DOE Hydrogen Program

2022 Annual Merit Review and Peer Evaluation Meeting

Decarbonizing Natural Gas

PI: Prof. Eric McFarland

Binary Chloride Salts as Catalysts for Methane to Hydrogen and Graphitic Powder

DE-EE0008845 AMR#P182

C ZERO

This presentation does not contain any proprietary, confidential, or otherwise restricted information

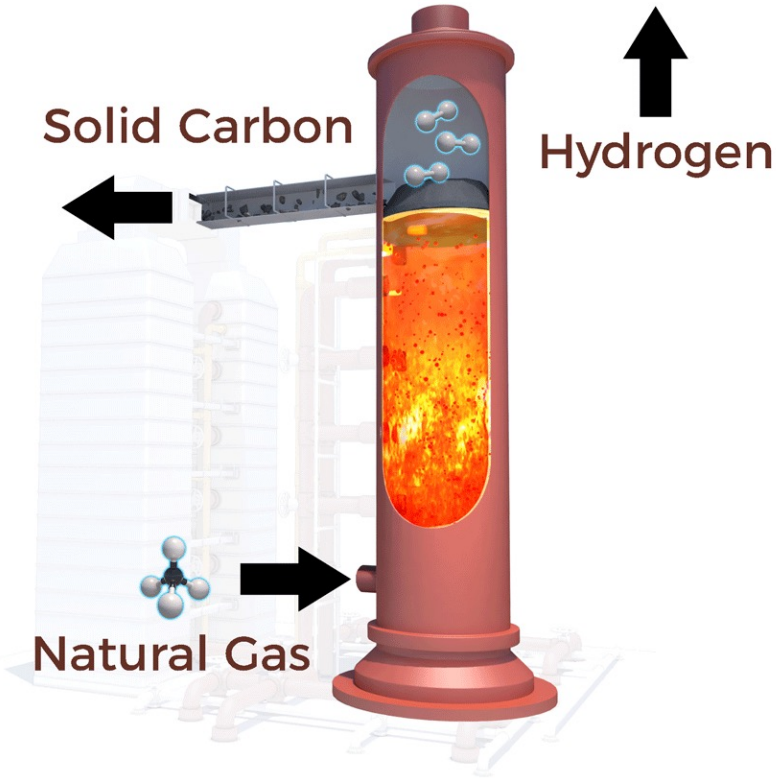
Project Goal & Approach

Idea

Key Challenges

- Carbon Removal
- Carbon Valorization
- Control Carbon
- Reactor Design
- Heat Integration
- Product Gas Cleanup

Goal



Project Goal: Develop scalable methane pyrolysis process that produces cheap low-emission hydrogen from natural gas

Overview

Demonstration of stable, active, melt system:

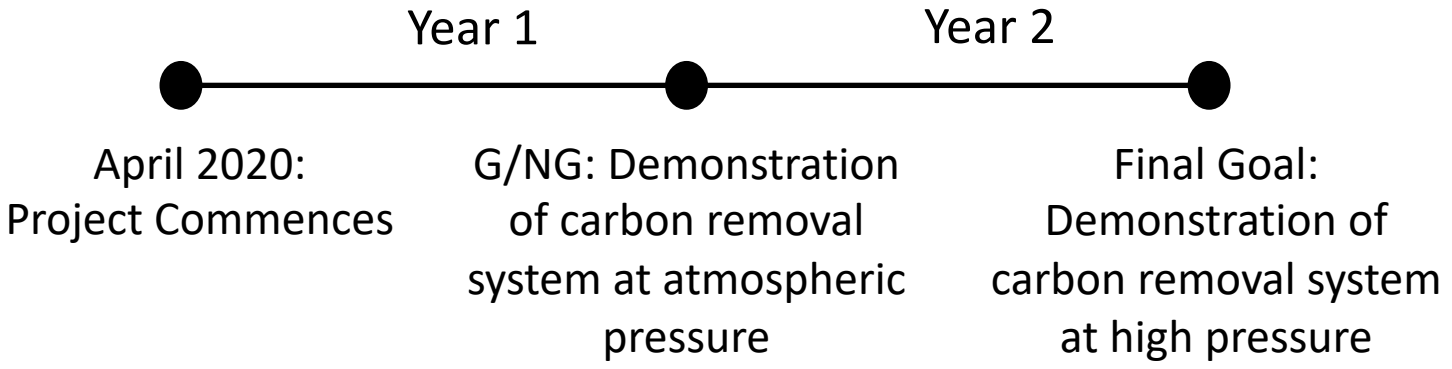
- ≥ 90% H_2 selectivity
- Graphitic carbon product that has properties favorable for battery anodes and additives

Design and construct a carbon removal system capable of:

- High Temperature (1000 C)
- Continuous carbon removal (≥ 24 hours)
- High Pressure (≥ 10 bar)

- Total Project Budget: $1.25MM
  - Total DOE Share: $999,878
  - Total Cost Share: $252,000
  - Total DOE Funds Spent*: $625,023
  - Total Cost Share Funds Spent*: $193,297

* As of 01/31/2022



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Company & Collaborators

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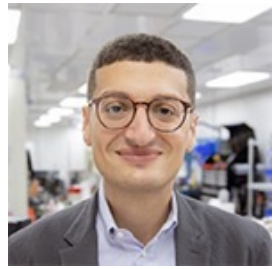

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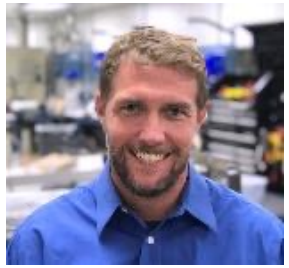

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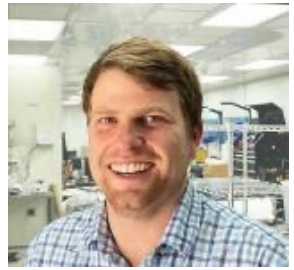

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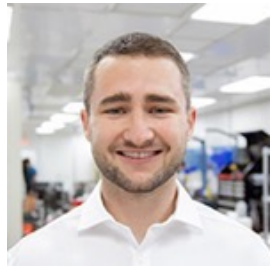
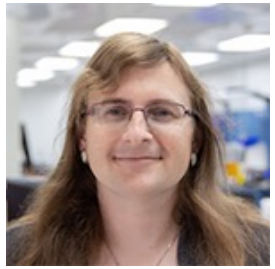


Henry Moise
Engineer



Ashley Carmichael
Lab & HSE Manager

Collaborators

Prof. Mike Gordon
UCSB

Prof. Raphaele Clement
UCSB

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Potential Impact

Project Goal: Demonstrate scalable methane pyrolysis process capable of carbon removal and valorization

Project Targets:

- Demonstration of stable, active, melt systems
- Design and construct a carbon removal system

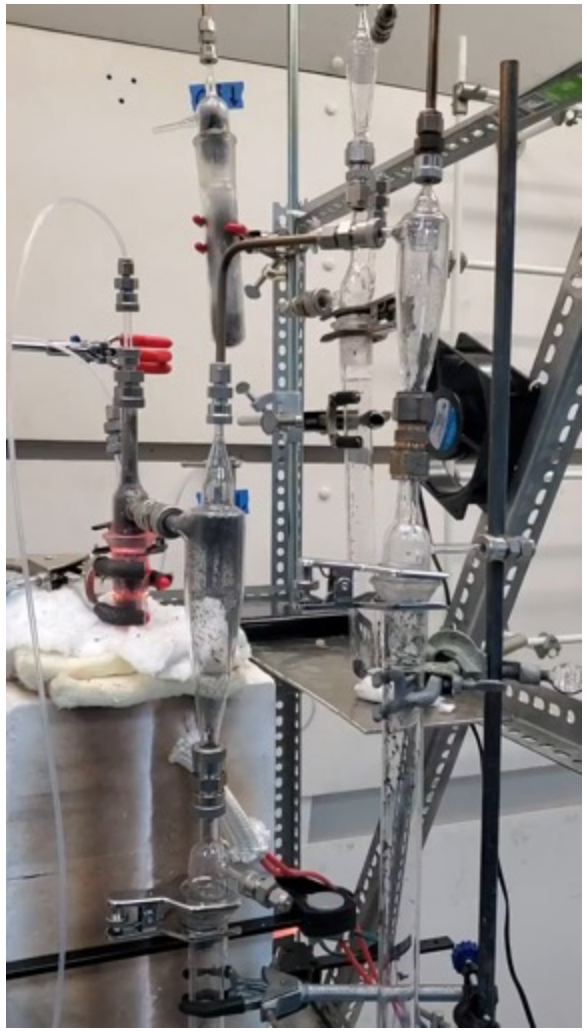
DOE Goal: Low-CO_2 emission Hydrogen <2 $/gge

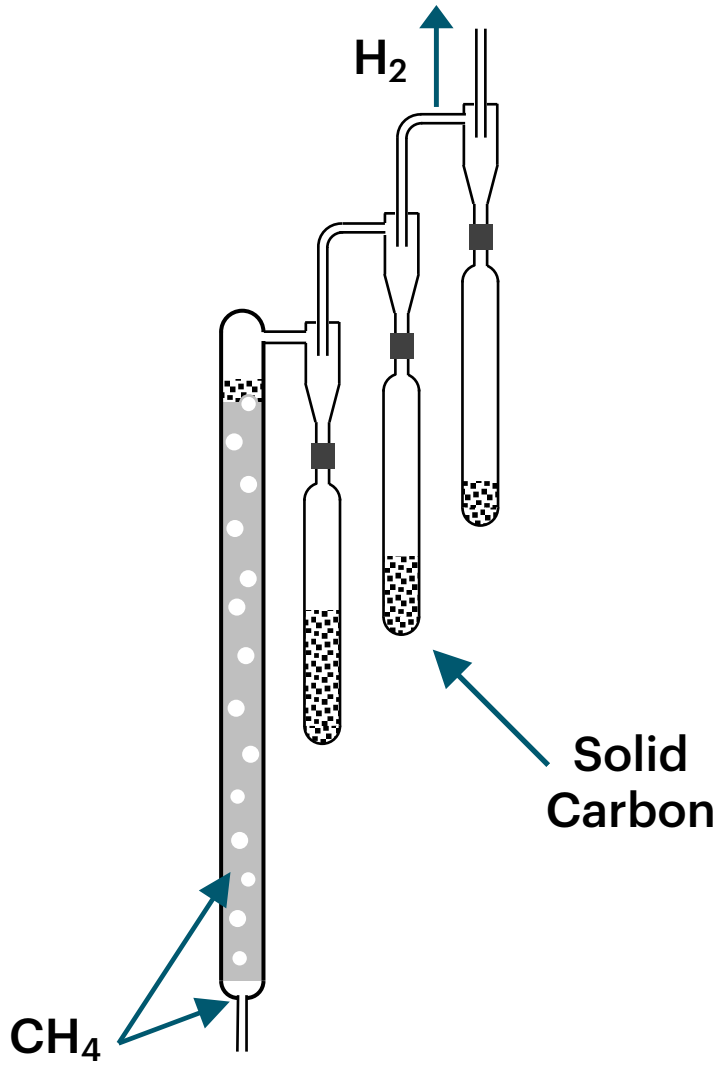
Potential Impact

- 75+% reduction in CO_2 emission from hydrogen production from natural gas
- Ability to do ‘carbon sequestration’ in locations that are not amenable to CO_2 sequestration
- Provide employees with expertise in the oil & gas space opportunities to work on clean energy technologies

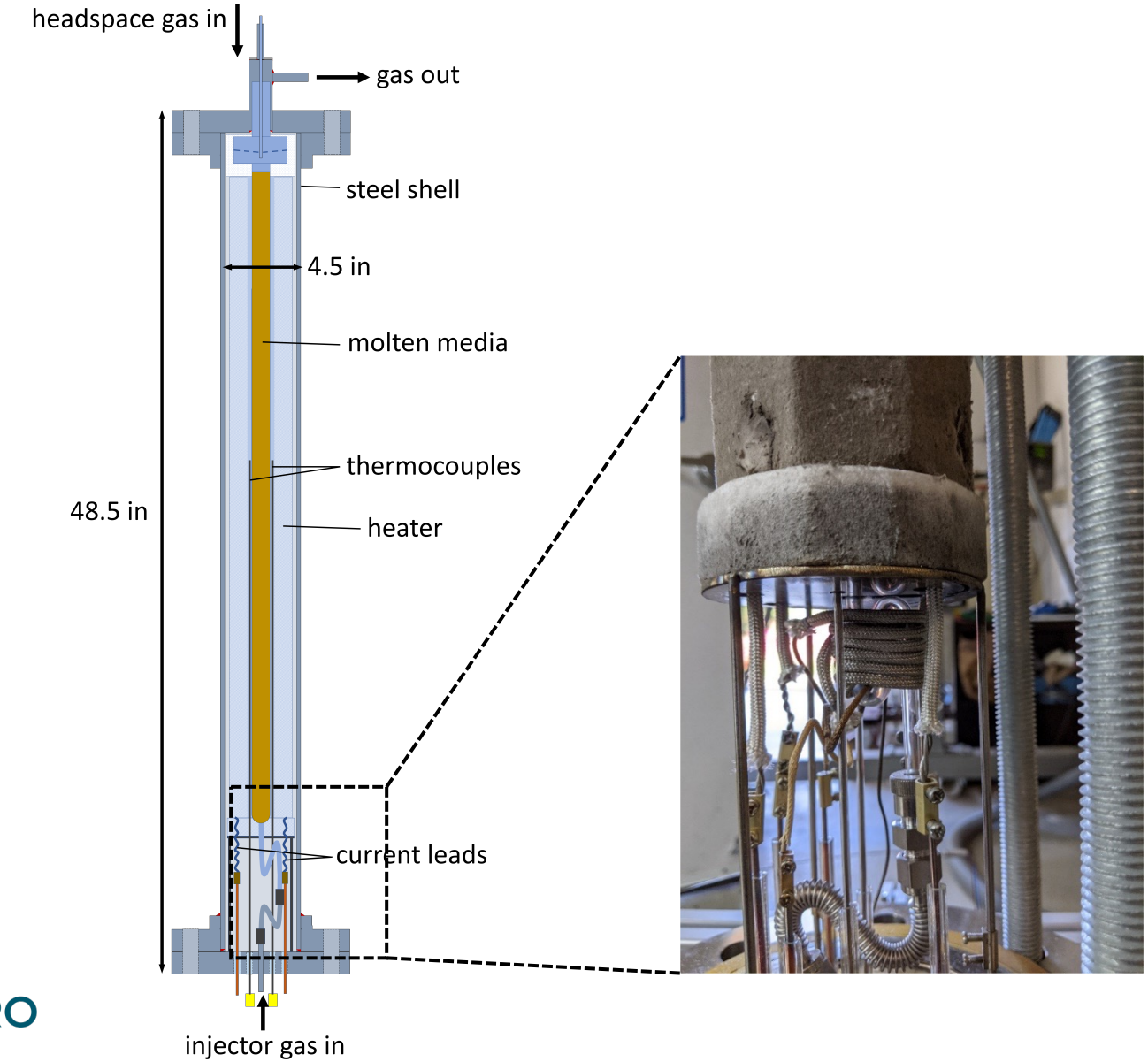
Task 2: Continuous Carbon Fluidization

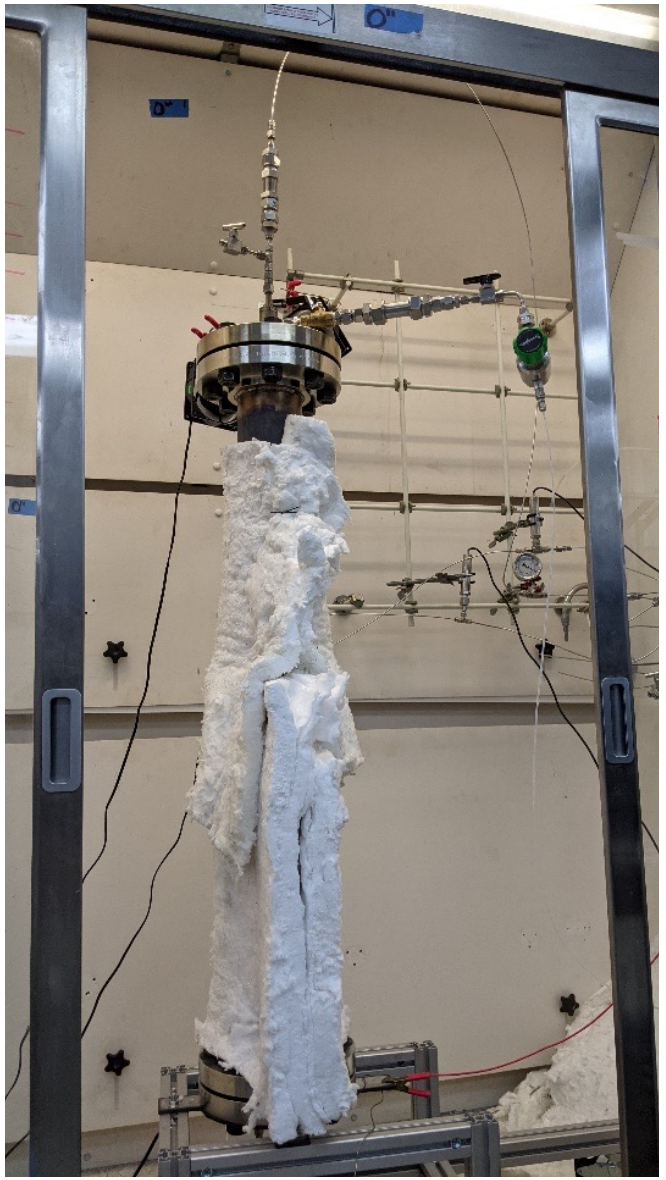
- Demonstrated continuous carbon removal from methane pyrolysis via fluidization (>24 hrs)
- 3-phase disengagement zone designed for minimal liquid carryover
- Carbon separation conducted via conventional gas/solid separation methods (cyclones in series)





Task 3: High Pressure Reactor Demonstration

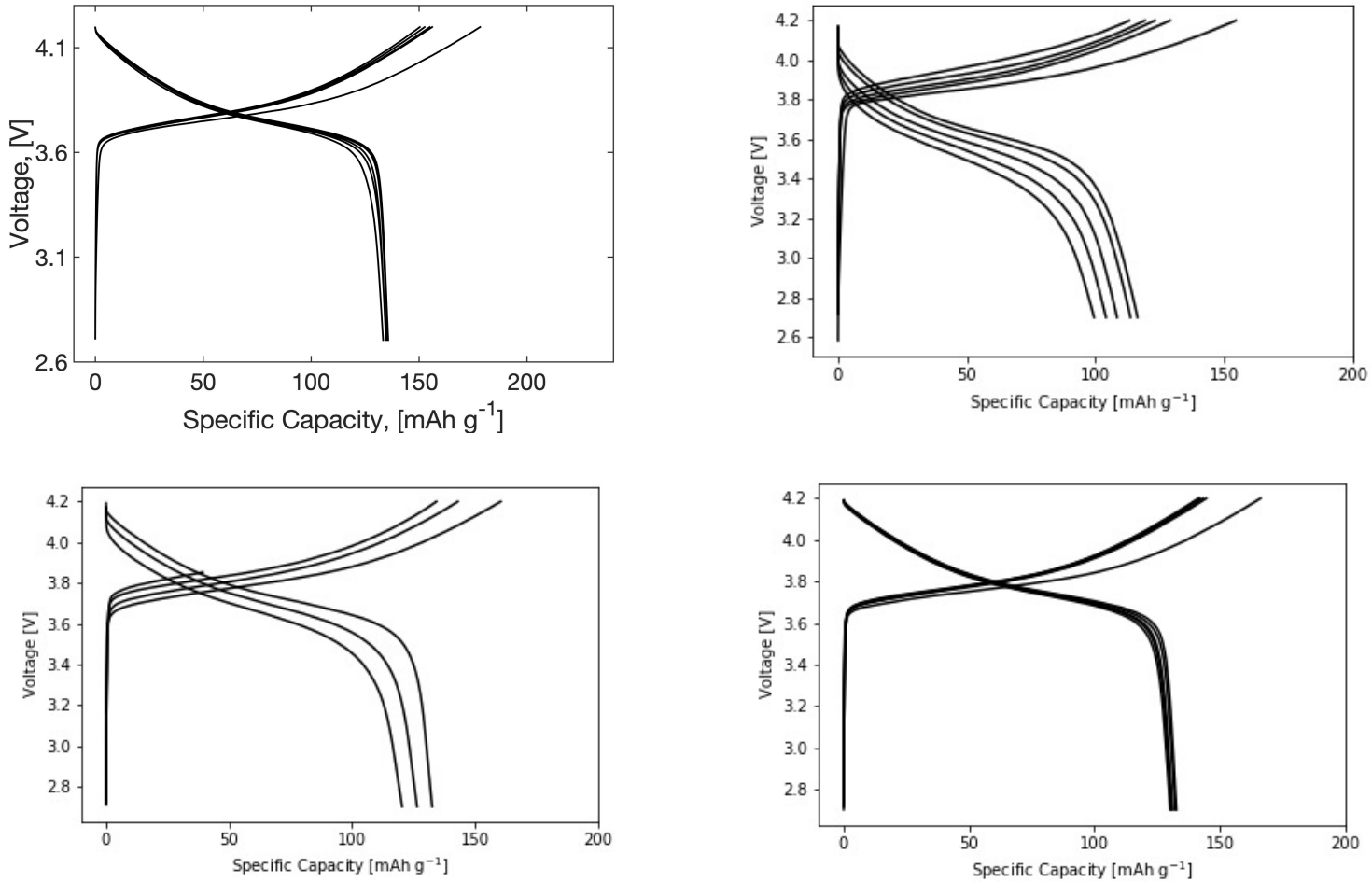




Task 3: High Pressure Reactor Demonstration

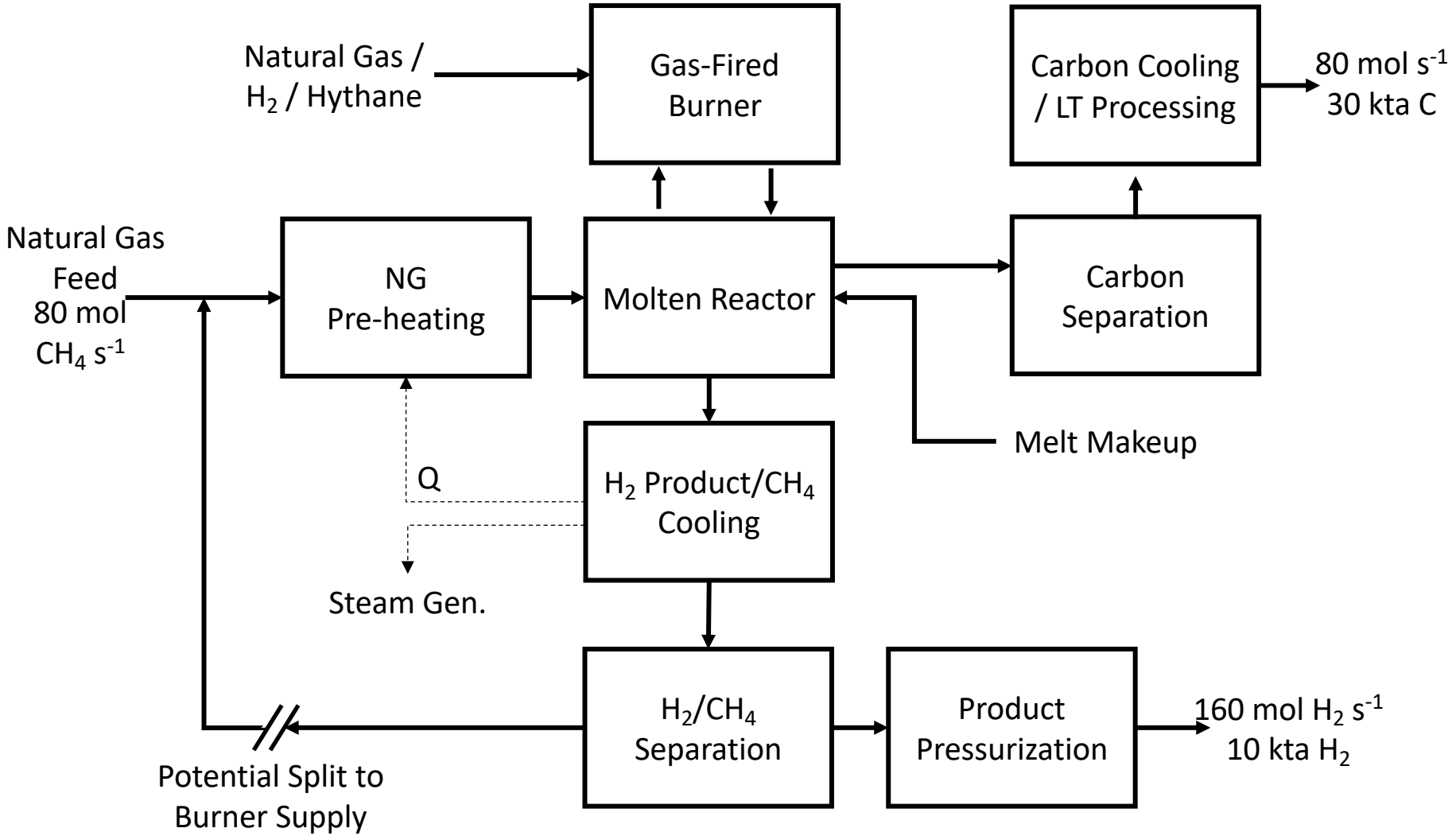
- High pressure (up to 20 bar) methane pyrolysis demonstrated with continuous carbon removal using internally heated reactors
- Stainless steel cyclones fabricated via additive manufacturing
- System successfully operated continuously for >6 hrs

Task 4: Electrochemistry Data for the Carbon



Voltage profiles for the first few charge-discharge cycles obtained on carbon-coated NMC111 at C/20 and over a voltage window from 2.7 V to 4.2V vs. Li/Li$^+$ in Li-ion half cells. All 4 carbon samples came from methane pyrolysis but with different post treatments

Task 5: Flow-Sheet – 10 KTA H_2



Responses to Previous Year's Reviewer Comments

AMR 2021 Comment	Response
Future work could include thermal integration pilot system design, including pressure swing adsorption tail gas heat recovery, resolution of potential coking issues, assessment of potential toxic waste production, salt recovery and purification for reuse, and characterization of produced gas content based on various feedstock assumptions. Additionally, the team should also consider how to achieve uniform pressure, temperature, bubble size, and space velocity to produce carbon with a more consistent, precise, and higher- value morphology.	While outside the scope of this project, C-Zero has been looking into many of these points including thermal integration, pilot system design, and achieving uniform pressures, temp, bubble size etc.
Considering the relatively short funding period, the project needs to focus on narrower and more achievable tasks to advance the key concepts. The project could choose to address potential scale-up challenges, including the reactor system, solids separation, catalyst recirculation, and product gas purification. The project should also clearly demonstrate the energy and greenhouse gas reduction benefits of its process against conventional SMR.	We have spent much of the past year focused on demonstrating continuous carbon removal from our system in both at atmospheric and pressurized system.
Based on the energy analysis, it seems that more of the effort should go toward solving the carbon separation step (Tasks 2/3). Optimization of the salt composition (Task 1) and assessing the carbon as a cathode material (Task 4) can come later.	See response above
The team should look further at the materials and corrosion aspects of the design. Several pathways (hydrogen embrittlement, halide-induced corrosion, carbon deposition, etc.) might severely limit the scale- up and increase the probability of unsafe conditions.	Materials and corrosion are critically important for this process and something that is being looked at extensively in this project

Proposed future work

- Task 1: Investigation of catalytic melt activity for the synthesis of carbon products
  - Measure in-situ methyl radical generation and dominant gas phase reaction intermediates. Demonstrate the nucleation and growth kinetics of solid carbon products.
- Task 2/3: Fabrication of high pressure carbon removal system
  - Finalize demonstration of carbon removal system capable of operation at 1000 C and 10 bar for > 24 hours
- Task 4: Analysis of carbon for battery and additives usage
  - Finalize testing carbon produced for battery anode use
- Task 5: Technoeconomic Analysis (TEA), Process Modelling, and Customer Discovery
  - Submit updated and refined Aspen model as process goes on with the goal of a process showing < 2 $/gge hydrogen production and carbon production cost < 1 $/kg

Summary

- **Task 2: Constructed and demonstrated carbon removal for methane pyrolysis via fluidization**
  - Significantly simpler than mechanical carbon removal and demonstrated at relevant pressure and temperature
- **Task 3: Fabrication of High Pressure Continuous Carbon Removal System**
  - Demonstrated methane pyrolysis and continuous carbon removal at >10 bar
- **Task 4: Analyzed several different carbons produced via methane pyrolysis for use as li-ion battery anodes**
  - Significant differences in activity observed depending on carbon post processing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Thank You!
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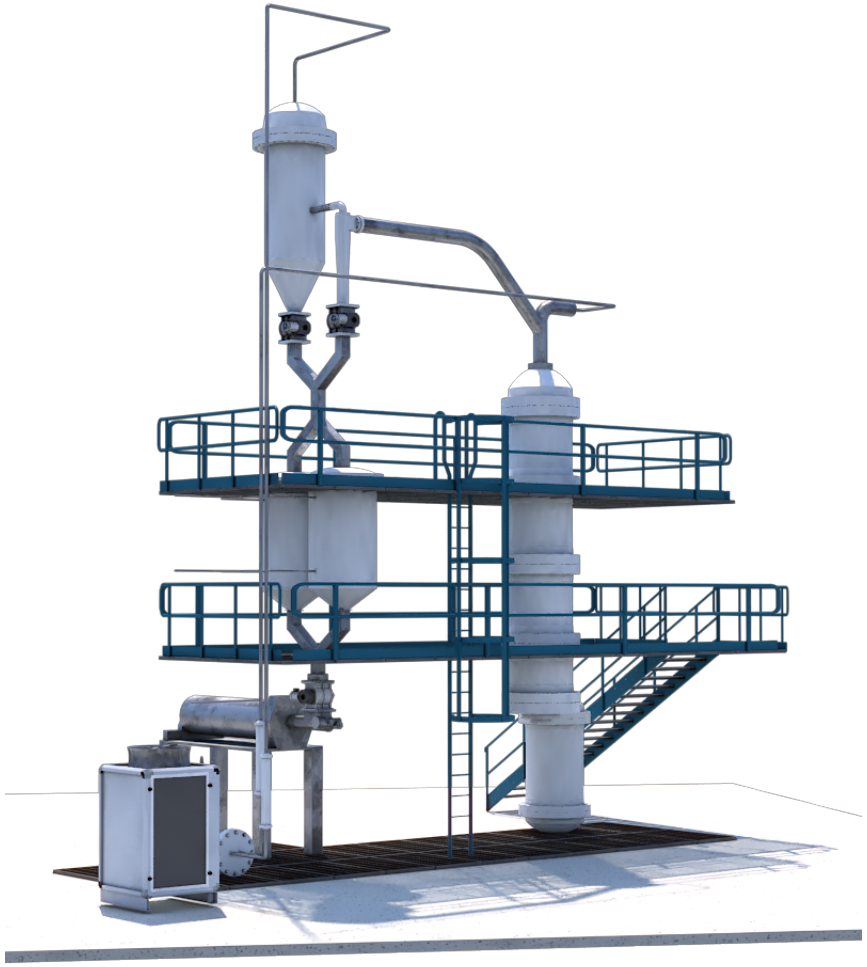
Technology Transfer Activities

- C-Zero is developing its first pilot plant with aims to operate by the end of the year
- EPC arm of C-Zero's largest investor, SK, interested in constructing and deploying C-Zero commercial units once the process has been sufficiently de-risked
- C-Zero has signed LOIs with utilities with >100 GW of natural gas electrical generation capacity
  - This would translate to >30 million tons of H_2 or ~3x current US H_2 production
- Patent 'Carbon separation and removal from molten media' published



Special Recognitions and Awards

- C-Zero awarded Early Stage Company of the Year in the 2022 Global Cleantech 100
- C-Zero was chosen as one of C&EN's 2021 10 Start-Ups to Watch