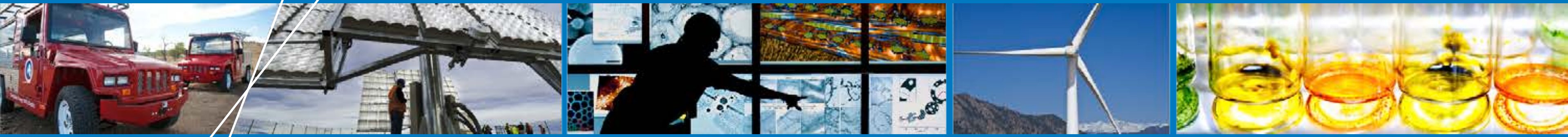
NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Hydrogen Storage Engineering
CENTER OF EXCELLENCE

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



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National Renewable Energy Laboratory (NREL)
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Project ID # ST008

Overview

Timeline

HSECoE start date: FY09
HSECoE end date: FY15
Percent complete: 70%

Budget

Total funding $1.8M

DOE Share 100%

Funding Received in FY12: $110K

Funding for FY13: $100K

Hydrogen Storage Engineering
CENTER OF EXCELLENCE

Barriers

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

Partners

Savanna River National Lab (SRNL), Pacific Northwest National Lab (PNNL), United Technologies Research Center (UTRC), Jet Propulsion Lab (JPL), Ford, General Motors (GM), Los Alamos National Lab (LANL), Oregon State University (OSU), University of Michigan (UM) the DOE Vehicle Technologies Program.

Relevance/Objectives

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

- Manage Hydrogen Storage Engineering Center of Excellence (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 well-to-wheels (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 Department of Energy (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 DOE technical targets
  - Relative in class and across class for materials systems
  - Relative to physical storage systems
  - Relative to conventional vehicles

Objectives: Energy Analysis

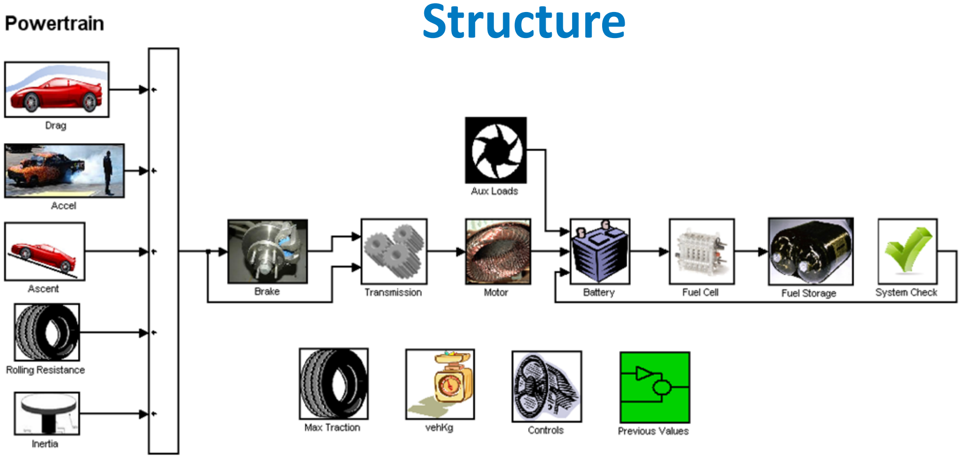
- Perform hydrogen storage system energy analysis to evaluate well-to-power-plant (WTPP) efficiency, Energy requirements, hydrogen cost and green house gas (GHG) emissions
    - Develop vehicle a level models and obtain fuel economy (FE) figures for energy analysis.
    - Obtain data from center partners on storage system designs (mass, volume, operating temperature (T) and pressure (P))/fuel interface/dispensing/station energy requirements.
    - Work with other teams (e.g. Hydrogen Delivery and Systems Analysis) and use existing data for H_2 production and distribution and tank production and carbon dioxide equivalent (CO_2e) emission factors (from GREET, H_2 A, etc.) to calculate WTPP efficiencies etc.
    - Adjust model inputs based on changes in storage system design and data to obtain final results.
    - FY13 focus is on 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

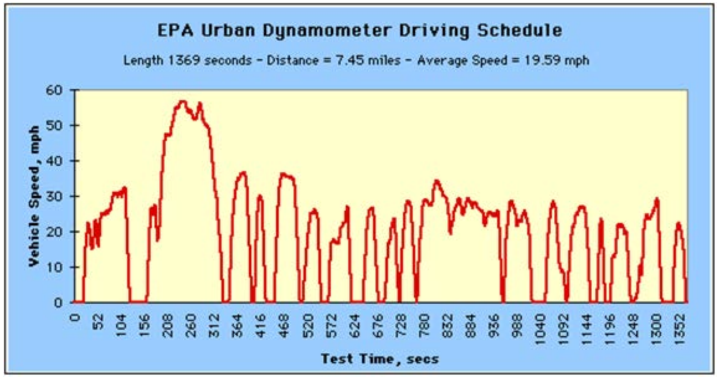
Date	Milestone or Go/No-Go Decision	Status
2/13	NREL will work center partners to set up and run vehicle simulations to evaluate the key volumetric, gravimetric, and on-board efficiency trade-offs over three test cases (drive cycles) and progress towards 2017 targets for two chemical hydrogen and two to three adsorbent system designs in support of final design selection for each material class for phase III work.	100%
8/13	Provide summary of scaled H2 storage system engineering material property input.	30%
9/13	Provide HSECoE appropriate engineering properties	30%
9/13	Calculate and model the well-to-powerplant (WTPP) efficiency for two adsorbent storage system designs and compare results relative to the 60% technical target.	50%
9/13	Calculate and model the well-to-powerplant (WTPP) efficiency for two chemical hydrogen (CH) storage system designs and compare results relative to the 60% technical target.	100%

Approach: Develop HSSIM (Vehicle Model)

Structure



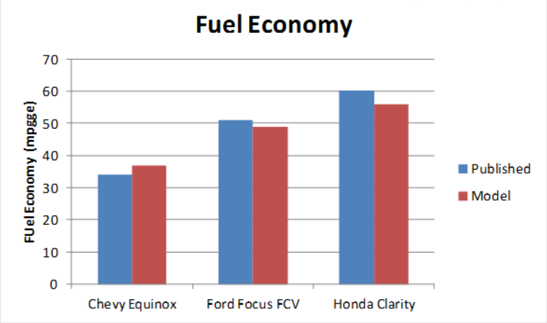
Drive Cycles

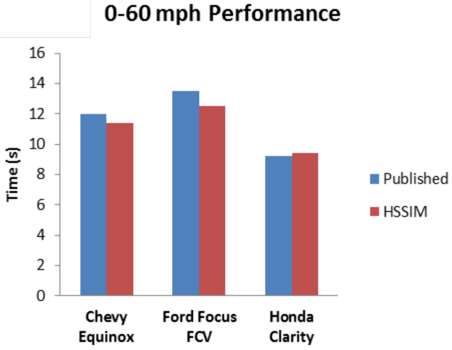


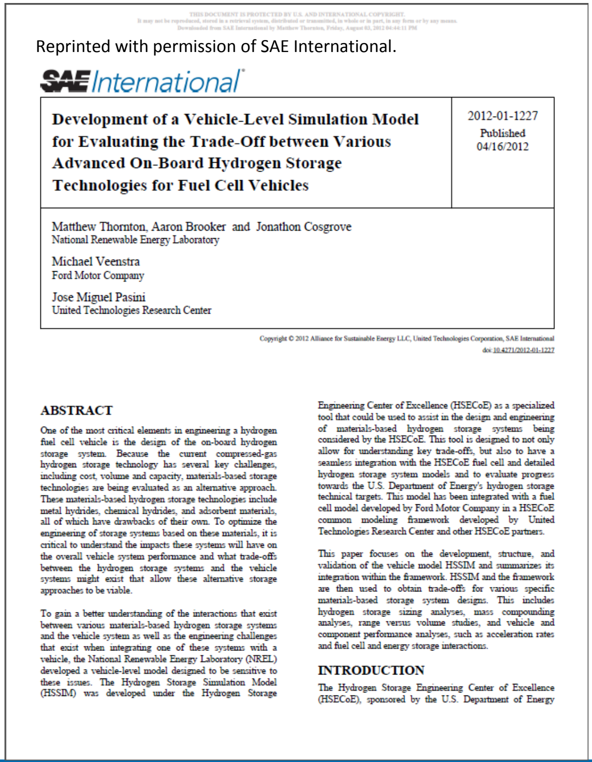
Output

- Fuel economy (mpgge) based on EPA adjusted five cycle estimate
- Range (miles) from adjusted mpgge
- Onboard efficiency (%)
- Hydrogen flow (moles/s)
- Vehicle performance (e.g. 0-60 mph time)

Validation







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Development of a Vehicle-Level Simulation Model for Evaluating the Trade-Off between Various Advanced On-Board Hydrogen Storage Technologies for Fuel Cell Vehicles

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ABSTRACT

One of the most critical elements in engineering a hydrogen fuel cell vehicle is the design of the on-board hydrogen storage system. Because the current compressed-gas hydrogen storage technology has several key challenges, including cost, volume and capacity, materials-based storage technologies are being evaluated as an alternative approach. These materials-based hydrogen storage technologies include metal hydrides, chemical hydrides, and adsorbent materials, all of which have drawbacks of their own. To optimize the engineering of storage systems based on these materials, it is critical to understand the impacts these systems will have on the overall vehicle system performance and what trade-offs between the hydrogen storage systems and the vehicle systems might exist that allow these alternative storage approaches to be viable.

To gain a better understanding of the interactions that exist between various materials-based hydrogen storage systems and the vehicle system as well as the engineering challenges that exist when integrating one of these systems with a vehicle, the National Renewable Energy Laboratory (NREL) developed a vehicle-level model designed to be sensitive to these issues. The Hydrogen Storage Simulation Model (HSSIM) was developed under the Hydrogen Storage Engineering Center of Excellence (HSECoE) as a specialized tool that could be used to assist in the design and engineering of materials-based hydrogen storage systems being considered by the HSECoE. This tool is designed to not only allow for understanding key trade-offs, but also to have a seamless integration with the HSECoE fuel cell and detailed hydrogen storage system models and to evaluate progress towards the U.S. Department of Energy's hydrogen storage technical targets. This model has been integrated with a fuel cell model developed by Ford Motor Company in a HSECoE common modeling framework developed by United Technologies Research Center and other HSECoE partners.

This paper focuses on the development, structure, and validation of the vehicle model HSSIM and summarizes its integration within the framework. HSSIM and the framework are then used to obtain trade-offs for various specific materials-based storage system designs. This includes hydrogen storage sizing analyses, mass compounding analyses, range versus volume studies, and vehicle and component performance analyses, such as acceleration rates and fuel cell and energy storage interactions.

INTRODUCTION

The Hydrogen Storage Engineering Center of Excellence (HSECoE), sponsored by the U.S. Department of Energy

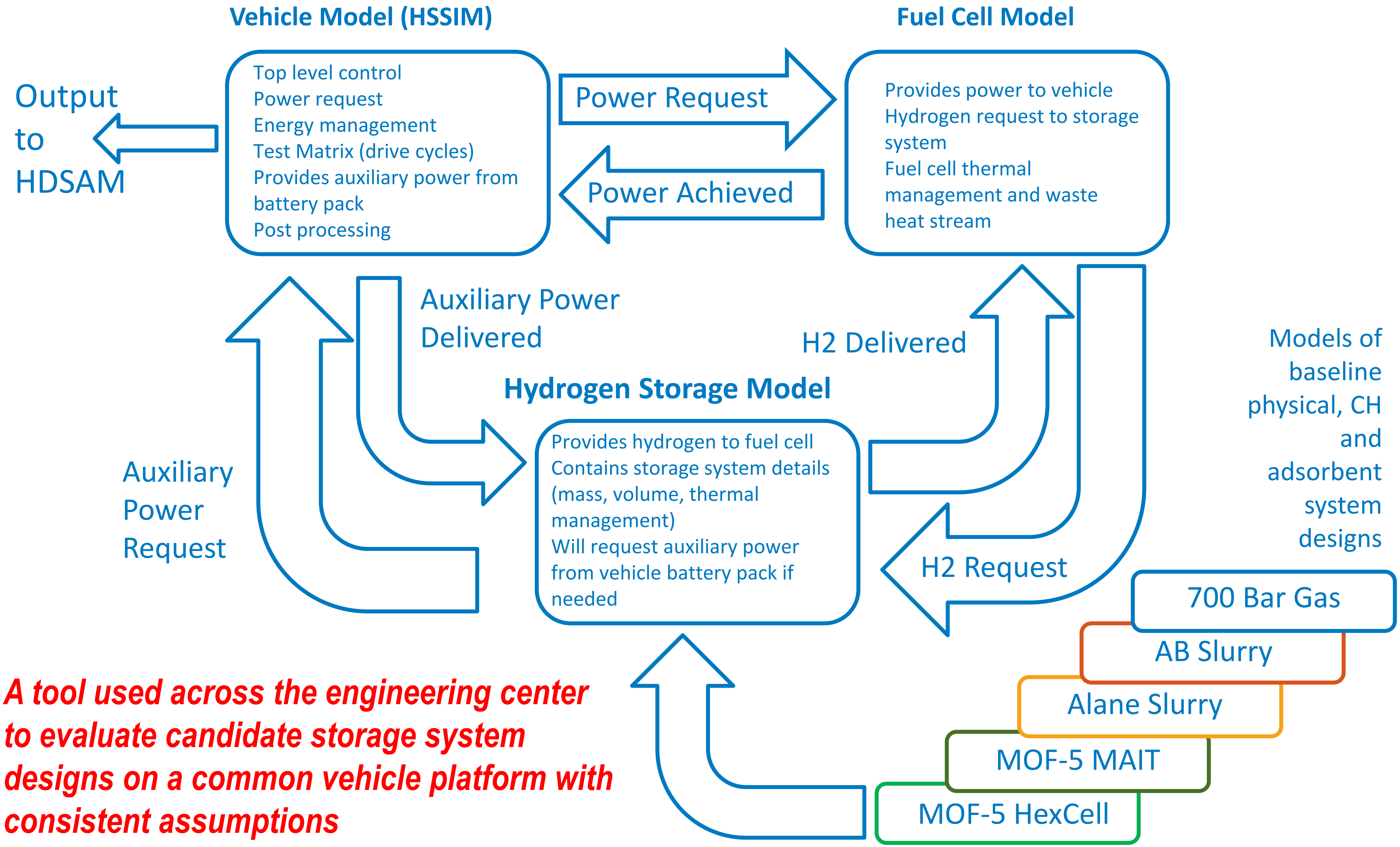
Approach: Vehicle Assumptions

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 Model (HSSIM)

- Top level control
- Power request
- Energy management
- Test Matrix (drive cycles)
- Provides auxiliary power from battery pack
- Post processing

Fuel Cell Model

- Provides power to vehicle
- Hydrogen request to storage system
- Fuel cell thermal management and waste heat stream

Hydrogen Storage Model

- Provides hydrogen to fuel cell
- Contains storage system details (mass, volume, thermal management)
- Will request auxiliary power from vehicle battery pack if needed

Models of baseline physical, CH and adsorbent system designs

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

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 hydrogen delivery components – pipelines, tube trailers, liquid hydrogen ($LH_{2)}$ 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 (WTPP), and GHGs (gms/mile)**

Approach: Energy Analysis Assumptions for HDSAM

Production: Steam Methane Reforming (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: 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.

- Provide measurements of relevant metal organic framework (MOF)-5 samples to validate models.

NREL's Sitaram PCTPro System with Temperature Stability Improvements to Measure Hydrogen Isotherms

Accomplishments: Vehicle Performance Summary-End of Phase I

Simulated vehicle performance results for Phase I 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)
Fluid AB	45	254	96	4.6	38.9
Alane	43	239	88	4.6	38.9
AX21 press FCHX	49	273	97	4.3	25.2
MOF5 Cmpct-FCHX	48	271	97	3.5	24.1
MOF5 Press FCHX	49	276	98	4.6	25.3
350 bar Compressed Gas	50	280	100	4.8	17.0
700 bar Compressed Gas	50	279	100	4.7	25.0

Phase I Results from 2012 AMR Presentation

Accomplishments: Vehicle Performance Summary-End of Phase II

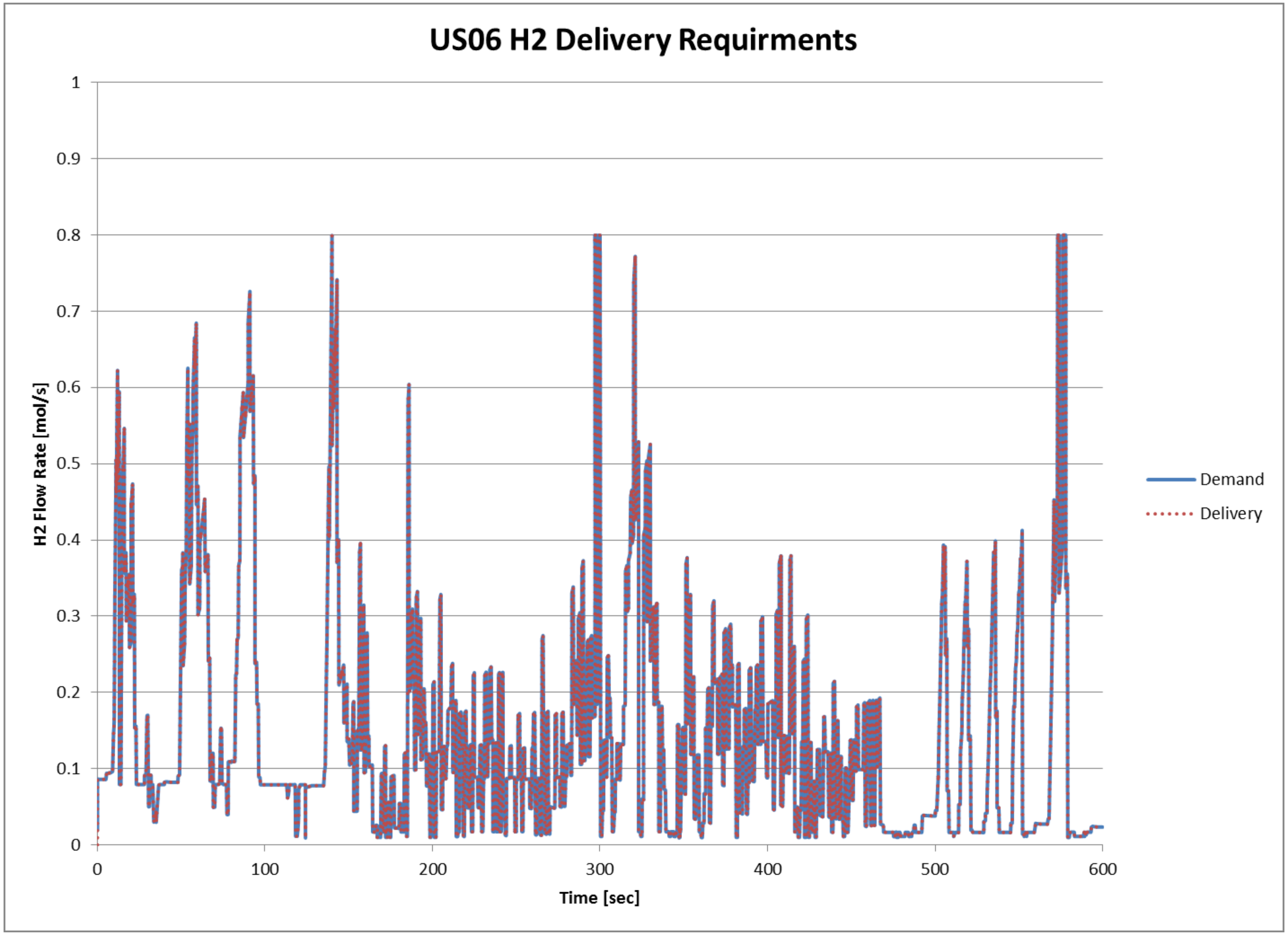
Simulated vehicle performance results for Phase II hydrogen storage systems with fixed on-board H2 (from framework)

Fixed on-board usable H2 = 5.6kg

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Range (mi)	On-Board Efficiency (%) UDDS/HFET	Gravimetric Density (wt. %)	Volumetric Density (g/l)	System Mass (kg)
Exothermic AB Slurry	47	264	97	4.2	36.8	137.1
Endothermic Alane Slurry	44	244	93	3.4	34.3	185.1
HexCell Powder MOF-5	49*	274*	92**	3.5	17.5	137.6
MATI Puck MOF-5 (.32g/cc)	48*	269*	97**	3.4	20.7	149.3
700 bar Compressed Gas	50	279	100	4.7	25.0	119.0

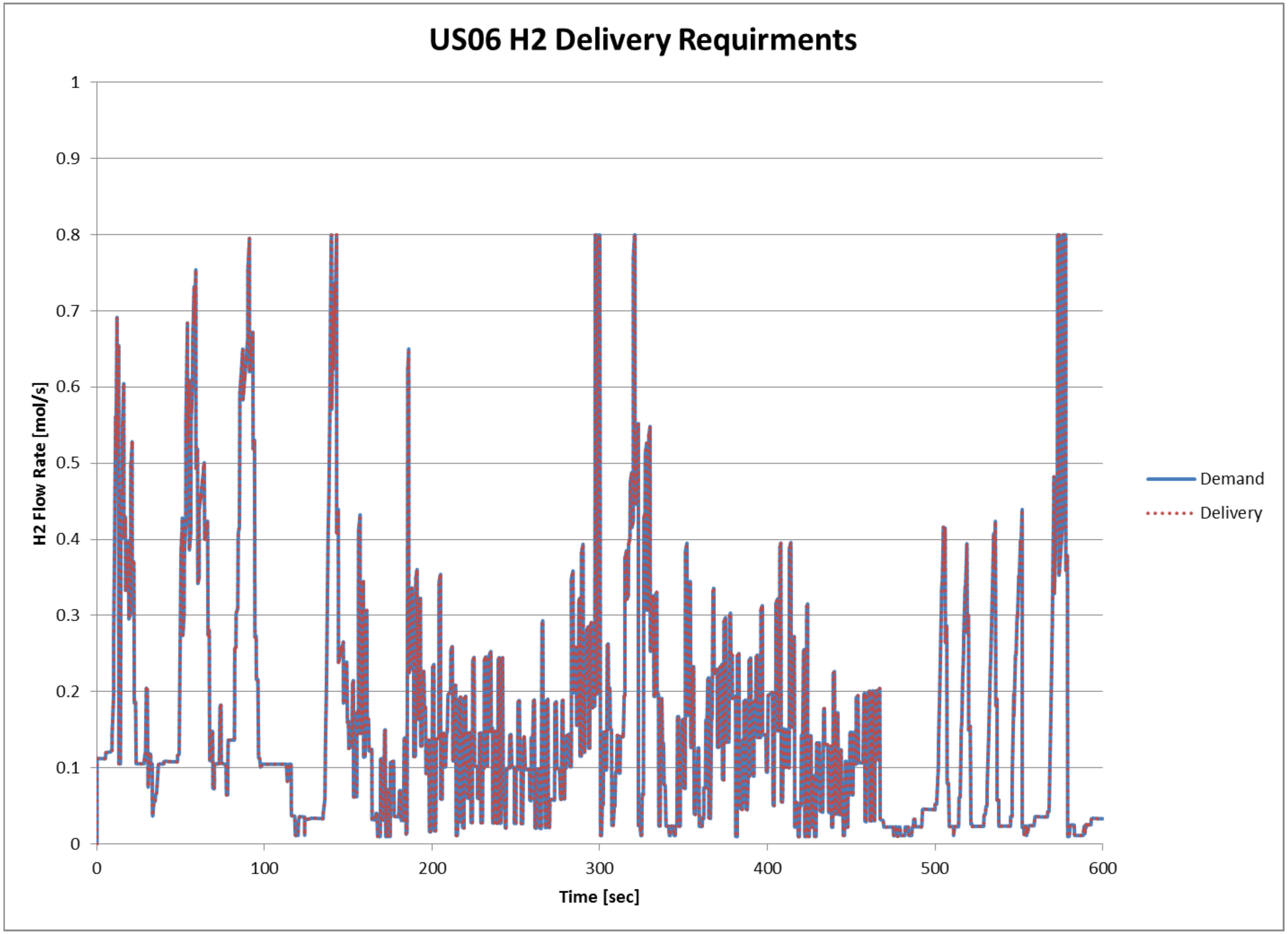
*Preliminary Model Results **Off Model Calculations

Accomplishment: US06-Aggressive Dive Cycle
H2 Delivery Requirements Exothermic AB Slurry



System meets drive cycle demands under aggressive driving conditions

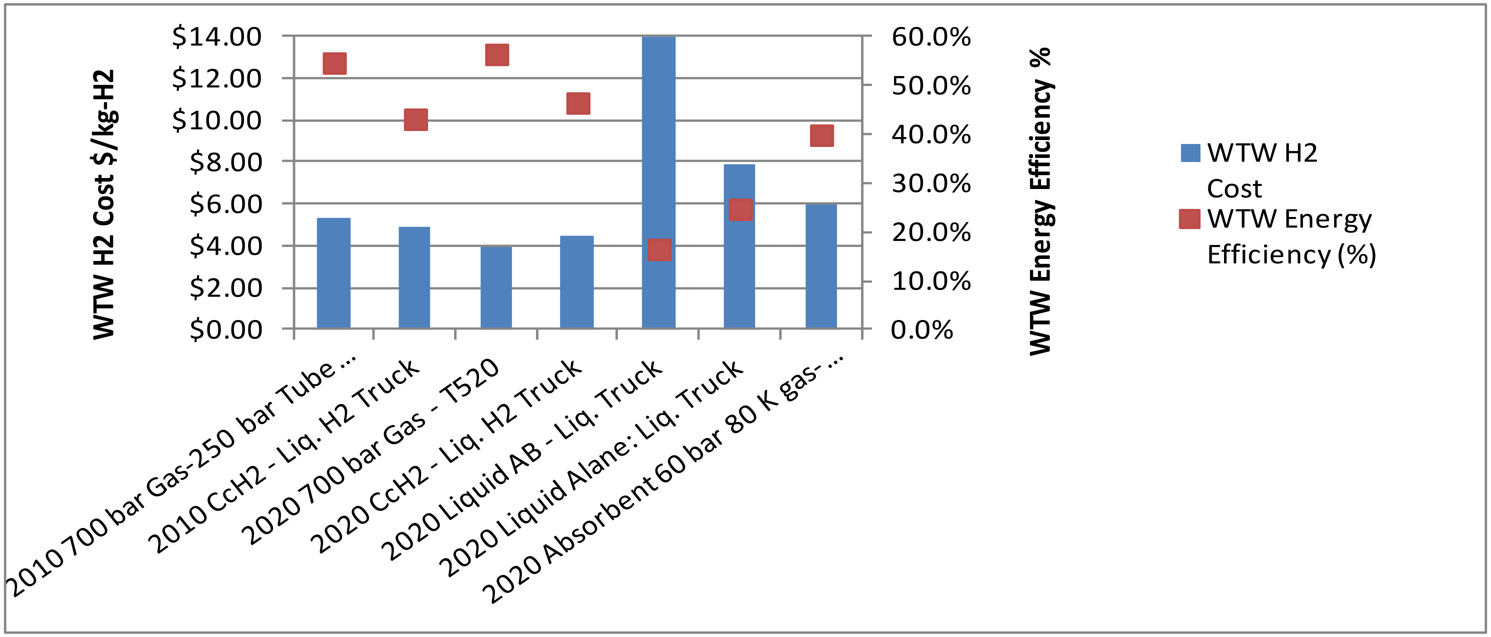
Accomplishment: US06-Aggressive Dive Cycle H2 Delivery Requirements Endothermic Alana Slurry



System meets drive cycle demands under aggressive driving conditions

Accomplishment: WTW Storage Systems Results

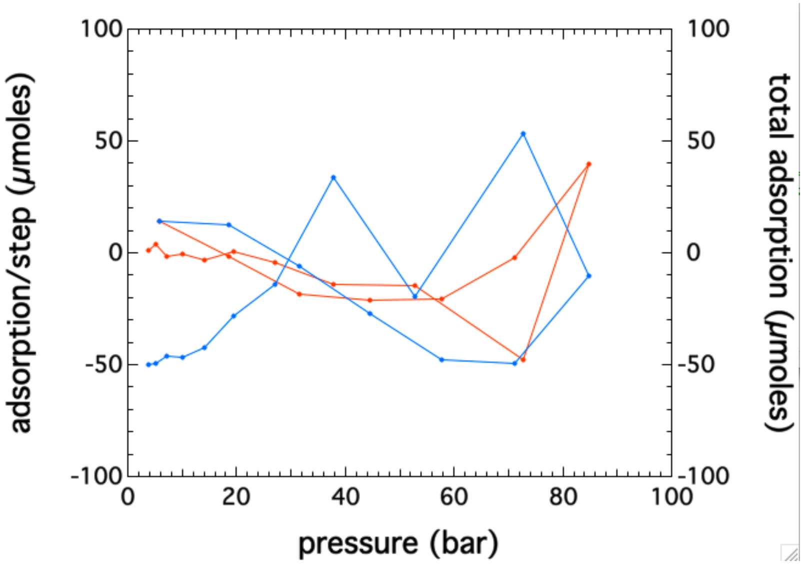
Draft—Preliminary Results	WTW H2 Cost ($/kg-H2)	WtW Energy Efficiency (%)	WTW GHG Emissions (gms/mile)	Volumetric Efficiency (gms-H2/L)
2010 700 bar Gas-250 bar Tube Trailer	$5.28	54.7%	240	25.6
2010 CcH2 - Liq. H2 Truck	$4.92	43.2%	322	41.8
2020 700 bar Gas - T520	$3.91	56.4%	230	25.6
2020 CcH2 - Liq. H2 Truck	$4.49	46.5%	289	41.8
2020 Liquid AB - Liq. Truck	$13.96	16.5%	915	41.4
2020 Liquid Alane: Liq. Truck	$7.89	24.7%	642	32.2
2020 Absorbent 60 bar 80 K gas-T340	$6.00	39.9%	407	24.1



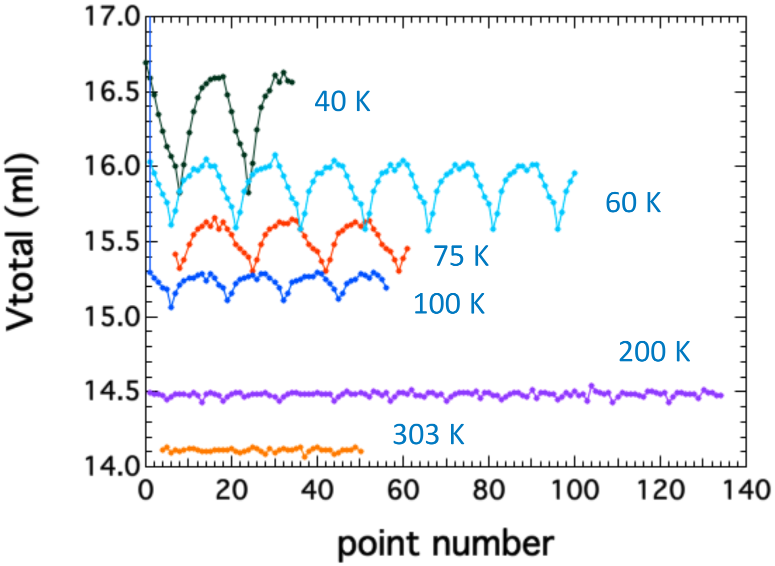
Accomplishment: Isotherm Measurement Method Calibration

Provided isotherm measurements on MOF-5 powder at 40 K and 60 K

- Systematic evaluation requiring the use of a He cyrostat cooler that can be adjusted to hold the sample at a temperature between 20 K and 330 K.
  - Calibration indicates appropriate temperature control & self-consistent zero measurements.
  - With a stainless steel tube sample holder, the thermal conductivity is an issue and a pressure dependence of the different volumes is observed, especially at lower temperatures.
  - This pressure dependence should not occur; not known why it is affecting the measurement.



Hydrogen adsorption of empty sample holder at 75 K. The data show that the instrument is providing a reasonable measure of zero adsorption as a function of pressure. Red: Adsorption per Step (left axis). Blue: Total Adsorption (right axis).



Adsorrption system calibration measurements with He show a pressure dependence for the volume that increases as the temperature decreases below 200K.

Accomplishment: Isotherm Measurement

Improved isotherm measurements at less than 75 K.

- Developed a “difference” technique that removes He calibration.
  - Measures H2 adsorption difference between 303 K (RT) and 40 K to 75 K. 303 K (RT) adsorption usually negligible.
  - Preliminary results: measured adsorption at 40 K with difference method is similar to the models.
- Redesigned cryostat sample holder to minimize pressure dependent effects.
- At this time, no additional work to improve the measurements is planned.

Pressure (Bar)	**Difference Method 100*(gH2/gsample)**	**A-D Model 100*(gH2/gsample)**
1.3	8.2	
1.5	8.3	8.5
1.8	8.5	
4		10.5

Preliminary difference method results compared with model at 40 K. The maximum adsorption from the model is approximately 10.5 g/gX100 at 4 bar. Additional measurements are needed to measure intermediate pressures.

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

Management of collaboration efforts across organizations is done through monthly and on-demand modeling team telecons, bi-annual face-to face-meetings and through SharePoint

Proposed Future Work

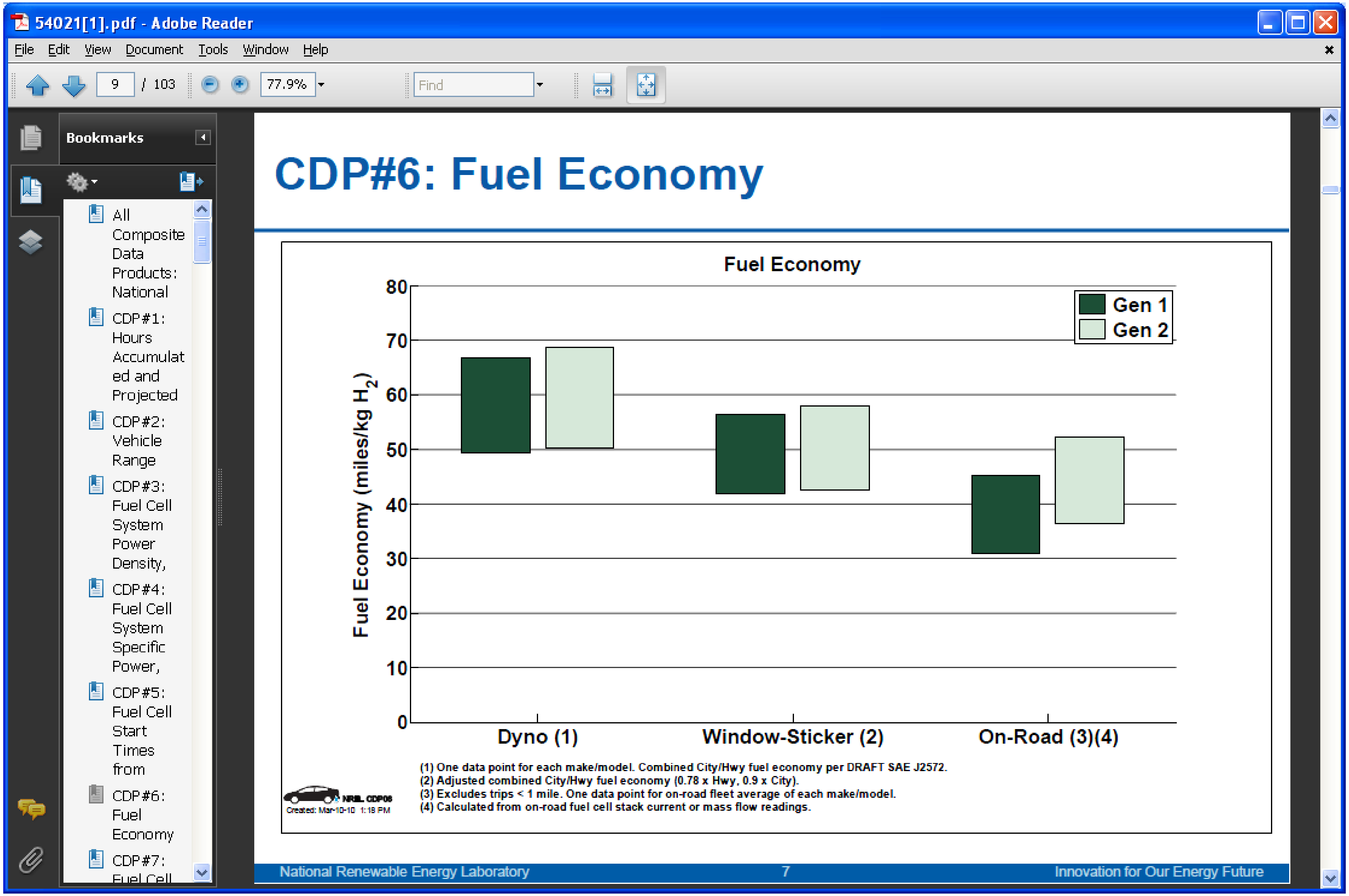
- Continue to run vehicle simulations to:
  - Evaluate the impact of changes to phase III storage system designs and refinements
  - Determine system demand/flow rate for phase III systems (based on US06 cycle)
  - Assist with public release and access of all center models
- Energy Analysis
  - Work complete
- Media engineering properties
  - Possibly provide hydrogen storage engineering properties for selected sorbent materials/pellets at the appropriate conditions to validate models.

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.

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Adjusted Five Cycle Fuel Economy Calculation (Window Sticker)

$$Adjusted\_City\_MPGGE = \frac{1}{0.003259 + \dfrac{1.1805}{Model\_City\_MPGGE}} \tag{1}$$

$$Adjusted\_Highway\_MPGGE = \frac{1}{0.001376 + \dfrac{1.3466}{Model\_Highway\_MPGGE}}$$

$$Adjusted\_Combined\_MPGGE = (Adjusted\_City\_MPGGE \bullet 0.55) + (Adjusted\_Highway\_MPGGE \bullet 0.45)$$