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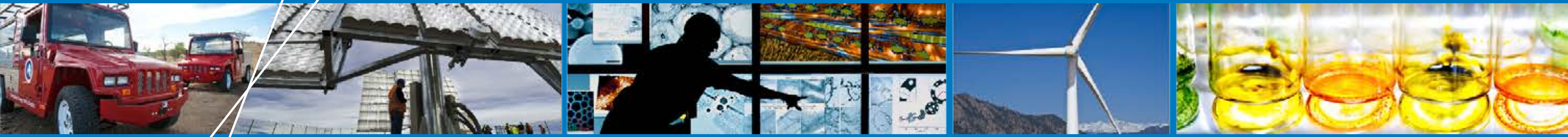
Hydrogen Storage Engineering
CENTER OF EXCELLENCE

System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage



Matthew Thornton
NREL
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Project ID # ST008

Overview

Timeline

HSECoE start date: FY09
HSECoE end date: FY14
Percent complete: 55%

Budget

Total funding $1.8M

DOE Share 100%

Funding Received in FY11: $320K

Funding for FY12: $110K

Barriers

- **System cost**
- **Charge/discharge rate**
- **System mass**
- **Systems volume**
- **Transient response**
- **Well-to-power plant efficiency**
- **Vehicle performance**

Partners

SRNL, PNNL, UTRC, UQTR, JPL, Ford, GM, LANL, OSU, BASF, UM the DOE Vehicle Technologies Program.

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Relevance/Objectives

System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage

- Manage HSECoE vehicle performance, cost and energy analysis technology area
- Vehicle Performance: Develop and apply model for evaluating hydrogen storage requirements, operation and performance tradeoffs at the vehicle system level.
- Energy Analysis: Coordinate hydrogen storage system WTW energy analysis to evaluate off-board energy impacts with a focus on storage system parameters, vehicle performance, and refueling interface sensitivities.
- Media engineering properties: Assist center in the identification and characterization of adsorbent materials that have the potential for meeting DOE technical targets for an onboard systems.

Objective: Vehicle Performance

- Develop and apply a model for evaluating hydrogen storage requirements, performance and cost trade-offs at the vehicle system level; e.g. Range, fuel economy, cost, efficiency, mass, volume, acceleration, on-board efficiency
- Provide high level evaluation (on a common basis) of the performance of materials based systems:
    - Relative to technical targets
    - Relative in class and across class for materials systems
    - Relative to physical storage systems
    - Relative to conventional vehicles

Objectives: Energy Analysis

- Perform hydrogen storage system energy analysis to evaluate WTPP efficiency, Energy requirements, H_2 cost and GHG emissions
  - Develop vehicle a level models and obtain FE figures for energy analysis.
  - Obtain data from center partners on storage system designs (mass, volume, operating T and P)/fuel interface/dispensing/station energy requirements.
  - Work with other teams (e.g. H_2 Delivery and systems analysis) and use existing data for H_2 production and distribution and tank production and CO_2e emission factors (GREET, H_2 A, etc.) and calculate WTPP efficiencies etc.
  - Adjust model inputs based on changes in storage system design and data to obtain final results.
  - FY12 focus is accounting for and understanding the impact of the thermal management (i.e. flow through cooling design for adsorbents) and off-board regeneration cycles for chemical hydride systems

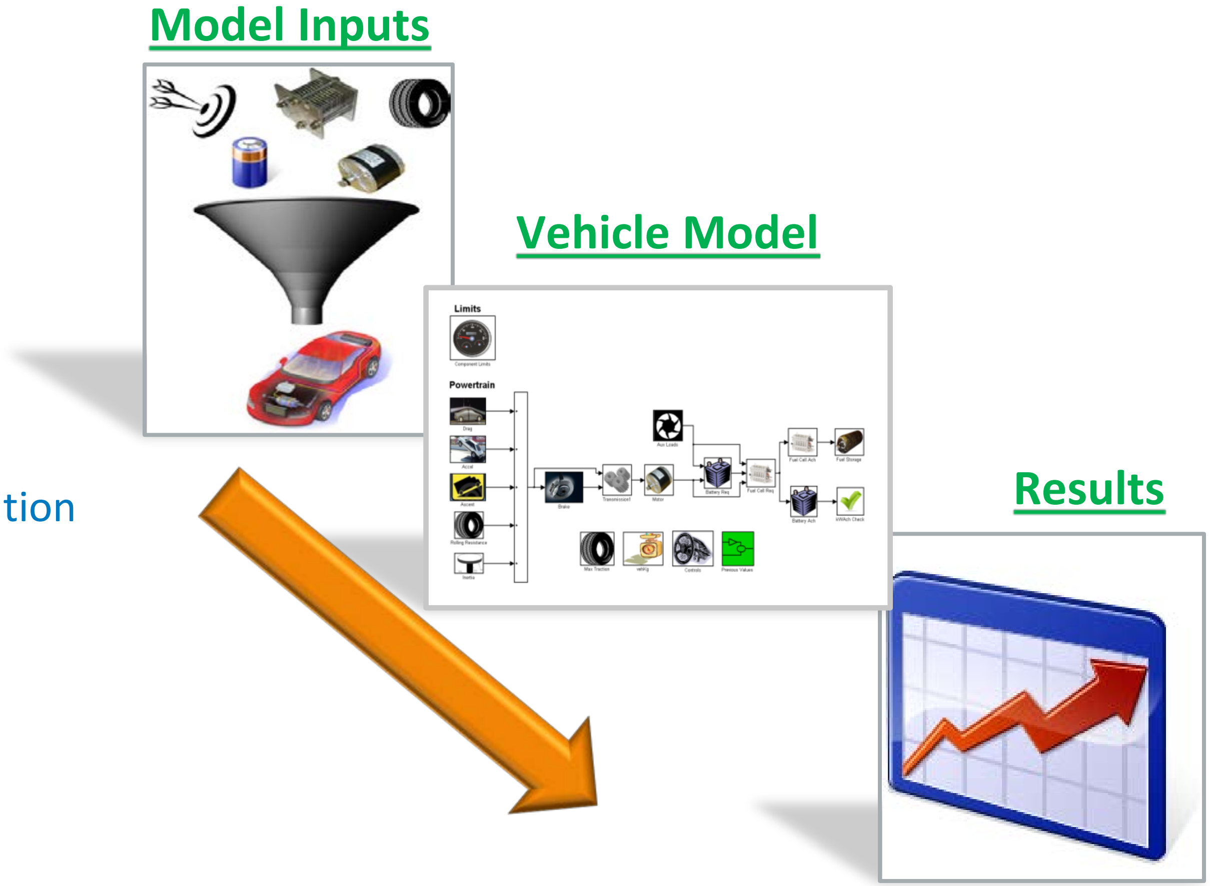
Milestones

Date	Milestone or Go/No-Go Decision	Status
9/12	Work with center and SSAWG partners to complete at least one well-to-wheel efficiency analysis for a sorbent-based storage design concept and compare it's energy efficiency versus the DOE 2017 minimum efficiency targets of 70% off-board and 90% on-board.	25%
2/12	Recommend materials for scaled H2 storage system engineering.	100%
9/12	Provide HSECoE appropriate engineering properties.	25%

Approach: Develop HSSIM (Vehicle Model)

HSSIM Structure

- **Model Inputs**
  - Vehicle characteristics
  - Fuel cell characteristics
  - H_2 storage system
- **Vehicle Model**
  - Power requirement calculation
  - Vehicle level test matrix
- **Results**
  - Fuel economy (mpgge)
  - Range (miles)
  - Vehicle mass (kg)
  - Onboard efficiency (%)
  - Hydrogen flow (moles/s)
  - Vehicle performance (e.g. 0-60 mph time)



A tool to be used across the engineering center to evaluate candidate storage system designs on a common vehicle platform with consistent assumptions

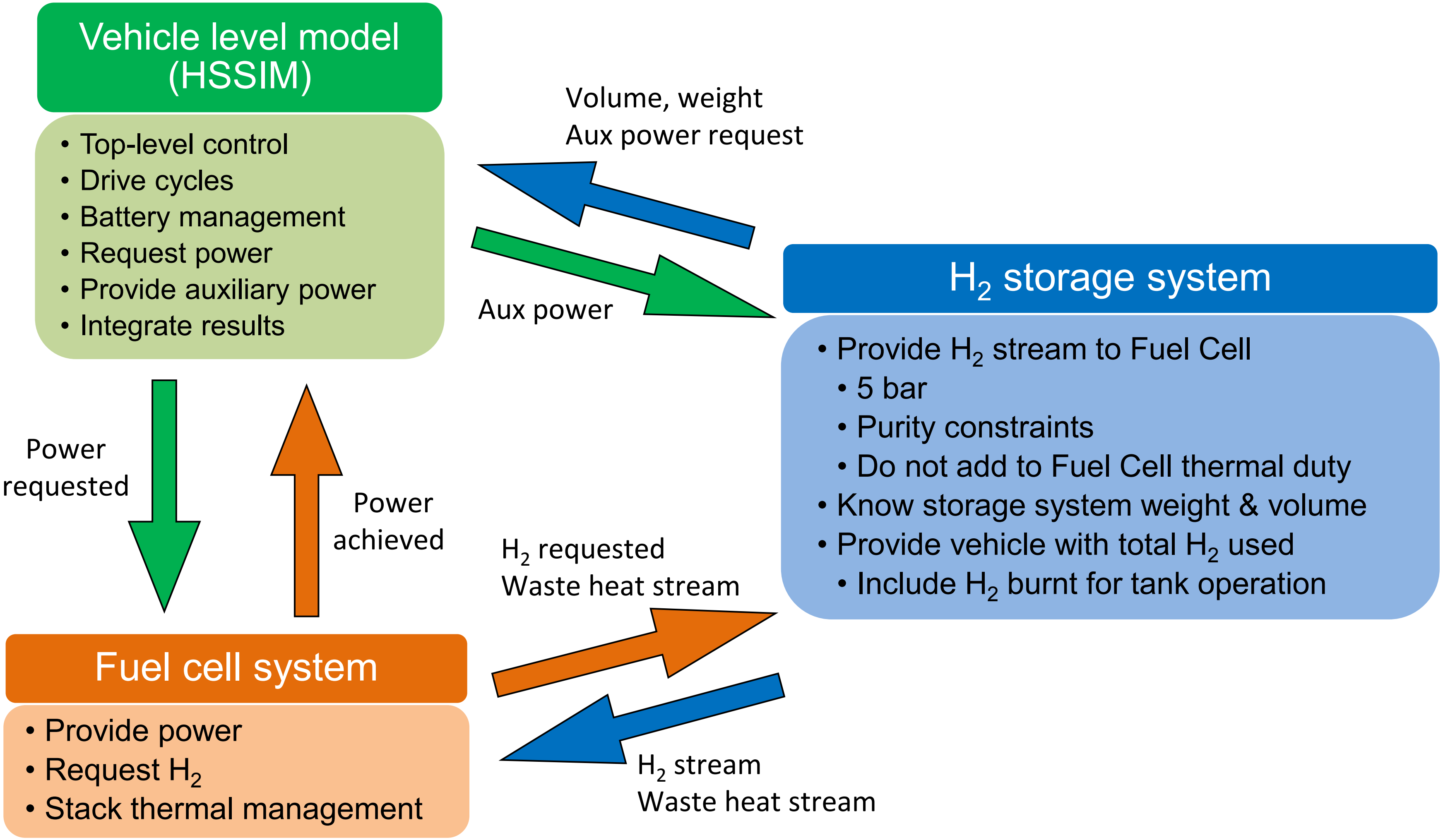
Approach: Vehicle Assumptions

- **Midsize Car Class (Family Sedan):**

Vehicle Attribute	**Units**	**Value**
Glider mass[1]	kg	1,104
Frontal area	m^2	2.2
Drag coefficient	–	0.29
Rolling Resistance	–	0.008
Tires	–	P195/65R15
Electric Motor	kW	100 (~85% eff.)
Energy Storage	kW/kWh	20/1 (40-80% SOC)

[1] Excludes fuel cell, hydrogen storage system, electric motor, power electronics, and energy storage system

Approach: Modeling Framework



Vehicle level model (HSSIM)

- Top-level control
- Drive cycles
- Battery management
- Request power
- Provide auxiliary power
- Integrate results

Volume, weight
Aux power request

Aux power

H_2 storage system

- Provide H_2 stream to Fuel Cell
  - 5 bar
  - Purity constraints
  - Do not add to Fuel Cell thermal duty
- Know storage system weight & volume
- Provide vehicle with total H_2 used
  - Include H_2 burnt for tank operation

Power requested

Power achieved

H_2 requested
Waste heat stream

Fuel cell system

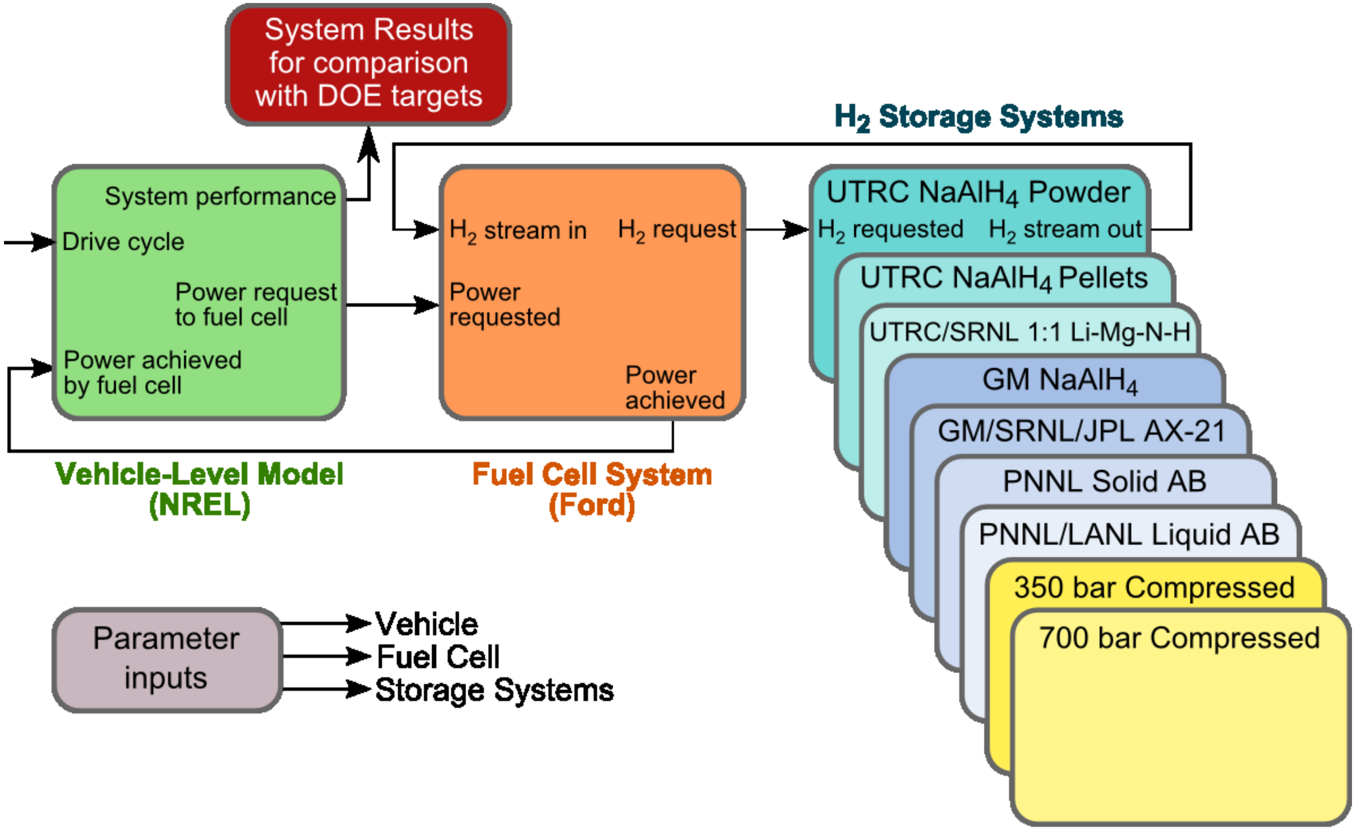
- Provide power
- Request H_2
- Stack thermal management

H_2 stream
Waste heat stream

Slide provided courtesy of José Miguel Pasini UTRC

Approach: Modeling Framework

Compare materials-based hydrogen storage systems on a common basis with defined interfaces and consistent assumptions



Slide provided courtesy of José Miguel Pasini UTRC

Approach: Energy and WTPP Analysis

Utilize H_2A Hydrogen Delivery Scenario Model (HDSAM)

- **Standardized Excel spreadsheet tool with the same H_2A approach to cost, energy efficiency and GHG emissions analysis but more complex**
- **Pre-loaded with current capital costs and utility costs of H_2 delivery components – pipelines, tube trailers, LH_2 trucks, terminals, refueling stations, etc.**
- **User specifies a delivery scenario:**
  - Urban or city and which city
  - Market penetration (%)
  - Transport mode (to terminal) and distance
  - Distribution mode (terminal to refueling stations)
- **Model calculates: delivery cost (\$/kg-H_2), energy efficiency (WTW (power plant)), and GHGs (gms/mile)**

Approach: Energy Analysis Assumptions for HDSAM

Production:	**SMR**
Market:	**Sacramento, 15% market penetration**
Plant (and Regen.):	**62 miles (100 km) from city gate**
Electricity:	**U.S. grid**
Large scale storage:	**Geologic, LH_2, liquid**
Transport:	**Plant to city gate terminal** • **GH2 – pipeline** • **LH2, liquid carrier – truck**
Distribution:	**City gate terminal to refueling stations – truck**
Refueling Station Size:	**1000 kg/day maximum (may be limited by one delivery per day or 9% coverage)**

Approach: Energy Analysis

Storage System	H_2 Delivery Cost ($/kg)	WTPP Efficiency (%)	WTW GHG (gms/mi)	Energy (Delivery) (kWh/kg-H_2)
60 Bar Adsorbent 40-120K (Flow through cooling) Al				
200 Bar Adsorbent 80-160K (Flow through cooling) CF				
60 Bar Adsorbent 80-160K (MATI HX) Al				
200 Bar Adsorbent 40-120K (MATI HX) CF				
CH exothermic (fluid AB)				
CH endothermic (Alane)				
350 Bar Pipeline	4.26	56.7	197	58.8
700 Bar Pipeline	4.71	54.4	208	61.2
Cold Gas 500 Bar	4.80	42.7	279	78.0

Approach: Media Engineering

Work with engineering center partners to identify potential materials and configurations that can be optimized with the appropriate thermal conductivity, sorption, and mechanical properties needed for integration in a hydrogen storage system

- Optimize AC pellet synthesis and capacities
  - Compare results between MSC-30, Missouri 3K, and Pyrolyzed Polyether ether ketone (PEEK) powders and pellets
  - Investigate the use of carbon fibers to improve pellet structure and possibly thermal conductivity

Accomplishments: Vehicle Performance Summary

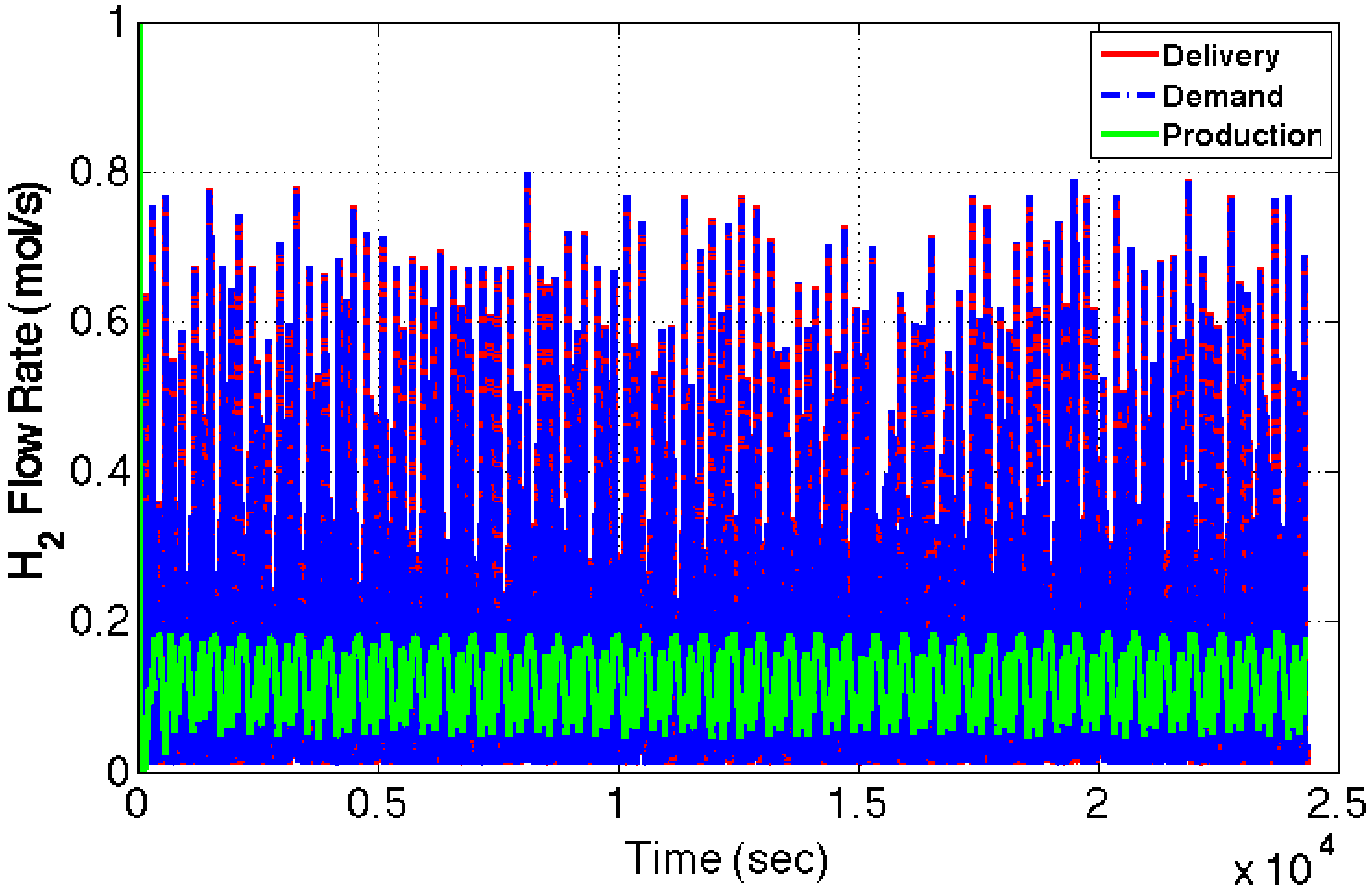
Example simulated vehicle performance results for various hydrogen storage systems with fixed on-board H2 (from framework)

Fixed on-board usable H2 =5.6kg

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Range (mi) 5.6kg H2	On-Board Efficiency (%) UDDS/HFET	Gravimetric Density (wt. %)	Volumetric Density (g/l)
AX21 press FCHX	48.7	273	97	4.3	25.2
MOF5 Cmpct- FCHX	48.3	271	97	3.5	24.1
MOF5 Press FCHX	49.3	276	98	4.6	25.3
Fluid AB	45.3	254	96	4.6	38.9
Alane	42.6	239	88	4.6	38.9
NaAlH4	36.4	204	77	1.2	11.39
TiCrMn	45.9	257	100	1.1	26.53
350 bar Compressed Gas	49.9	280	100	4.8	17.03
700 bar Compressed Gas	49.9	279	100	4.7	25.01

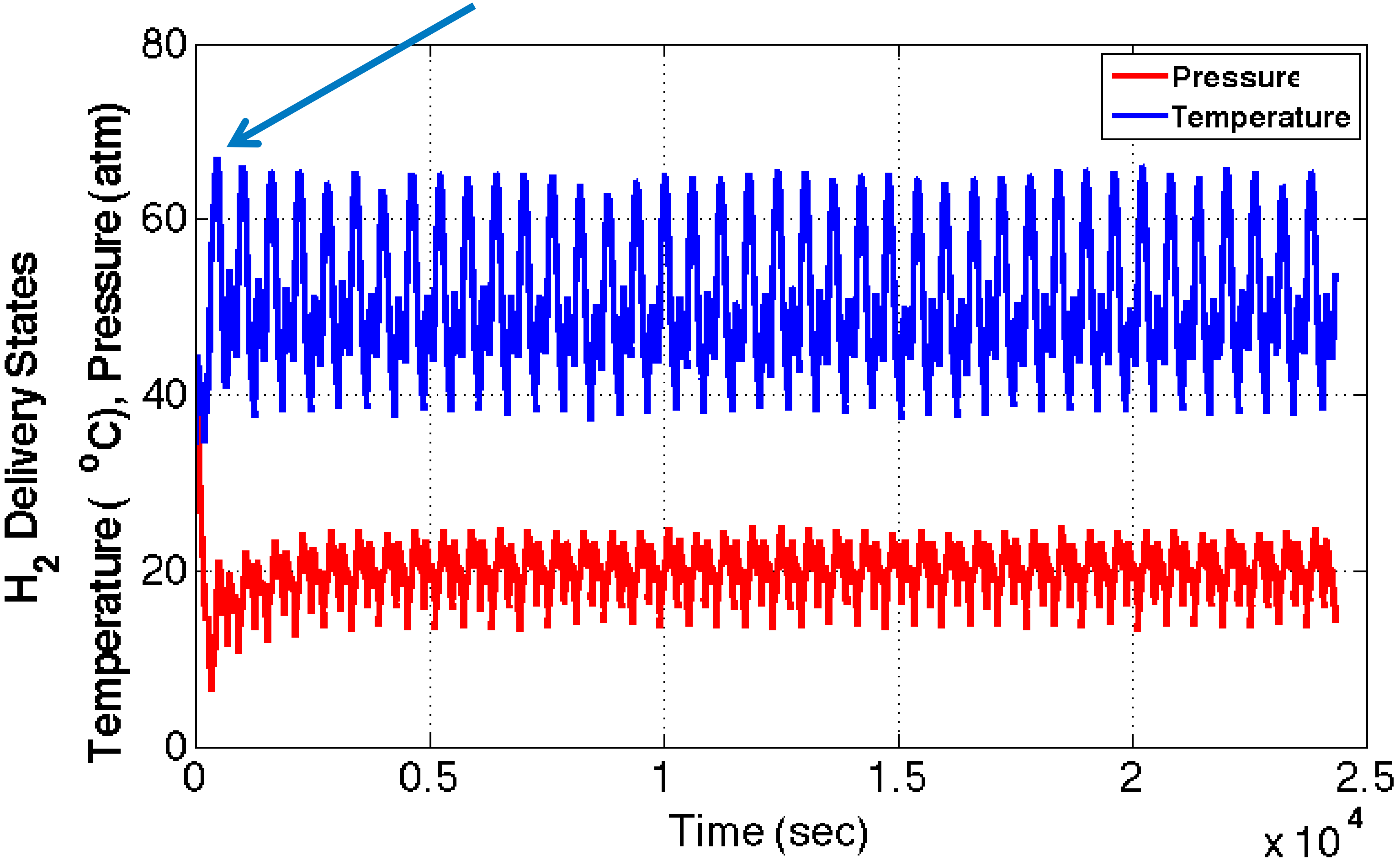
Accomplishments: H_2 Flow Rate for Alane System (CH endothermic) Over US06 Cycle Analysis

Met US06 H_2 Delivery Requirements



Accomplishments: H_2 Delivery States for Alane System Over US06 Cycle Analysis

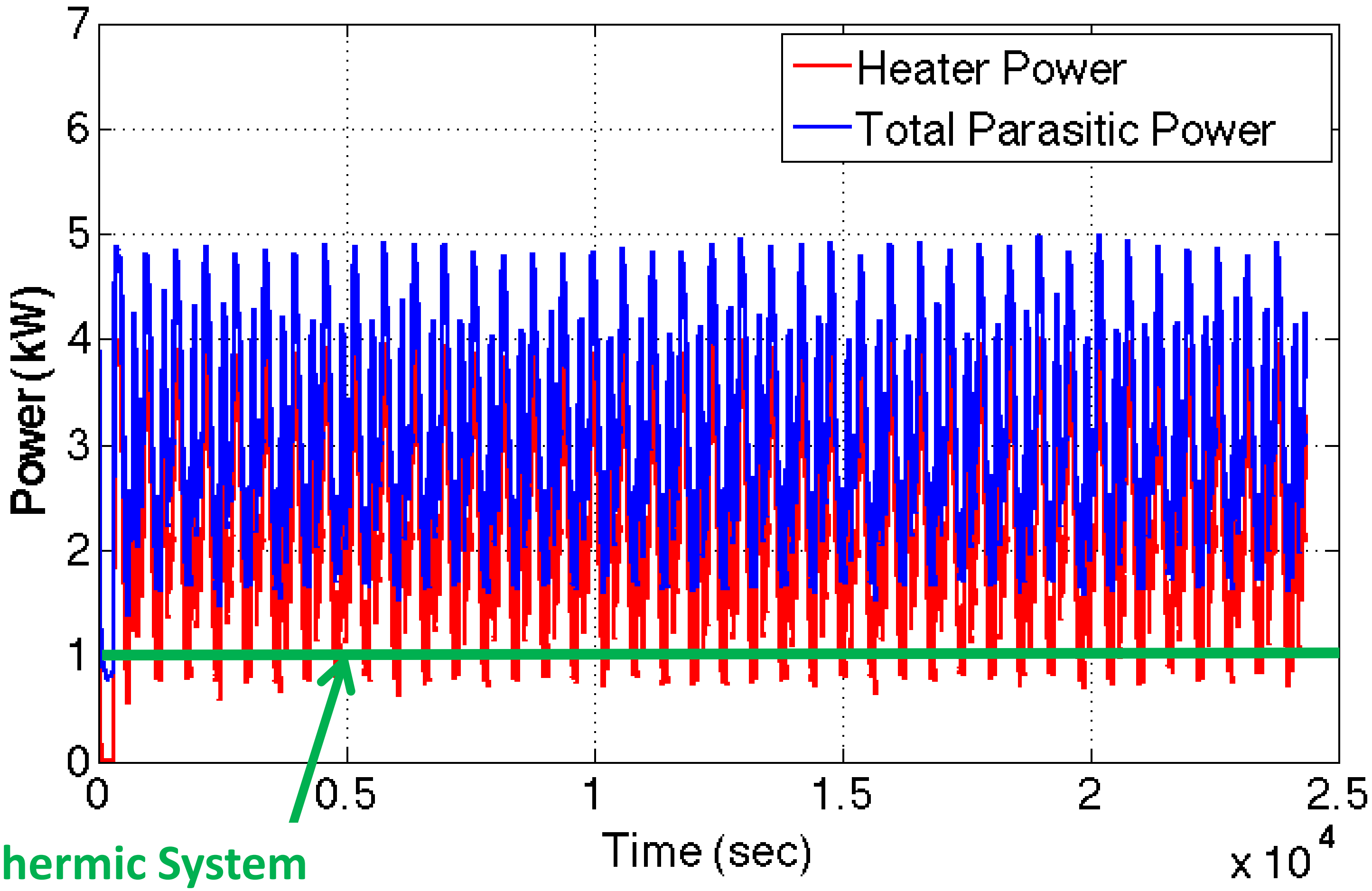
Maximum H_2 Delivery Temperature 66ºC



Met H2 Delivery Temperature and Pressure Requirements

Accomplishments: On-board Efficiency Over US06 Analysis for Alane System

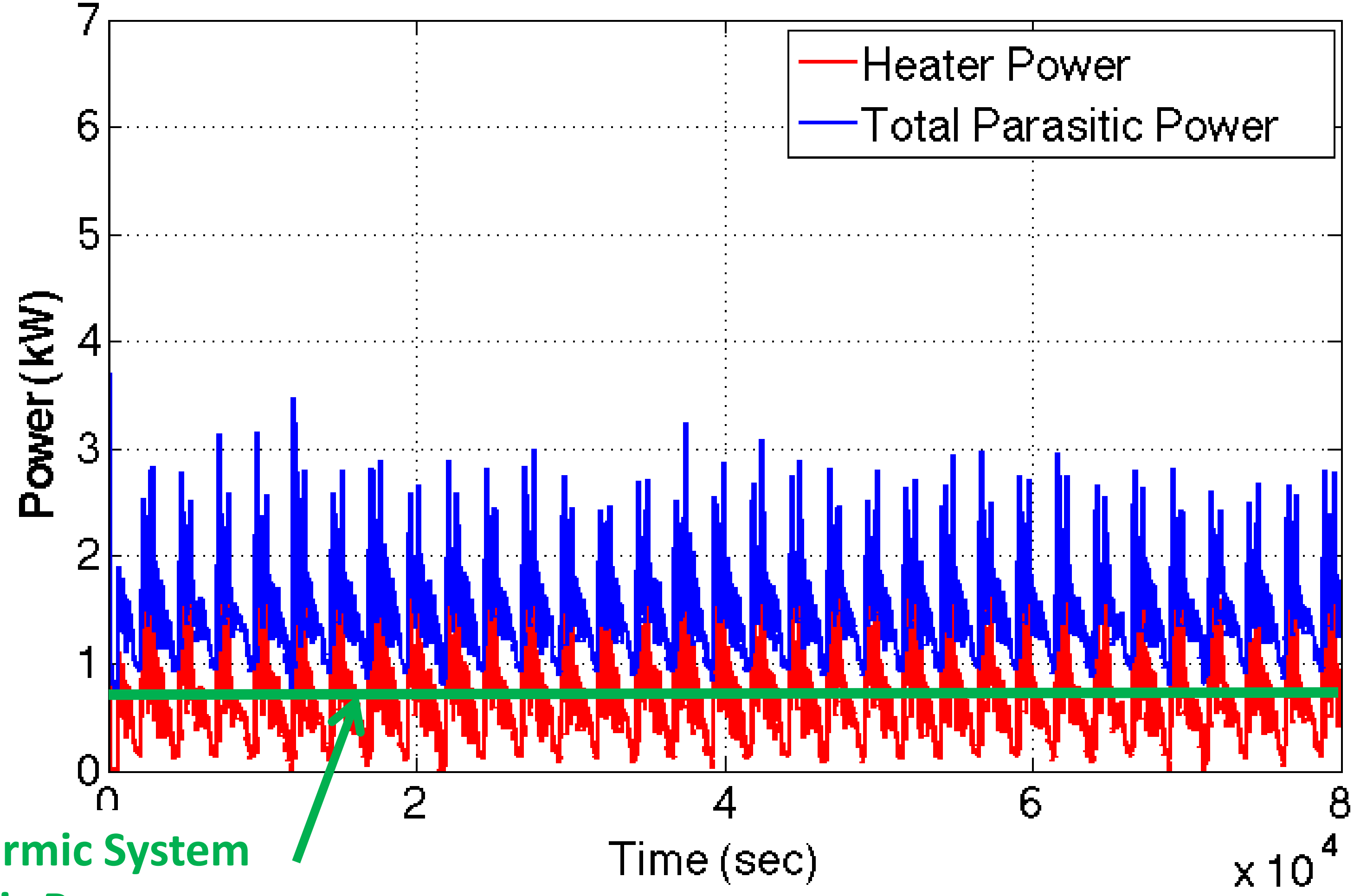
On Board Efficiency = 87%, Did not Meet 90% Target



Exothermic System Parasitic Power

Accomplishments: On-board Efficiency Over Cold FTP Analysis for Alane System

On Board Efficiency = 81%, Did not Meet 90% Target



Exothermic System Parasitic Power

Results: Fixed Volumetric Effects on Range Analysis

Example simulated volume effects on vehicle range and on board usable H2 (from framework) for various adsorbent system designs

For three fixed volumes scenarios 140/205/253 liters

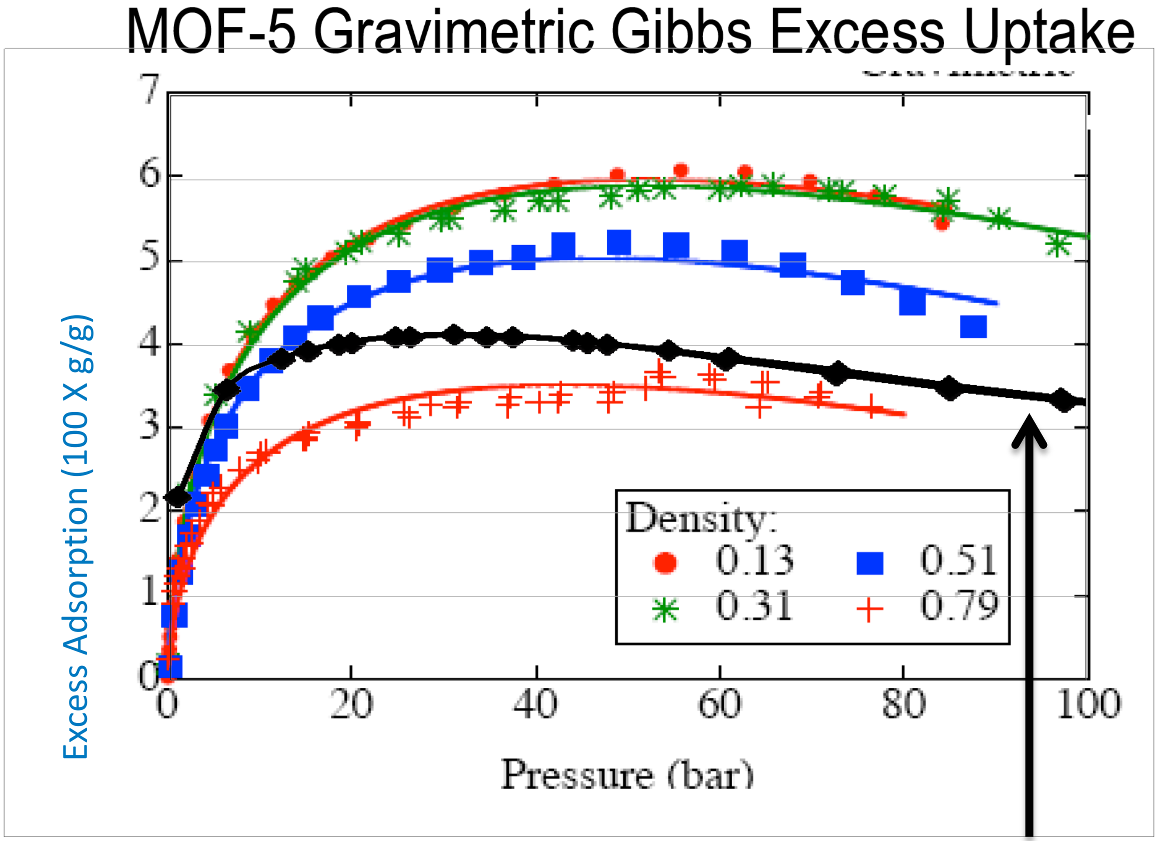
Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Usable H2 (kg)	Range (mi) Usable H2	Gravimetric Capacity Weight Percent	Volumetric Capacity (g/l)	Volume (L)
Powder MOF-5 60bar 80k Al	51.11	2.00	102.20	2.80	12.86	140[1]
Powder MOF-5 60bar 40k CF	51.30	4.20	215.50	6.61	29.84	140
0.52g/cc MOF-5 200bar 80k Al	50.47	3.35	169.10	2.68	23.94	140
0.52g/cc MOF-5 200bar 40k CF	50.62	4.60	232.90	4.18	32.59	140
Powder MOF-5 60bar 80k Al	50.95	2.80	142.70	3.15	13.67	205
Powder MOF-5 60bar 40k CF	50.97	6.70	341.50	7.97	32.64	205
0.52g/cc MOF-5 200bar 80k Al	49.93	5.35	267.10	2.92	26.11	205
0.52g/cc MOF-5 200bar 40k CF	50.18	7.30	366.30	4.61	35.51	205
Powder MOF-5 60bar 80k Al	50.73	3.60	182.60	3.39	14.18	253
Powder MOF-5 60bar 40k CF	50.89	8.60	437.60	8.68	33.96	253
0.52g/cc MOF-5 200bar 80k Al	49.32	6.85	337.90	3.02	27.05	253
0.52g/cc MOF-5 200bar 40k CF	49.71	9.30	462.30	4.77	39.56	253

[1] *Actual volume used = 155.56L which represents the lowest value in the data set available.*

Accomplishments: Activated Carbon Pellet Development

Optimize AC pellet synthesis and capacities

- Carbon fibers improve pellet structure and possibly thermal conductivity
- Pellets made with MSC-30, Pyrolyzed PVDF, and carbon fibers behave similarly to MOF-5 pressed materials as a function of bulk density

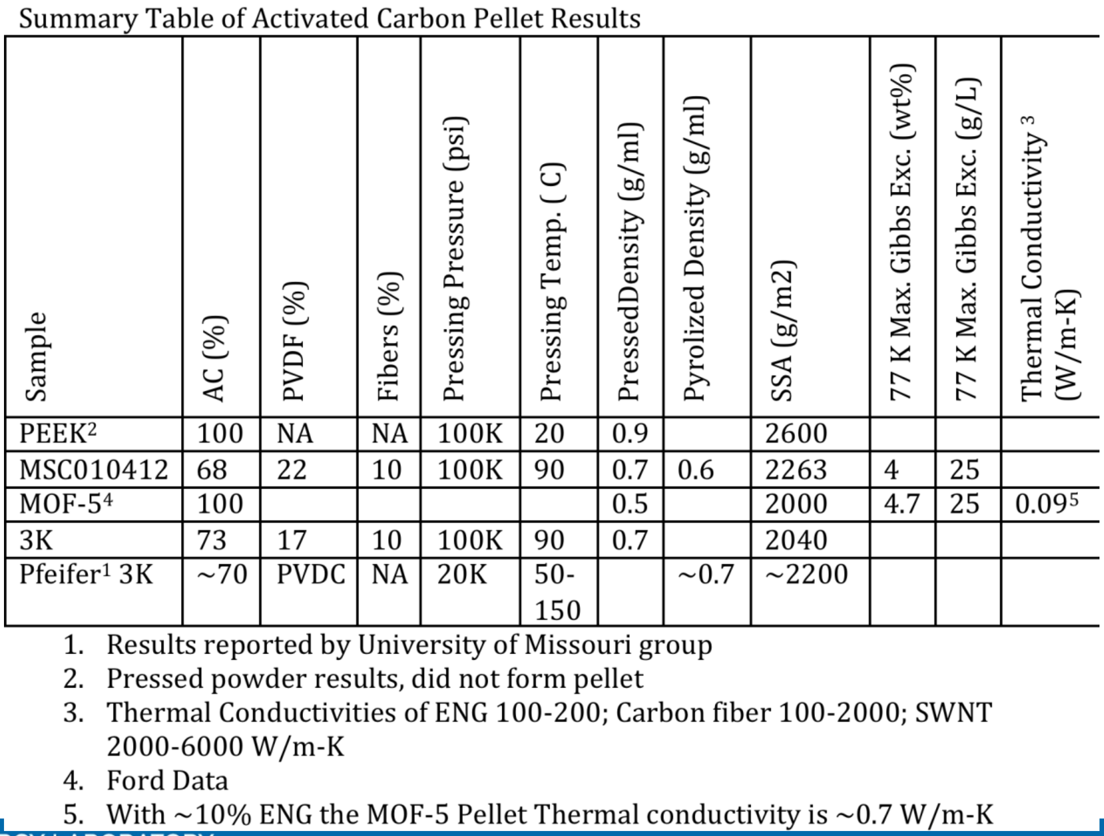


MSC30 PVDF Pyrolized Pellet with Fiber, 0.6 g/ml

Accomplishments: AC and MOF-5 Pellets Similar Performance

Optimize AC pellet synthesis and capacities

- Approximately, standard correlation between BET and H_2 capacity for pellets
  - i.e. ~1 wt% max. Gibbs Excess per 500 m^2/g)
- MSC-30, Missouri 3K, and Missouri pellet results agree
  - Similar to MOF-5 pellet volumetric and gravimetric capacities on a per bulk density basis
  - A little improvement could be made with more optimized pores
    - e.g. using pyrolyzed polyether ether ketone (PEEK) material



Summary Table of Activated Carbon Pellet Results

Sample	AC (%)	PVDF (%)	Fibers (%)	Pressing Pressure (psi)	Pressing Temp. (C)	PressedDensity (g/ml)	Pyrolized Density (g/ml)	SSA (g/m2)	77 K Max. Gibbs Exc. (wt%)	77 K Max. Gibbs Exc. (g/L)	Thermal Conductivity [3] (W/m-K)
PEEK[2]	100	NA	NA	100K	20	0.9		2600			
MSC010412	68	22	10	100K	90	0.7	0.6	2263	4	25	
MOF-5[4]	100					0.5		2000	4.7	25	0.095[5]
3K	73	17	10	100K	90	0.7		2040			
Pfeifer[1] 3K	~70	PVDC	NA	20K	50-150		~0.7	~2200			

1. Results reported by University of Missouri group
2. Pressed powder results, did not form pellet
3. Thermal Conductivities of ENG 100-200; Carbon fiber 100-2000; SWNT 2000-6000 W/m-K
4. Ford Data
5. With ~10% ENG the MOF-5 Pellet Thermal conductivity is ~0.7 W/m-K

Collaboration and Coordination

Key Collaborators:

UTRC-Model integration and model Framework

Ford-FC model, model integration and MOF-5 data

SRNL-Adsorbent models

PNL-Chemical Hydride models

GM-Metal Hydride models

LANL-Chemical Hydride data

UM-Adsorbent data

ANL-System/energy analysis

Proposed Future Work

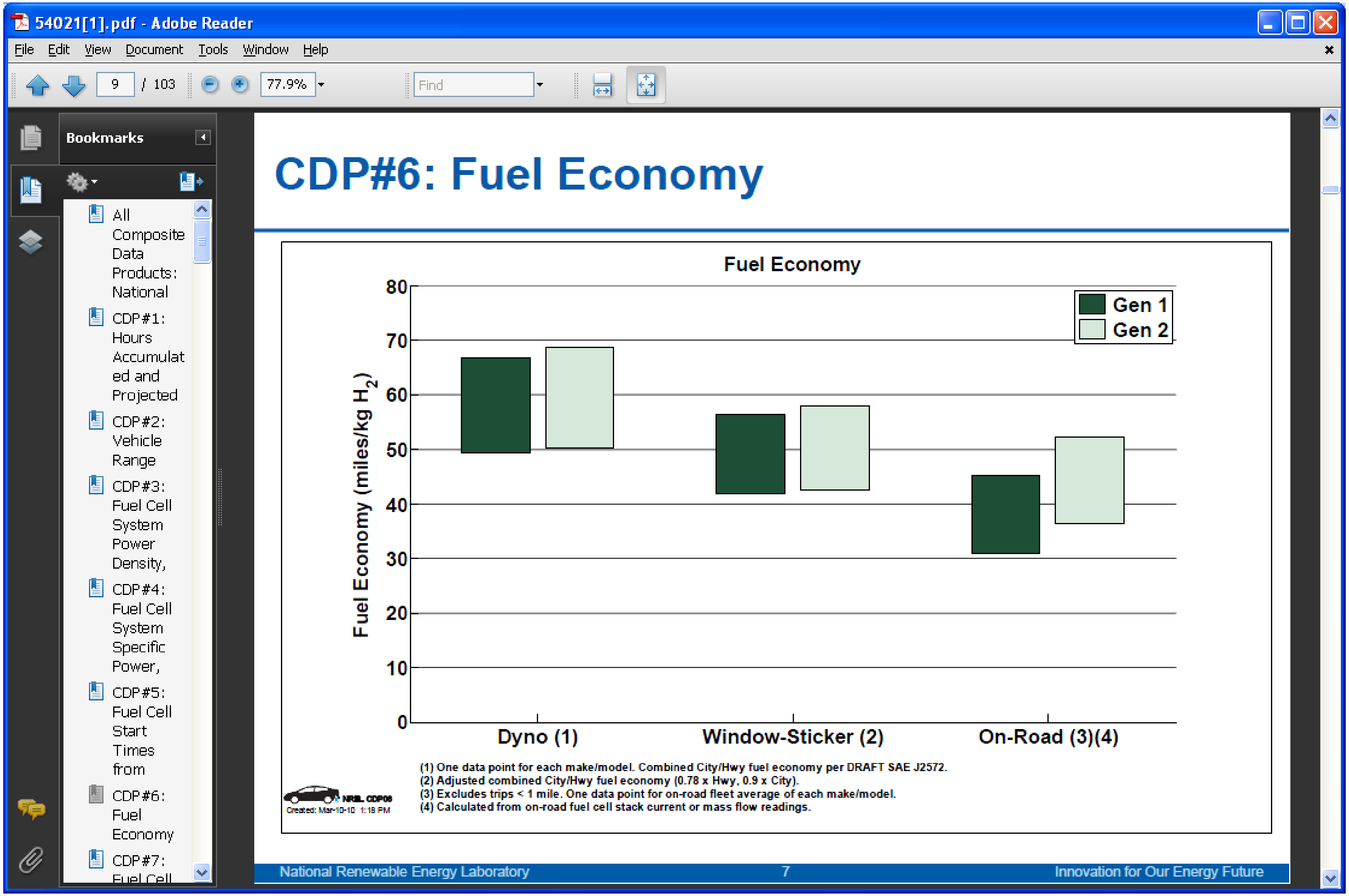
- Continue to run vehicle simulations to:
  - Refine storage systems sizing
  - Evaluate progress toward tech targets
  - Evaluate the impact of changes to existing storage system designs—refine system designs
  - Determine system demand/flow rate for phase III systems (based on US06 cycle)
- Energy Analysis
  - Model and calculate WTPP efficiencies, hydrogen cost, energy requirements and GHG emissions for adsorbent and CH Phase II systems
- Media engineering properties
  - Provide hydrogen storage engineering properties for selected sorbent materials/pellets as a function of temperature from ~30 K to 300K

Summary

- Manage HSECoE vehicle performance, cost and energy analysis technology area
- Vehicle Performance: Develop and apply model for evaluating hydrogen storage requirements, operation and performance tradeoffs at the vehicle system level.
- Energy Analysis: Coordinate hydrogen storage system WTW energy analysis to evaluate off-board energy impacts with a focus on storage system parameters, vehicle performance, and refueling interface sensitivities.
- Media engineering properties: Assist center in the identification and characterization of sorbent materials that have the potential for meeting DOE technical targets for an onboard systems.

Technical Back-Up Slides

FE Validation,



CDP#6: Fuel Economy

(1) One data point for each make/model. Combined City/Hwy fuel economy per DRAFT SAE J2572.
(2) Adjusted combined City/Hwy fuel economy (0.78 x Hwy, 0.9 x City).
(3) Excludes trips < 1 mile. One data point for on-road fleet average of each make/model.
(4) Calculated from on-road fuel cell stack current or mass flow readings.