Determining the Value Proposition of Materials-based Hydrogen Storage for Stationary Bulk Storage of Hydrogen

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Project ID: ST288

Project Goals

- Evaluate the capability and design of materials-based stationary bulk hydrogen storage for backup power applications (starting with fuel cell powered data centers)
- Leverage technoeconomic models developed by NREL to understand the value proposition of hydrogen and fuel cells for data centers to determine a priority list of reversible materials
- Develop a detailed model to identify validate the suitability of a metal hydride-based storage system and identify parameters and designs that yield the most significant improvements in performance

Overview

Timeline and Budget

FY20 DOE Lab Call Project:

- Project Start Date: 10/01/2020
- FY20 DOE Funding (if applicable): $0
- FY21 Planned DOE Funding (if applicable): $500K ($300K SRNL/$200K NREL)
- Total DOE Funds Received to Date**: $500K** Since the project started

Barriers

- Barriers addressed
  - TEA analysis for cost challenges
  - Heat source availability and system size
  - Ability of system to supply H2 flowrate to power a 20MW data center for 72 hours at the required fuel cell pressure
  - Identify transient heat required rate for hydrogen discharge

Partners

- Project lead: Bruce Hardy, SRNL
- Co-PI: Mark Ruth, NREL
- Savannah River National Laboratory
- National Renewable Energy Laboratory

Relevance/Potential Impact

- Fuel cells are a potential means supplying for backup power (in renewable form) to a data center
- Although there have been demonstrations and case studies for materials-based bulk storage of H_2, none have reported the value-proposition from a techno-economic perspective
- The March 2019, the DOE HFTO workshop focused on understanding the R&D gaps and business case for fuel cell powered data centers
- Hydrogen storage was identified as an areas for advancement to increase acceptance of fuel cells for primary or back-up power sources for data centers
  - Although viable, compressed and liquid H_2 had shortcomings that could be cost-prohibitive for liquid or cryogenic H_2
  - Metal hydrides have features that have the potential for promising and competitive solutions

Approach

Hydrogen fuel cells & metal hydride storage to provide data center backup power

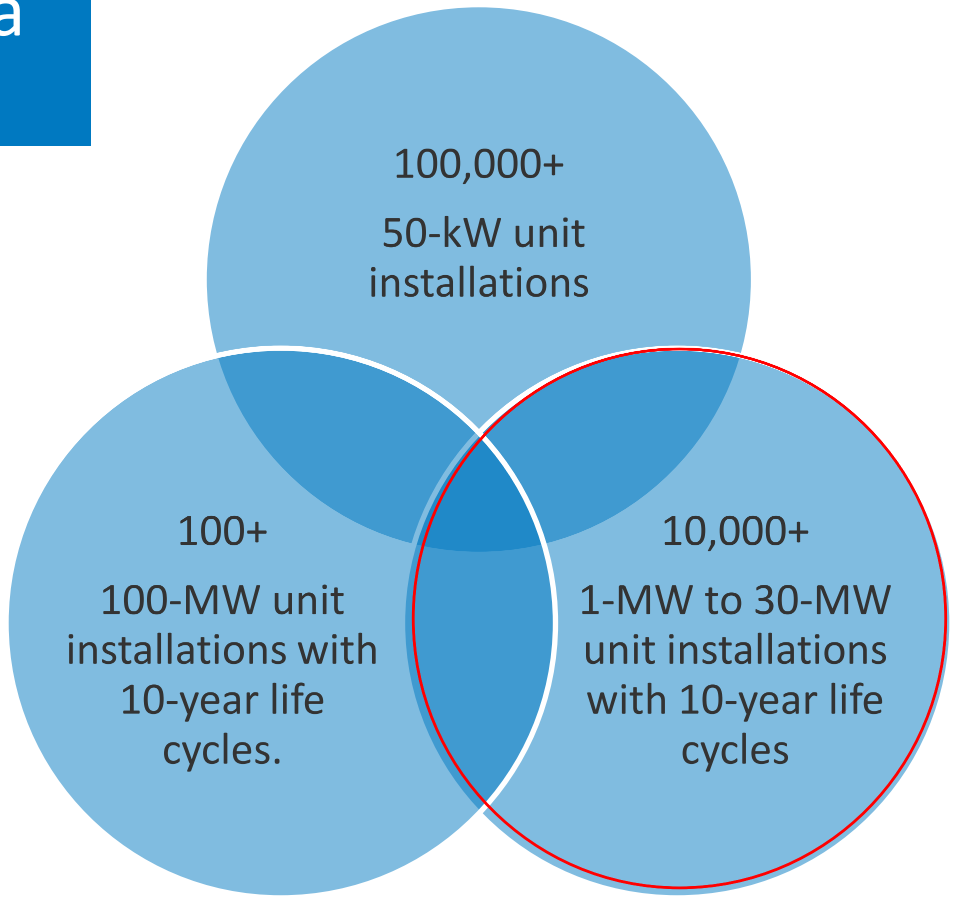
Why Backup Scenario?

- Diesel generators are becoming more difficult to permit
  - Air quality
  - Noise
- A fuel cell backup system
  - Least disruptive to current data center designs
  - Less hydrogen needed on annual basis (though individual events could still stress current merchant market)

Why 5 MW data center?

- 10,000+ data centers in this size range
- Will likely include backup systems (<1 MW may not)
- Corresponds to class (high-end) of data center that may value efficiency, clean power
- May include separated facilities with thermal integrations

Number of sites for size range



100,000+

50-kW unit installations

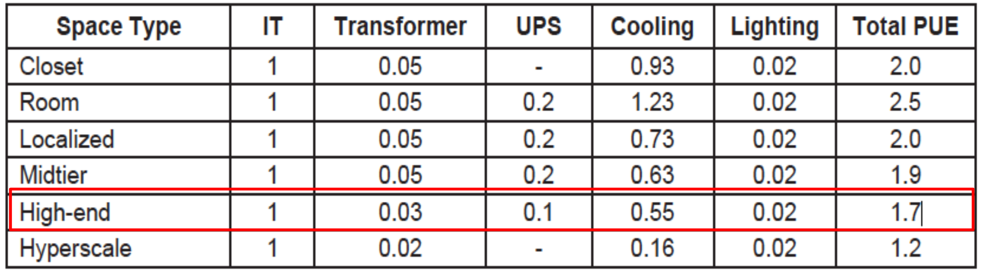
100+

100-MW unit installations with 10-year life cycles.

10,000+

1-MW to 30-MW unit installations with 10-year life cycles

Table 4. 2014 PUE by Space Type



Space Type	IT	Transformer	UPS	Cooling	Lighting	Total PUE
Closet	1	0.05	-	0.93	0.02	2.0
Room	1	0.05	0.2	1.23	0.02	2.5
Localized	1	0.05	0.2	0.73	0.02	2.0
Midtier	1	0.05	0.2	0.63	0.02	1.9
High-end	1	0.03	0.1	0.55	0.02	1.7
Hyperscale	1	0.02	-	0.16	0.02	1.2

Approach

Analysis includes techno-economic analysis, performance/integration, and space considerations

Techno-economic Analysis

- Initial capital cost comparison for comparing to installation cost of diesel generators (backup scenario)
- Levelized cost of energy (LCOE) analysis for better understanding of scenario impact

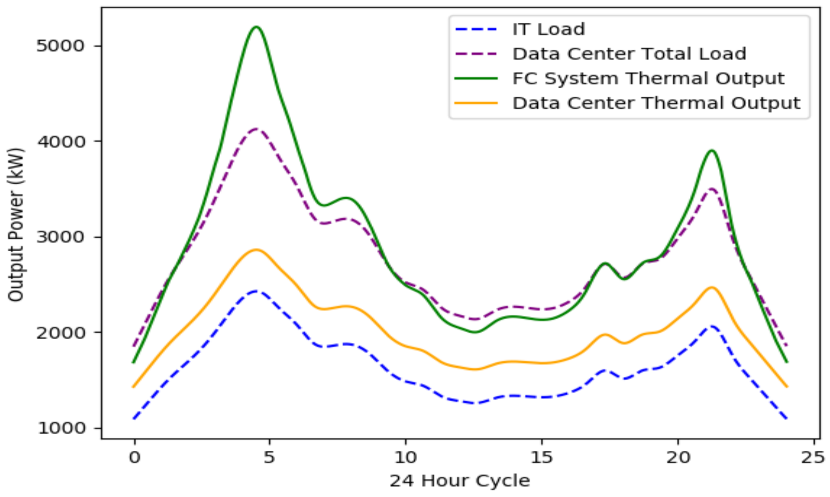
Performance/integration analysis

- Characteristics needed for system design
- Thermal options for integration with either fuel cell or data center as source of heat

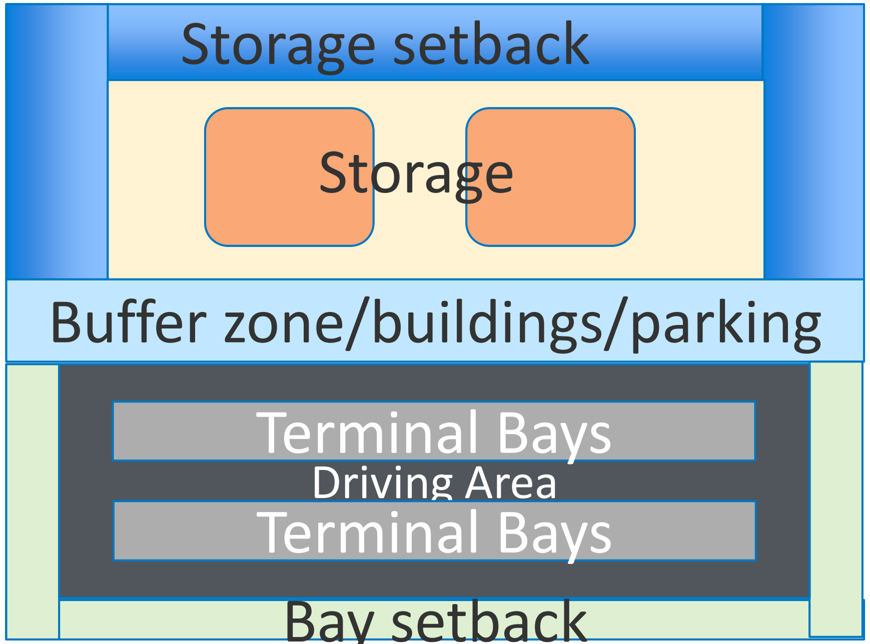
Space considerations

- Advantages of siting metal hydrides for stationary storage versus gaseous or liquid
- Five initial layouts that include delivered H_2, onsite H_2 production, and trailers versus stationary storage options

Data center load with thermal



Infrastructure layout – metal hydrides


Storage setback

Storage

Buffer zone/buildings/parking

Terminal Bays

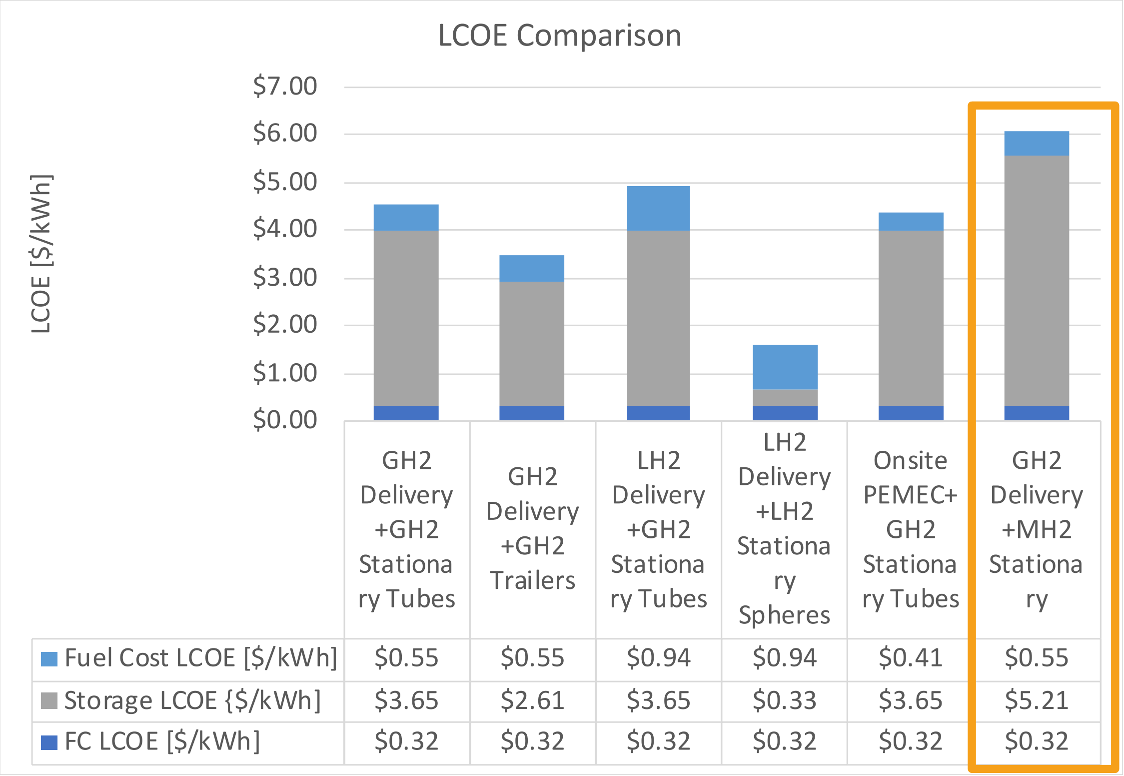
Driving Area

Terminal Bays

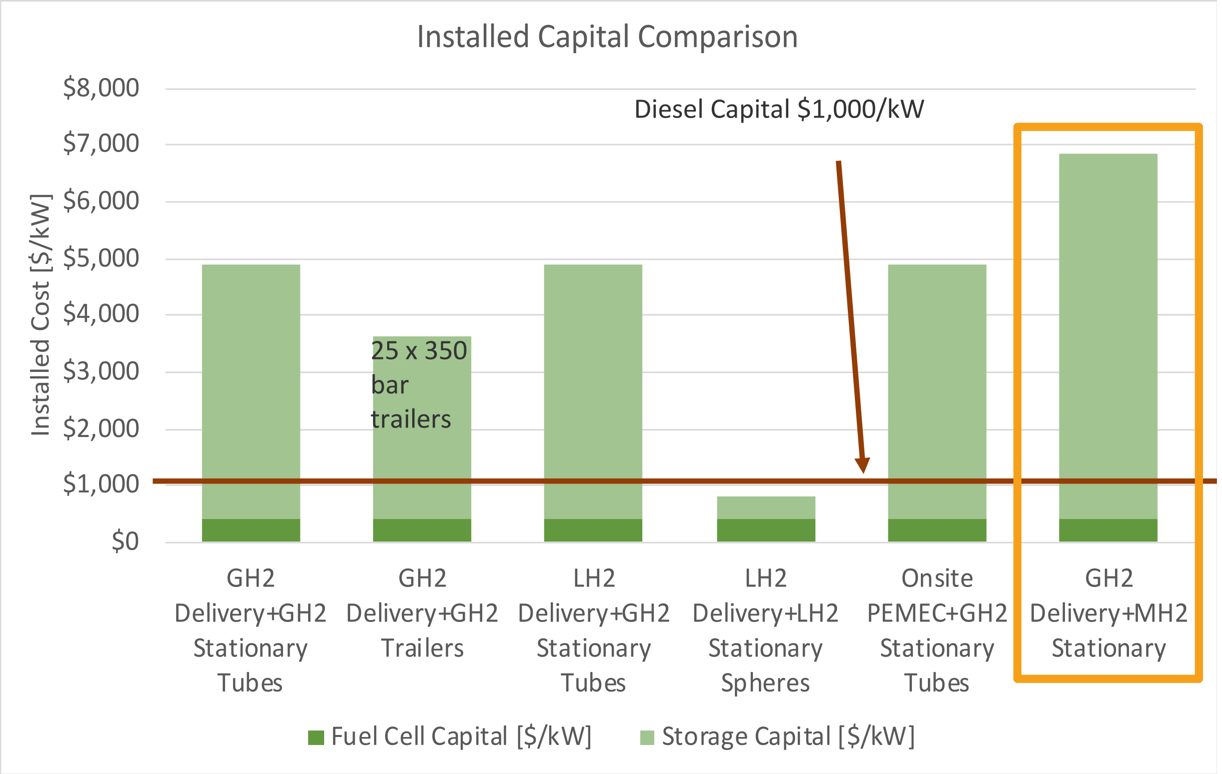
Bay setback

Accomplishments

Initial TEA results indicate cost challenges



	GH2 Delivery +GH2 Stationary Tubes	GH2 Delivery +GH2 Trailers	LH2 Delivery +GH2 Stationary Tubes	LH2 Delivery +LH2 Stationary Spheres	Onsite PEMEC+ GH2 Stationary Tubes	GH2 Delivery +MH2 Stationary
Fuel Cost LCOE [$/kWh]	$0.55	$0.55	$0.94	$0.94	$0.41	$0.55
Storage LCOE {$/kWh]	$3.65	$2.61	$3.65	$0.33	$3.65	$5.21
FC LCOE [$/kWh]	$0.32	$0.32	$0.32	$0.32	$0.32	$0.32



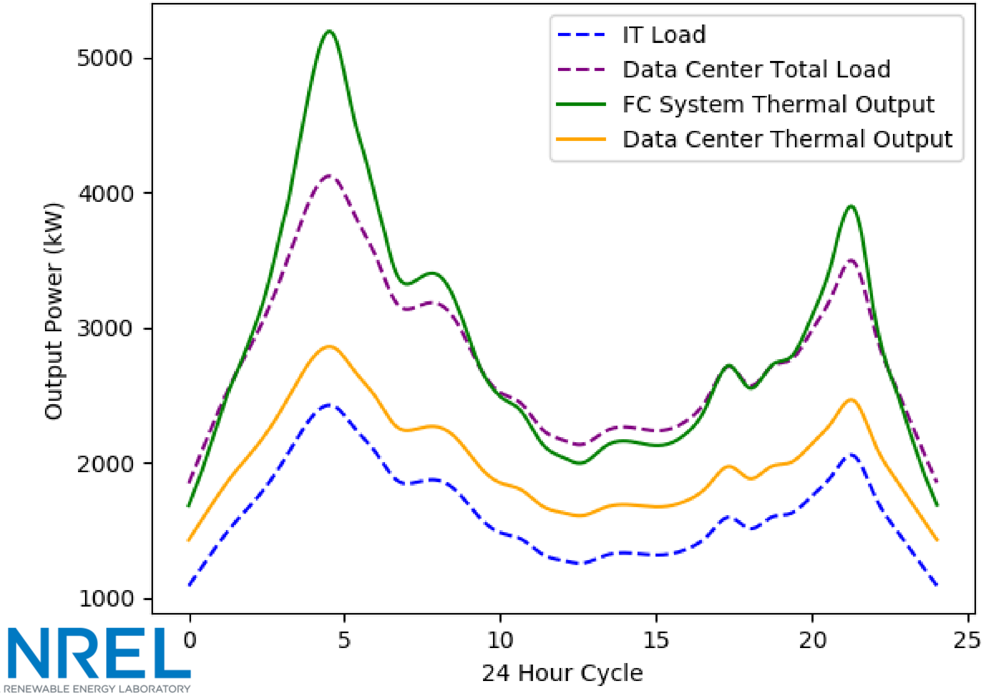
- Preliminary results for TEA: capital cost, LCOE
  - Assumptions still in progress
  - Metal hydride costs $1,430/kg

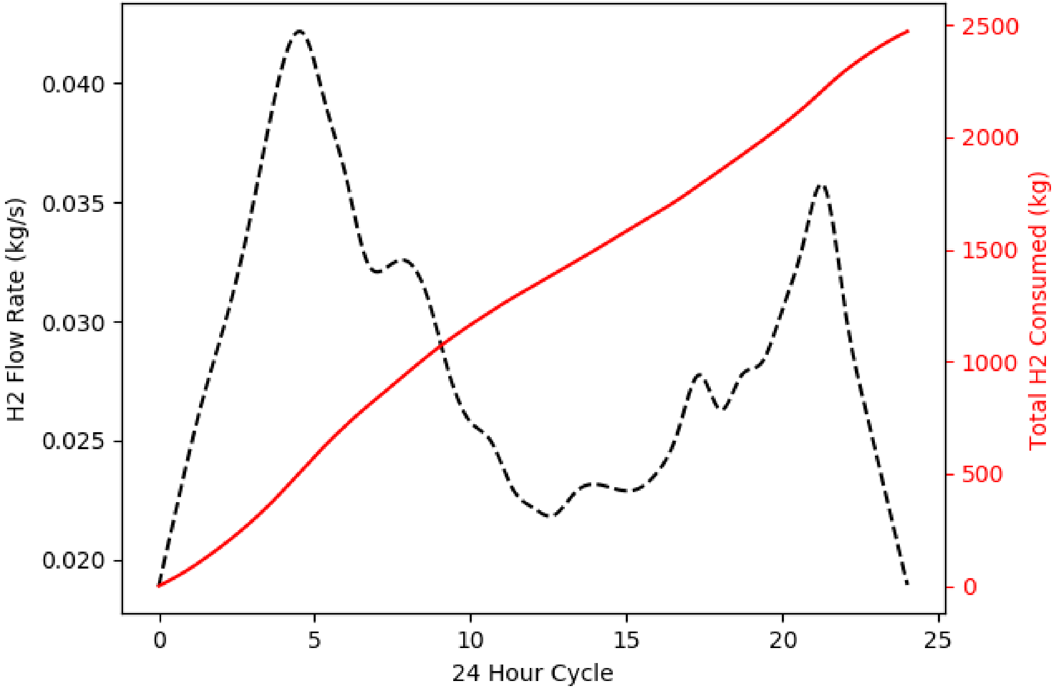
Accomplishments

Preliminary results show fuel cells are the priority heat source

- Fuel cell shows greater thermal output availability compared to the data center system
- Output heat can be captured and assist in keeping the metal hydride storage system at the required thermal setpoints

- Hydrogen flow rate and flow ramping required from metal hydride storage is dependent on IT load demand
- Results shown are based on a 24 hour, carbon aware data center load





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Accomplishments

Metal hydrides potentially have the smallest footprint

- Preliminary footprint calculations for 5 initial scenarios
- Layouts adapted from HDSAM
- Space allowances adapted from HDSAM/NFPA2
- Scenario: 22,526 kg H_2

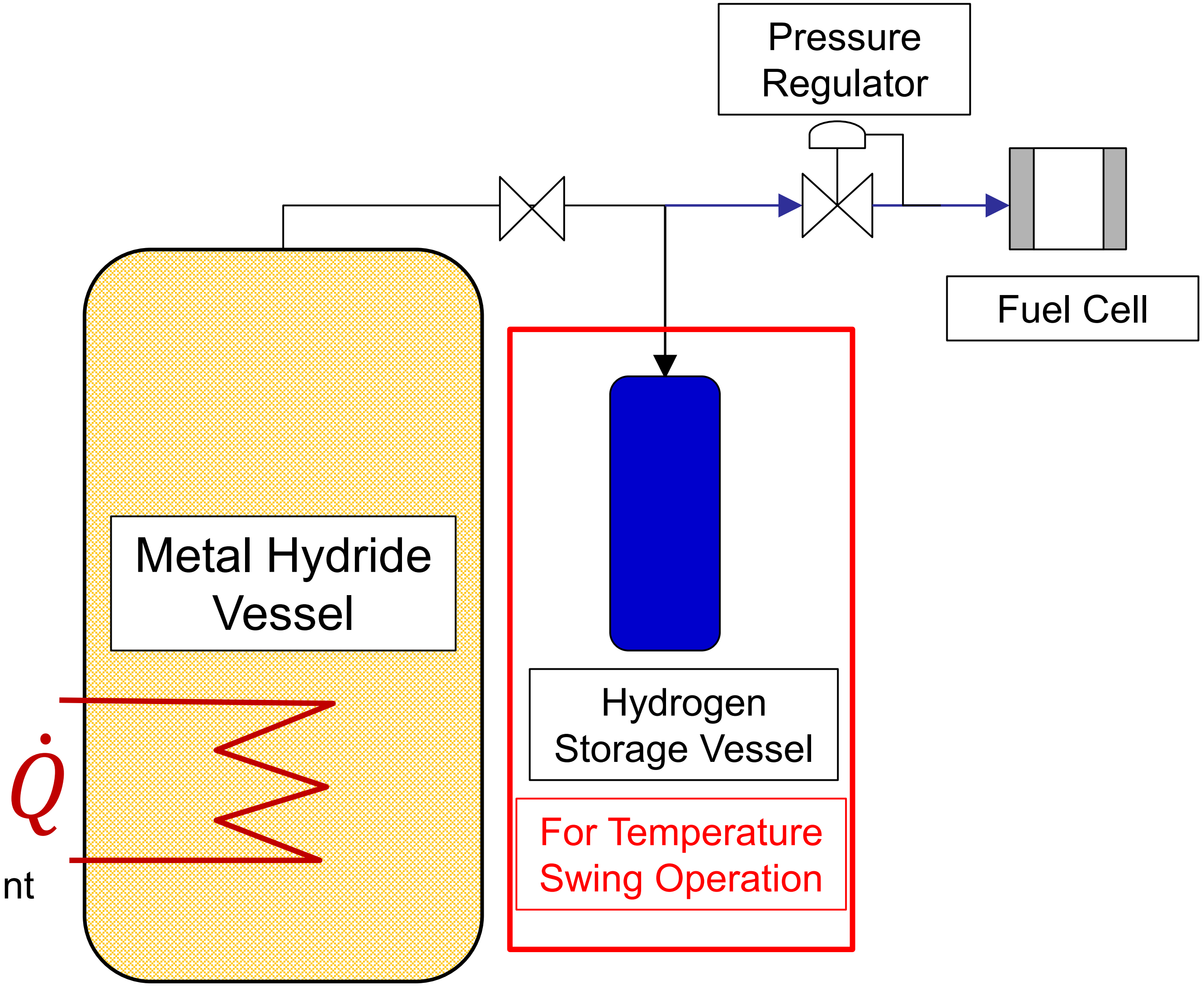
- Metal Hydride assumptions
  - (Ti0.97Zr0.03)1.1Cr1.6Mn0.4 (preliminary model)
  - MH_2 Volume supplied by SRNL, 1 tank assumed
  - Distance around storage and time to charge taken from GH_2 assumptions

Scenario	Storage Setback [m2]	Storage length [m]	Storage width [m]	Storage area [m2]	Buffer [m2]	Terminal Bay Length [m]	Terminal Bay area [m2]	Driving area [m2]	Bay Setback [m2]	PEMEC Plant [m2]	Total Area [m2]
GH_2 Stationary Storage	3,701	103	12	1,226	2,575	31	677	1,691	2,141	0	**12,012**
GH_2 + PEMEC	3,701	103	12	1,226	2,575	5	110	405	1,110	613	**9,740**
GH_2 Trailers	0	0	0	0	3,125	125	625	3,105	3,555	0	**10,410**
LH_2 Stationary Storage	2,806	38	38	1,444	2,100	12	269	1,413	1,413	0	**9,445**
MH_2 Stationary Storage	1,625	14	10	148	1,504	31	677	1,691	1,691	0	**7,337**

Approach

Preliminary Models for Storage System

- Simultaneously solves coupled ODE’s:
  - Mass and energy conservation
  - Chemical kinetics
  - Thermodynamics
  - Ancillary constitutive properties
- Calculates
  - Required metal hydride mass and volume
  - Temperature and pressure transients
  - Required transient heating power
    - Includes temperature of supplied heat
  - Transient depletion of hydrogen remaining in metal hydride
    - Needed to efficiently determine the required amount of metal hydride



Schematic of Storage System

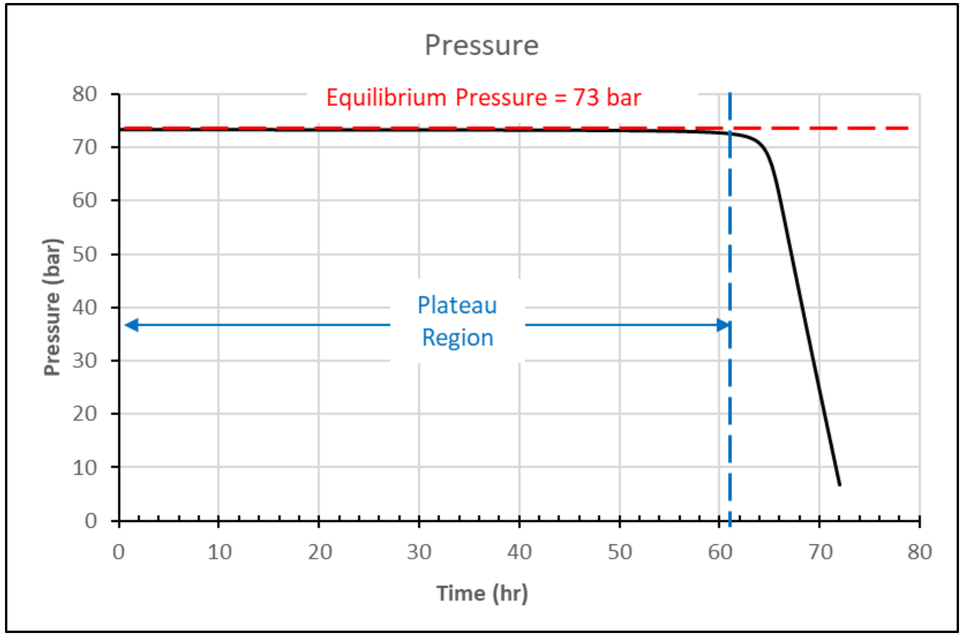
Storage System Operation

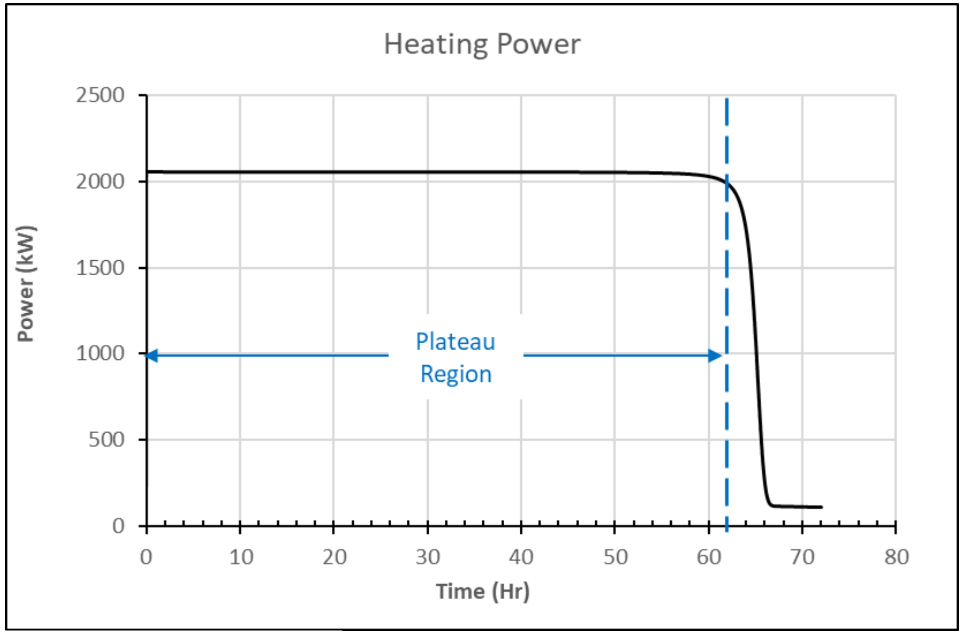
- Hydrogen desorption via pressure swing or temperature swing
  - Initial temperature is ambient (assumed to be 295K)
  - Initial pressure is equilibrium pressure at the ambient temperature
  - Operates for 72 hours
  - Supply 6 bar of pressure to fuel cell
  - Total of 90,000 kg of hydrogen is required to power the data center
  - Metal hydride expands on uptake of hydrogen & contracts on discharge
- Pressure swing
  - Metal hydride has high pressure at ambient temperature
  - Hydrogen is discharged while heat is supplied to the MH to maintain constant temperature
- Temperature Swing
  - Metal hydride is heated to raise pressure to meet fuel cell requirements
    - Pressure transient from initial to operating pressure is specified
  - After reaching target pressure, discharge is initiated
  - Heat is supplied to maintain pressure

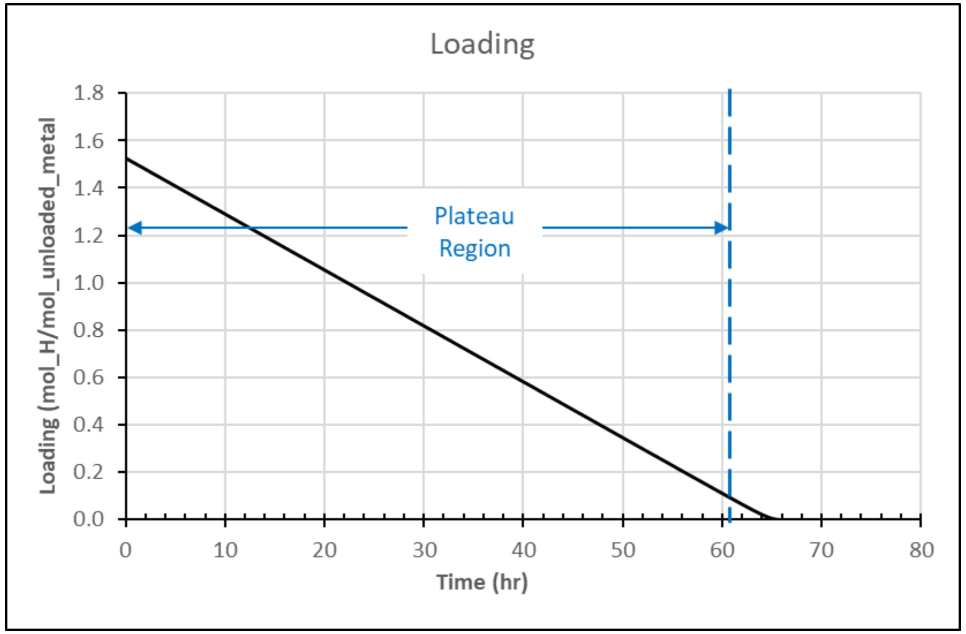
Accomplishments

Pressure Swing Model

- Metal Hydride $(Ti_{0.97}Zr_{0.03})_{1.1}Cr_{1.6}Mn_{0.4}$
- Duration 72 hours
- H_2 Outflow 1249 kg/hr
- Equilibrium Pressure at 295K is 72.4 bar
- Metal Hydride Volume is 3050 m^3
- Metal Hydride Mass is $9.4X10^6$ kg







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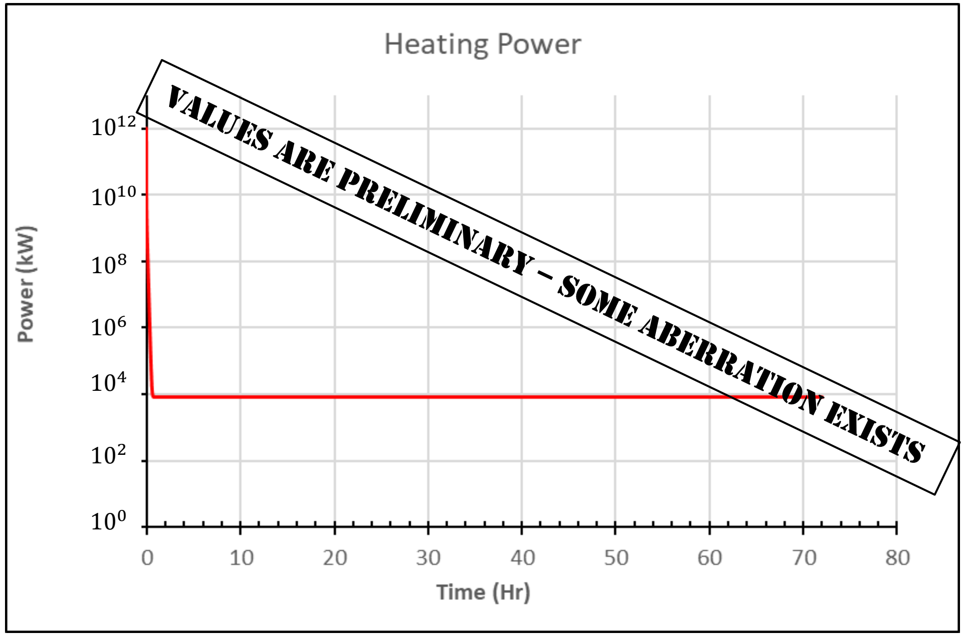
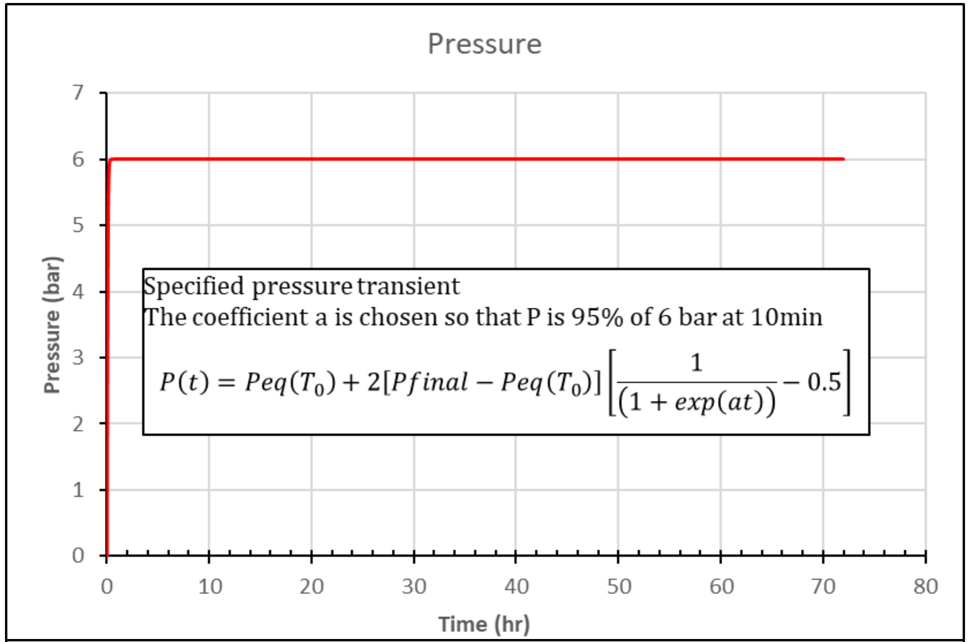
Temperature Swing Model

- Metal hydride $1/3Na_3AlH_6 \leftrightarrow NaH + 1/3\ Al + 1/2\ H_2$
- Duration 72 hours
- Pressure transient is specified
    - At 295K equilibrium pressure is ~ 0.01 bar
- H_2 outflow 1250 kg/hr
- Metal hydride volume is 9009 m^3
- Metal hydride mass is $3.05X10^6$ kg

System would require a tank of pressurized H_2 for rapid starting

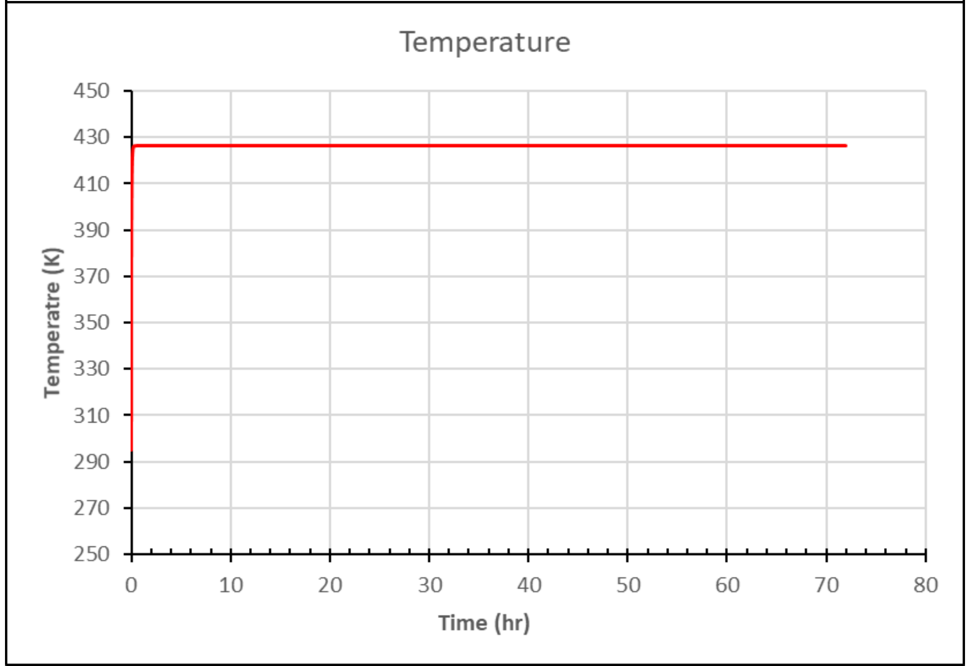


VALUES ARE PRELIMINARY – SOME ABERRATION EXISTS



Specified pressure transient
The coefficient a is chosen so that P is 95% of 6 bar at 10min

$$P(t) = Peq(T_0) + 2[Pfinal - Peq(T_0)]\left[\frac{1}{(1+exp(at))} - 0.5\right]$$



Collaboration and Coordination

- The SRNL/NREL team manages their respective personnel, budgets and coordinates tasks and schedules between both organizations to meet program objectives
  - Meetings are held as needed to update progress and address technical risks based on progress
- NREL Tasks
  - Development and application of a techno-economic modeling framework for evaluating materials and system properties against bulk application targets
  - Techno-economic assessment operating strategy, capital costs for the electrolysis-storage-fuel cell system, estimation of renewable electricity costs summarized in a levelized cost of electricity (LCOE) provided to the data center that can then be compared with other options summarized in a levelized cost of electricity (LCOE) for comparison with other options
- SRNL Tasks
  - Development and application of numerical model for a materials-based bulk storage system
  - Prediction of H_2 storage system size, mass and operating parameters for input to the NREL techno-economic analysis
  - Determination of preferred modes of operation and storage material properties for optimal thermodynamic efficiency and cost
  - Review existing codes and standards for stationary storage of H2, such as ASME Boiler and Pressure Vessel Code and NFPA 2

Remaining Challenges and Barriers

- Maintain acceptable system cost in terms of LCOE
  - Improve analysis of MH charging strategies
  - Improve characterization of opportunities to use available heat
- Identify suitable MH properties
  - To achieve fuel cell supply pressure
  - Reasonable initial pressure
  - High hydrogen capacity
  - Low reaction enthalpy (to have discharge with reasonable heating power)
- Determine system design that minimizes required MH volume and mass

Proposed Future Work

All Items are proposed as follow-ons to the current project

- Develop detailed spatially dependent transient model to determine rate of heat transfer to MH, as opposed to assuming instant, uniform distribution of power
- Perform technoeconomic analysis of heat exchangers for MH bed -
- Perform technoeconomic analysis of competitive MH's
- Determine range of desirable MH properties and compare to existing MH's
  - Includes MH mixtures
- Obtain MH data, suitable for engineering design, for a range of MH's
- Optimize system operation, i.e. temperature swing, pressure swing and hybrid systems with respect of LCOE and thermodynamic efficiency
- Improve monetization estimates for land area at data centers
- Extend program from investigation of back-up fuel cell power to continuous power operation and 100% green energy opportunities

Any proposed future work is subject to change based on funding levels

Summary

- Preliminary model is working
  - 2 types of metal hydrides were modeled
    - Complex (temperature swing) and intermetallic (pressure swing) MH
    - Not intended to be optimal, but had available properties
- Found that for simplistic bulk system (one large MH vessel) a pressure swing is favorable due to:
  - Immediately available fuel cell pressure
  - Lower heating power
- Other possibilities
  - Hybrid pressure swing/temperature swing system
  - Temperature swing system that includes
    - An H_2 pressure storage tank
    - And/or array of Individual small MH vessels that can be independently heated (smaller sequential power demand)
- Technoeconomic analysis
  - Initial techno-economic results identified breakdown of cost challenges
  - Preliminary results show fuel cells are the principal source of waste heat for the data center
  - Indicated that metal hydrides potentially have the smallest footprint

Technical Backup and Additional Information

Technology Transfer Activities

- NA

Progress Toward DOE Targets or Milestones

- Milestone 1, End Date 12/31/2020
  - *Successful screening of materials and system (containment and BOP), operating at large scale, based on application requirements, that would be likely candidates to demonstrate a viable path to reach the techno-economic targets compared to traditional bulk hydrogen storage.*
  - **Performed initial screening of materials for a 20MW data center.**
- Milestone 2, End Date 3/31/2021
  - *Presentation on the initial TEA of an optimal data center using a reversable material-based hydrogen storage system including the LCOE of the computational units.*
  - **Techno-economic analysis was used to compare LCOE and capital cost with bulk hydrogen storage.**
- Milestone 3, End Date 6/30/2021
  - *Provide a detailed system model (material, containment and BOP), operating at large scale, based on application requirements, demonstrating a viable path to reach the techno-economic targets compared to traditional bulk hydrogen storage.*
  - **Developed preliminary full-scale model and used it to describe system operation for pressure-swing and temperature-swing hydrogen discharge.**
- Milestone 3, End Date 6/30/2021
  - *Publish a gap assessment report that outlines an R&D pathway which will include the identification of any required material and system R&D gaps that should be addressed for a materials-based stationary bulk storage to meet DOE's Ultimate high-volume cost targets for bulk stationary storage ranging from \$450 - \$600/kg-H2 stored.*
  - **Currently using detailed model to identify gaps in available MH properties that preclude meeting targets for cost and performance targets.**