Evaluation of Life Support Candidate Technology for 100% Oxygen Recovery

Connor Thompson – Western Oregon University
Mentor: Dr. Morgan B. Abney – Marshall Space Flight Center – ES62
Co-Mentors: Bill Barnet and Chris Stanley – Marshall Space Flight Center – ES62

Introduction

Table 1. The Sabatier reaction.

Sabatier Reaction
$CO_2 + 4H_2 \Leftrightarrow CH_4 + 2H_2O$

- Current life support onboard the International Space Station (ISS) utilizes a Sabatier based oxygen recovery system which results in approximately 50% O_2 recovery from CO_2
- Resulting water is stored for future use and CH_4 is vented out of the vessel, resulting in a net loss of hydrogen needed to react with CO_2
- The Bosch process is of interest as there is the potential for zero net H_2 loss and therefore 100% O_2 recovery

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.

Step 1 (RWGSr):	<u>RWGS</u> $CO_2 + H_2 \leftrightarrow CO + H_2O$
Step 2 (CFR):	<u>Boudouard</u> $2CO \leftrightarrow C_{(s)} + CO_2$
	<u>CO Hydrogenation</u> $CO + H_2 \leftrightarrow C_{(s)} + H_2O$
<u>Overall Bosch Process:</u>	$CO_2 + H_2 \leftrightarrow C_{(s)} + 2H_2O$

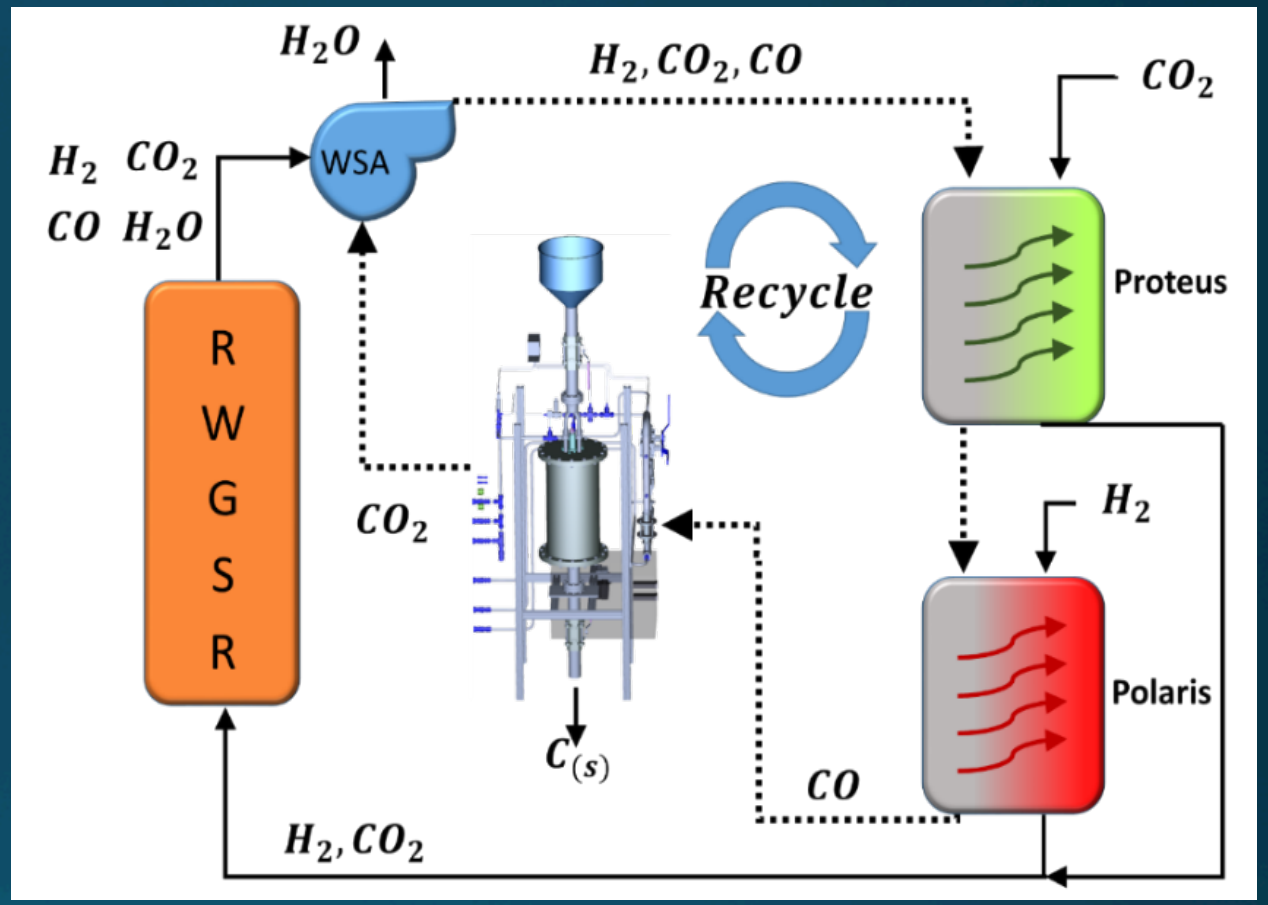

Figure 1. S-Bosch Flow Diagram.

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

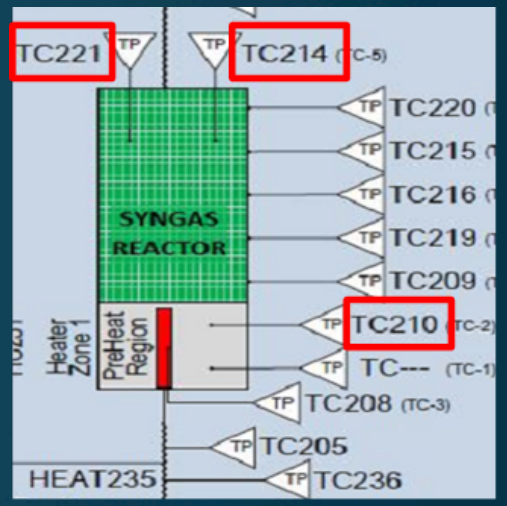

Figure 4. Location of Thermocouples of interest.

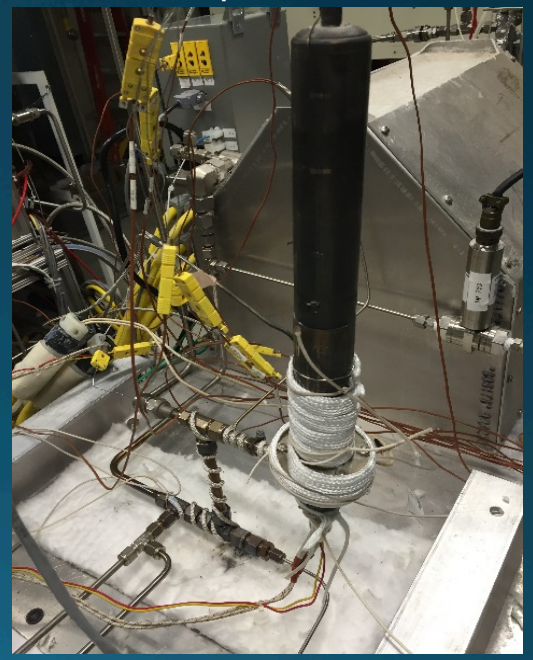

Figure 5. PCI RWGSr in Heater Configuration #2.

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

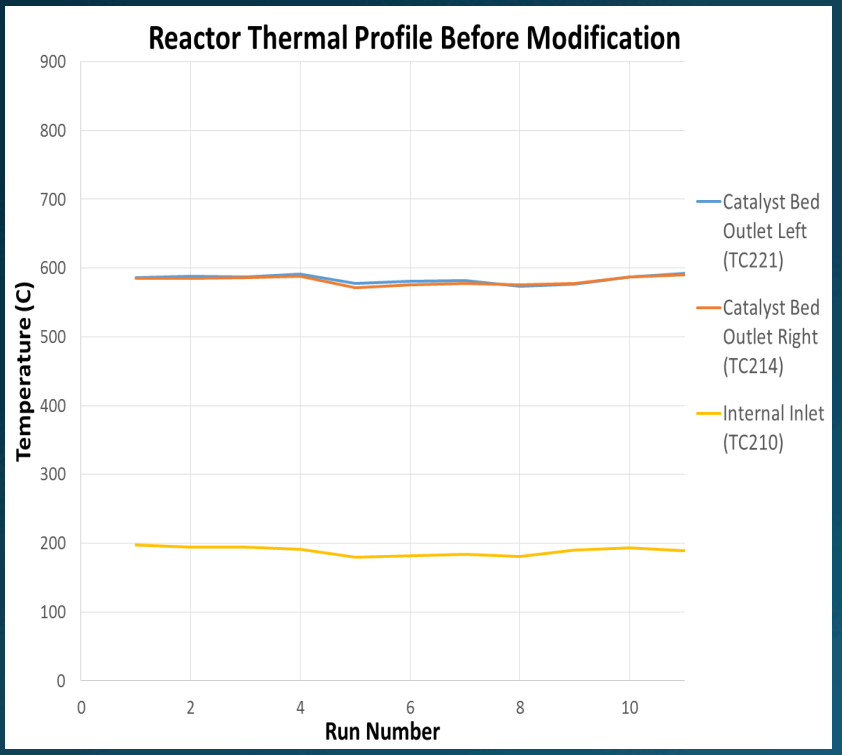

Figure 10. Temperature Gradient Before Modification.

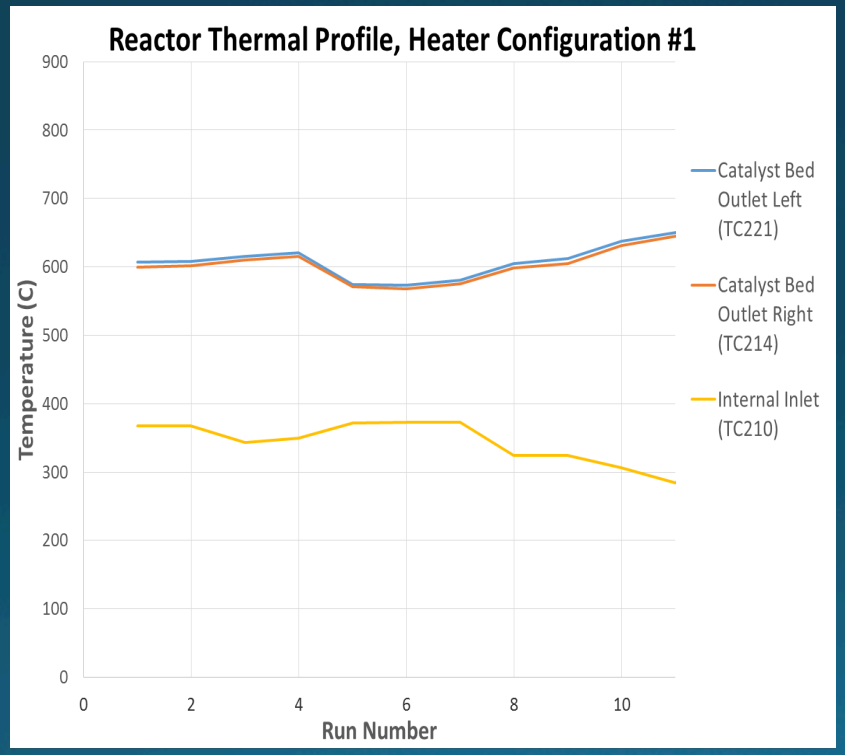

Figure 11. Temperature Gradient in Heater Configuration #1.

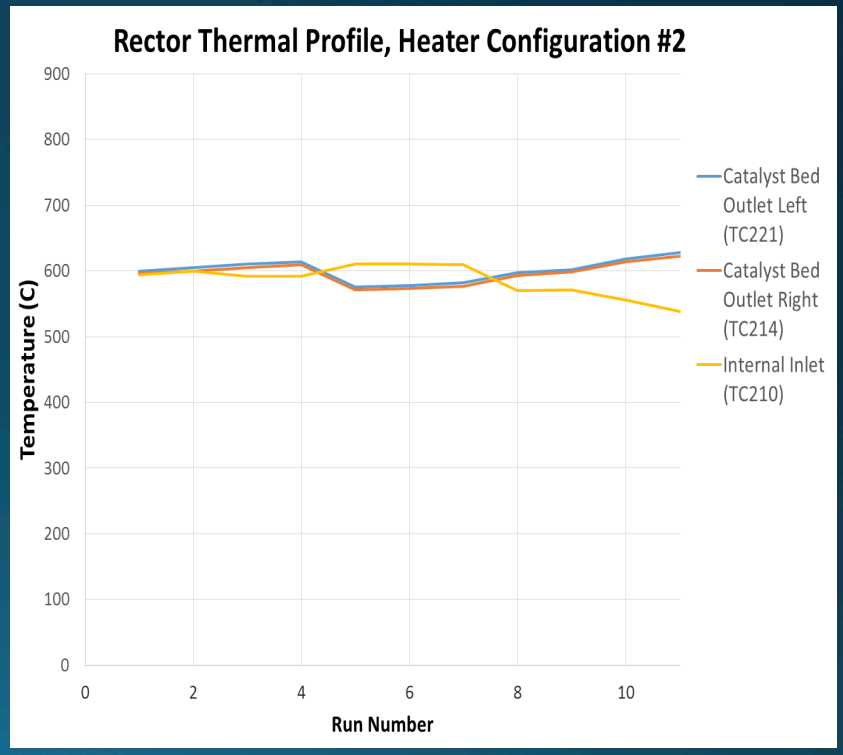

Figure 12. Temperature Gradient in Heater Configuration #2.

Results and Discussion

PCI RWGSr Testing (Reactor Performance)

- CO_2 conversion was compared with thermodynamic equilibrium
- Overall, reactor performance was acceptable before and after modification as conversion was near thermodynamic equilibrium

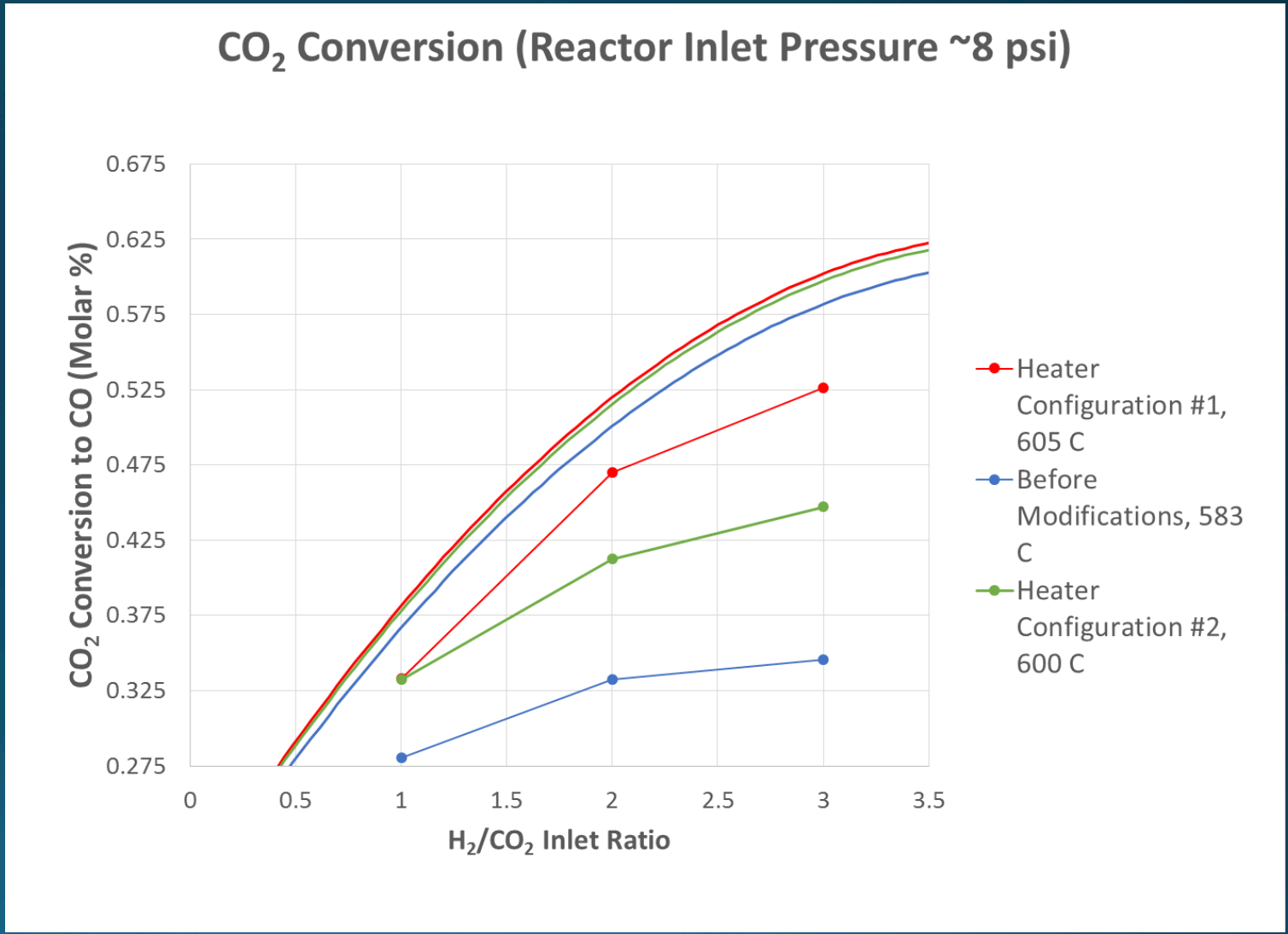

Figure 13. CO_2 Conversion Compared to Thermodynamic Equilibrium.

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% H_2/50 mol% N_2 mixture was flown through the reactor to reduce the catalyst
- For CO Hydrogenation testing the reactant feed was composed of H_2 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: $r_c = k_7 P_\alpha^{CO} P_\beta^{H_2}$

Model 2: $r_c = k_8 (P_{CO} P_{H_2})^h$

Where $k_x = Ae^{-E_x/RT}$

- "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 steel wool

Calculated Hydrogenation Constants	
α	1.17
β	0.55
h	0.55
E_7	48.34 kJ/mol
E_8	35.92 kJ/mol

Table 3. Calculated Rate Constants.

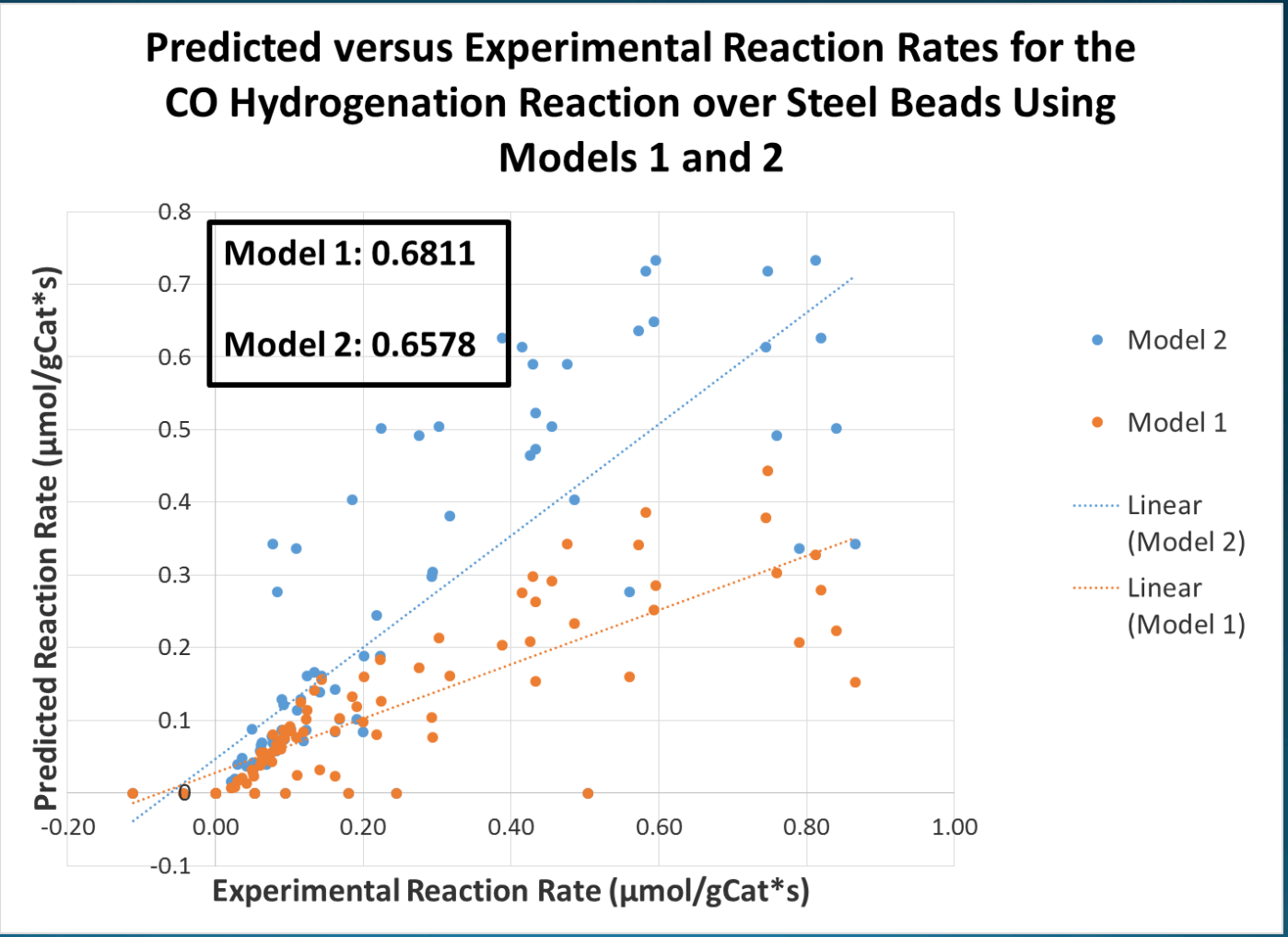

Figure 8. Predicted Reaction Rate Versus Experimental.

Results and Discussion

Steel Bead Kinetic Analysis (Boudouard Reaction)

- Three proposed reaction mechanisms, although two result in the same rate expression

Model A: $r_c = kP_{CO} / (1 + K_A P_{CO})^2$

Model B: $r_c = kP^2_{CO} / (1 + K_A P_{CO})^2$

Table 4. Calculated Activation Energies.

Energy of Activation	
Model A:	127.77 kJ/mol
Model B:	228.57 kJ/mol

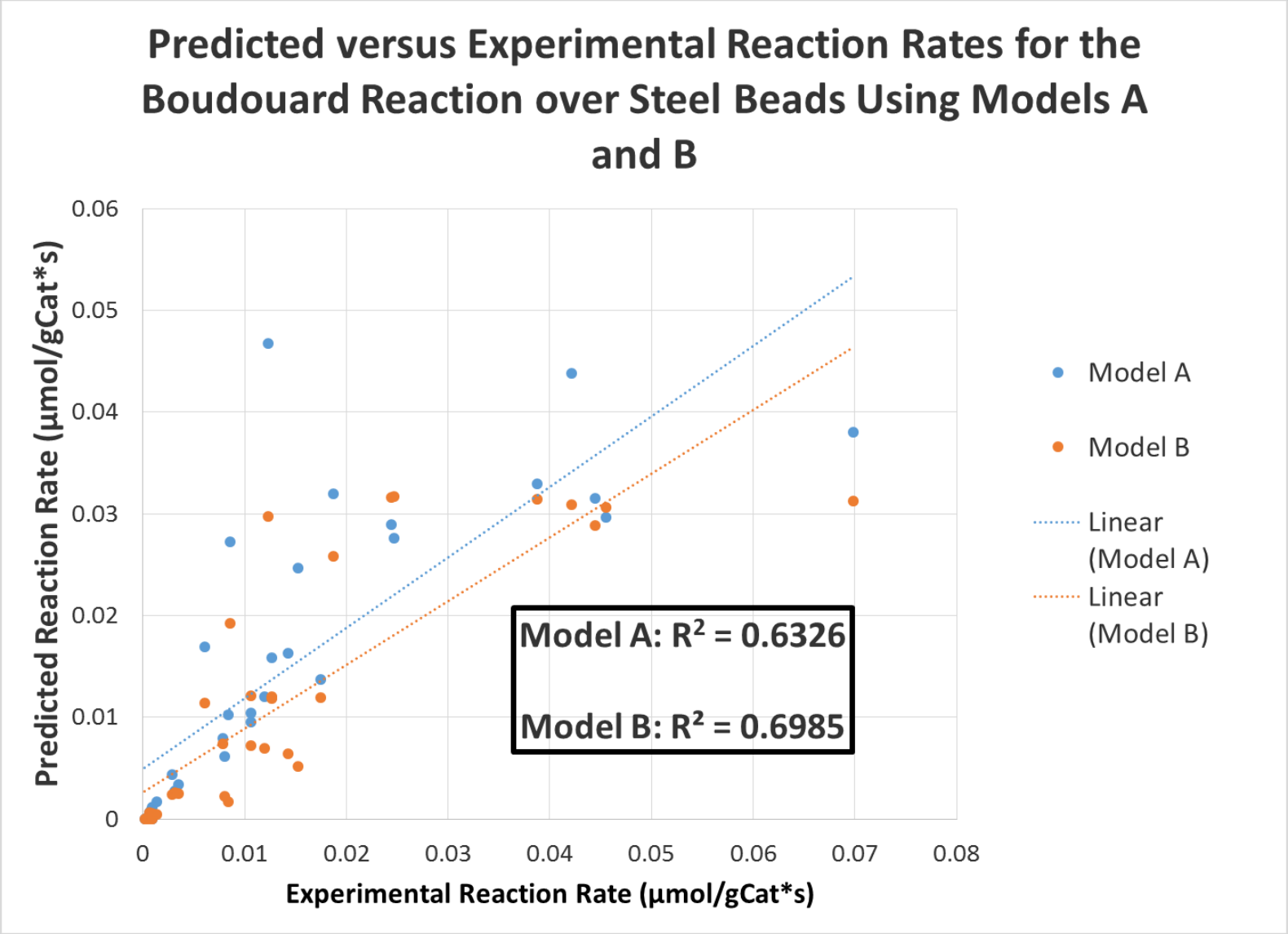

Figure 9. Predicted Reaction Rate Versus Experimental.

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 a 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

Figure 6. Outer Annulus Casing.

Figure 7. CCFR Test Stand Design.

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

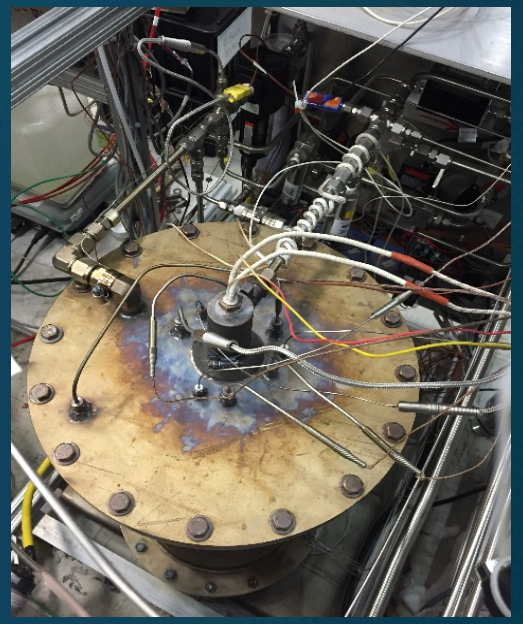

Figure 14. BCFR Integrated into the Test Stand.

Figure 15. Current CCFR Status.

Figure 16. CCFR Test Stand Progress.

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

[1]Abney, M. B., Kent, R. A., Mansell, J. M., "Operation Conditions and Reactor Robustness for Advanced Oxygen Recovery using Bosch Technology", NASA Marshall Space Flight Center, Huntsville, AL, 2015.

[2]Abney, M. B., Mansell, J. M., DuMez, S., Thomas, J., Cooper, C., and Long, D. "Ongoing Development of a Series Bosch Reactor System," NASA Marshall Space Flight Center, Huntsville, AL, 2013.

[3]Abney, M. B., Mansell, J. M., Rabenberg, E., Stanley, C. M., Edmunson, J., Alleman, J. E., and Chen, K. "Series-Bosch Technology for Oxygen Recovery During Lunar or Martian Surface Missions," International Conference on Environmental Systems. Tucson, Arizona, 2014.

[4]Abney, M. B., Mansell, J. M., "The Bosch Process – Performance of a Developmental Reactor and Experimental Evaluation of Alternative Catalysts", American Institute of Aeronautics and Astronautics, NASA Marshall Space Flight Center, Huntsville, AL, 2010.

[5]Everett, M.R., "The Kinetics of Carbon Deposition Reactions in High-Temperature Gas-Cooled Reactors," D.P.Report 500, Atomic Energy Establishment, Winfrith, 1967.

[6]Kareeri, A. A., Zughbi, H. D., Al-Ali, H. H., "Simulation of Flow Distribution in Radial Flow Reactors", Industrial & Engineering Chemistry Research, Department of Chemical Engineering, King Fahd University of Petroleum & Minerals, Dhahram, Saudi Ariabia, 2006.

[7]Manning, M.P., "An Investigation of the Bosch Process," Massachusetts Institute of Technology Dissertation, 1976.