr Testing

- Reactor pressure was varied between 3 psia, 5 psia, and 8 psia
- Catalyst bed internal outlet temperature was varied
- Reactant feed $H_2$ to CO molar ratio was varied between 1:1, 2:1, and 3:1
- Internal catalyst bed outlet temperature (TC221 and TC214) was compared with internal inlet temperature (TC210) to determine the temperature gradient
- Reactor was tested with two heater modification configurations

Figure 4. Location of Thermocouples of interest.

Figure 5. PCI RWGSr in Heater Configuration #2.
Results and Discussion
PCI RWGSr Testing (Internal Temperature Gradient)

- In heater configuration #2 the temperature gradient was reduced to approximately 0 °C to 75 °C in completed testing.

Figure 10. Temperature Gradient Before Modification.
Figure 11. Temperature Gradient in Heater Configuration #1.
Figure 12. Temperature Gradient in Heater Configuration #2.
Results and Discussion

PCI RWGSr Testing (Reactor Performance)

• CO₂ conversion was compared with thermodynamic equilibrium

• Overall, reactor performance was acceptable before and after modification as conversion was near thermodynamic equilibrium

Figure 13. CO₂ Conversion Compared to Thermodynamic Equilibrium.
Conclusions

• The PCI RWGSr internal temperature gradient was essentially eliminated in the modified reactor in heater configuration #2

Future Work

• A carbon formation test will be performed on the PCI RWGSr
Materials and Methods

Steel Bead Kinetic Analysis

- Boudouard and CO Hydrogenation reactions were characterized over an Amasteel S-660 steel bead catalyst using the Carbon Dioxide Reduction Catalyst Test Stand (COR-CaTS)
- Temperature was varied, while pressure remained constant
- 60g of steel beads were pre-treated and packed in a quartz tube
- Prior to testing, a 50 mol% H₂/50 mol% N₂ mixture was flown through the reactor to reduce the catalyst
- For CO Hydrogenation testing the reactant feed was composed of H₂ and CO
- For Boudouard testing the reactant feed contained only CO
- Flow was maintained until outlet flow composition reached steady state

Figure 2. Amasteel S-660 Steel Beads.

Figure 3. COR-CaTS Assembly.
Results and Discussion

Steel Bead Kinetic Analysis (CO Hydrogenation)

- There are two proposed rate expressions\(^4\)
  
  **Model 1:** \( r \downarrow c = k \downarrow 7 \ P \uparrow \alpha \downarrow CO \ P \uparrow \beta \downarrow H \downarrow 2 \)
  
  **Model 2:** \( r \downarrow c = k \downarrow 8 \ (P \downarrow CO \ P \downarrow H \downarrow 2 \ ) \uparrow h \)

  Where \( k \downarrow x = Ae \uparrow -E \downarrow x /RT \)

- “h” closely matches the values reported by Manning (0.42±0.10) and Everett (0.50) over steel wool catalysts\(^7,5\)
- Activation energies are lower than the 70 kJ/mol reported by Manning over a steel wool.

### Table 3. Calculated Rate Constants.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>1.17</td>
</tr>
<tr>
<td>( \beta )</td>
<td>0.55</td>
</tr>
<tr>
<td>( h )</td>
<td>0.55</td>
</tr>
<tr>
<td>( E_7 )</td>
<td>48.34 kJ/mol</td>
</tr>
<tr>
<td>( E_8 )</td>
<td>35.92 kJ/mol</td>
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</tbody>
</table>

**Figure 8.** Predicted Reaction Rate Versus Experimental Reaction Rate for the CO Hydrogenation Reaction over Steel Beads Using Models 1 and 2.
Results and Discussion

Steel Bead Kinetic Analysis (Boudouard Reaction)

- Three proposed reaction mechanisms, although two result in the same rate expression
  - Model A: $r \downarrow c = kP \downarrow CO / (1 + K \downarrow A \ P \downarrow CO)^\frac{1}{2}$
  - Model B: $r \downarrow c = kP^2 \downarrow CO / (1 + K \downarrow A \ P \downarrow CO)^\frac{1}{2}$

<table>
<thead>
<tr>
<th>Energy of Activation</th>
<th>Model A</th>
<th>127.77 kJ/mol</th>
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<tbody>
<tr>
<td>Model B</td>
<td>228.57 kJ/mol</td>
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Table 4. Calculated Activation Energies.

Figure 9. Predicted Reaction Rate Versus Experimental.
Conclusions

• Since both CO Hydrogenation and Boudouard reactions occur simultaneously, a better model would be a hybrid of the two

Future Work

• Rate constants will be incorporated into future CFR design
Materials and Methods

CFR Modification and Assembly

- It was reported that uniform flow within a radial flow reactor is achieved when the ratio of the cross-sectional area of the inner to outer flow channels is one\(^6\)
- Both the BCFR and CCFR were fitted with an outer annulus casing
- BCFR was packed with pre-treated Amasteel S-660 steel beads assembled and reintegrated into the BCFR test stand
- Both CCFR assembly and CCFR test stand build-up was initiated, but not completed due to time constraints
Results and Discussion

CFR Modification and Assembly

- BCFR modification, assembly, and integration was competed
- CCFR modification was complete, but assembly was not
- CCFR test stand build-up was also not completed
Conclusions

• The BCFR is now ready for future testing
• CCFR modification was completed, but assembly was not
• Significant progress was made on CCFR test stand build-up, although it was not completed

Future Work

• BCFR will be tested to determine if the modification were successful in improving reactor performance
• CCFR will continue to be assembled and integrated into the test stand for future testing
Acknowledgments

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References


