NATIONAL RENEWABLE ENERGY LABORATORY

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

2011 DOE Hydrogen and Fuel Cell Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting

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Overview

Timeline

HSECoE start date: FY09
HSECoE end date: FY14
Percent complete: 35%

Budget

Total funding $1.8M
FY 2009: $425K
FY 2010: $660K
FY 2011: $400K

Hydrogen Storage Engineering
CENTER OF EXCELLENCE

Barriers

- System cost
- Charge/discharge rate
- System mass
- Systems volume
- Life-cycle GHG emissions
- Transient response
- Well-to-power plant efficiency

Partners

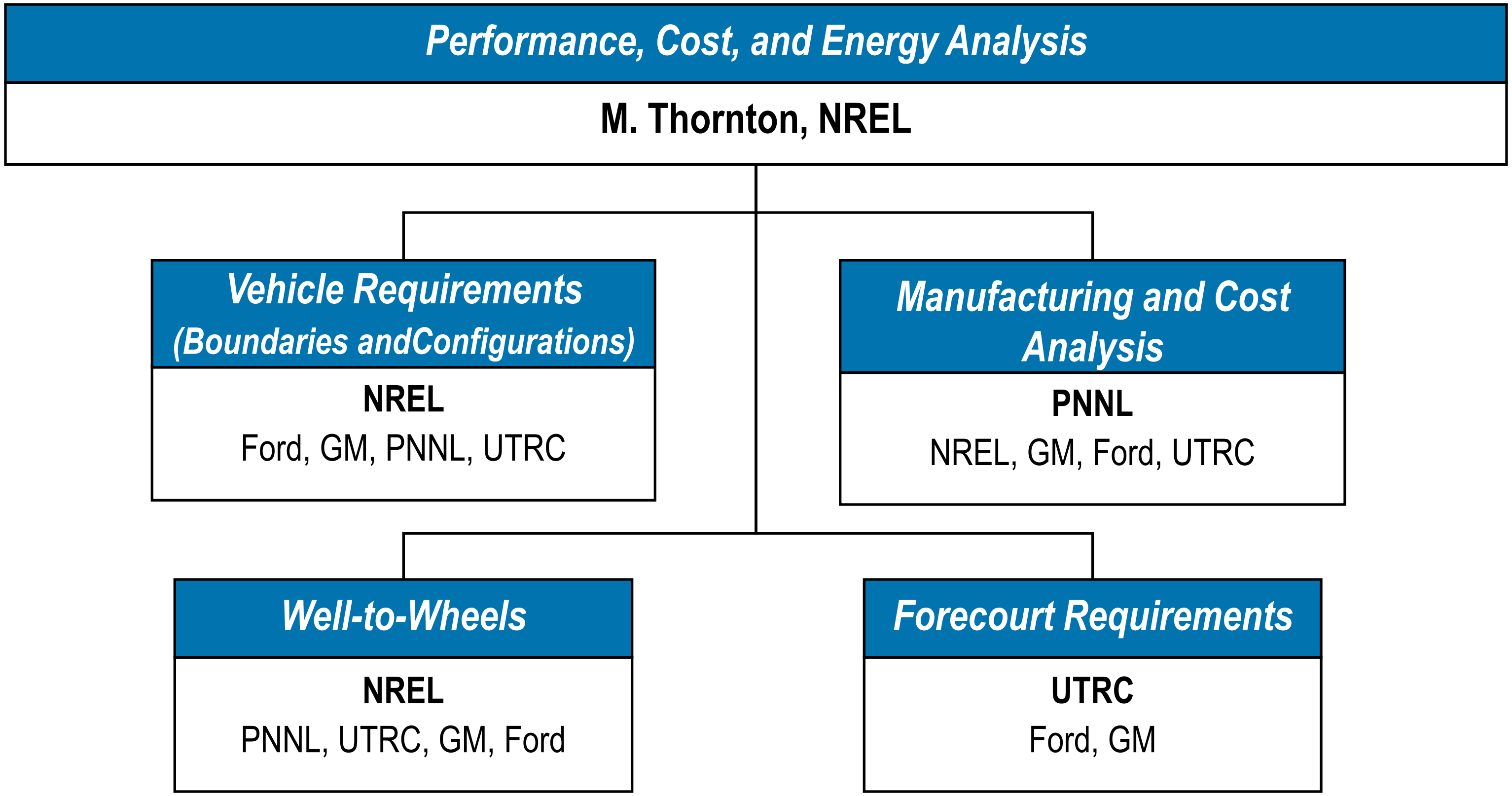
SRNL, PNNL, UTRC, UQTR, JPL, Ford, GM, LANL, OSU,BASF, DOE HSCoE, DOE MHCoE, the DOE Vehicle Technologies Program.

Objectives

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

- Manage HSECoE performance, cost and energy analysis technology area
- Vehicle Requirements: Develop and apply model for evaluating hydrogen storage requirements, performance, and cost tradeoffs at the vehicle system level.
- Well-to-wheels: Perform hydrogen storage system WTW energy analysis to evaluate GHG 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 as an onboard systems.

Performance, Cost, and Energy Analysis Technology Area Management



Objectives – Vehicle Requirements

- Develop and apply a model for evaluating hydrogen storage requirements, performance and cost trade-offs at the vehicle system level; e.g. Range, cost, size, efficiency, mass, performance, on-board efficiency
- Model application will identify
  - Storage system sizing
  - Relative importance/sensitivity of tradeoffs
  - Critical tech targets
  - Pathways to meet GO/NO-GO criteria
  - Important trends
  - Assumptions that are “driving” vehicle design and H_2 storage requirements

Objectives – Well-to-Wheels Analysis

- Perform hydrogen storage system WTW energy analysis to evaluate GHG impacts
  - Develop vehicle a level models and obtain FE figures for overall WTW analysis.
  - Obtain data from center partners on storage system designs (mass, volume, operating T and P)/fuel interface/dispensing/station energy requirements.
  - Use existing data for H_2 production and distribution and tank production and CO_2e emission factors (GREET, H2A, etc.) and calculate WTV (power plant) efficiencies.
  - Adjust model inputs based on changes in storage system design and data to obtain final results.

Objectives – Media Engineering Properties

- Work with Hydrogen Storage Center of Excellence and community to identify potential materials for engineering analysis.
  - Technology Team Co-Lead: Hydrogen Storage Materials Center of Excellence Collaborations, in the Materials Operating Requirements (MOR) Technology Area
- Measure and characterize promising sorption material properties for onboard hydrogen storage engineering analysis.
  - Technology Team Lead: Adsorbent Material Properties, in MOR Technology Area
- Provide detailed material property input and guidance for analysis and design of hydrogen storage systems optimized for sorption materials.

Accomplishments – Vehicle Requirements

Created a Hydrogen Storage Vehicle Model (HSSIM)

Generate higher level component models

Hydrogen **S**torage

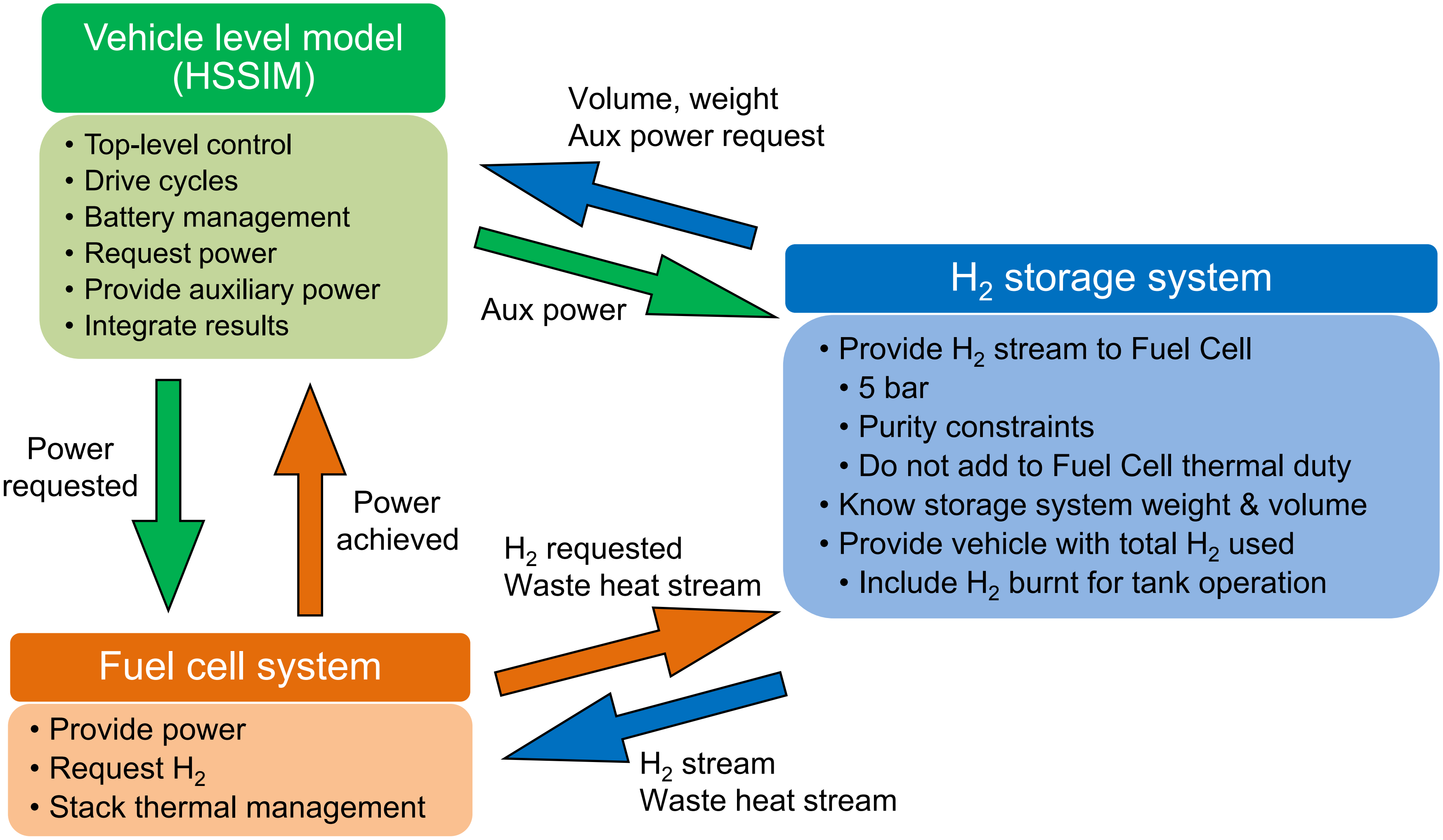
SIMulator

Run faster simulations

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

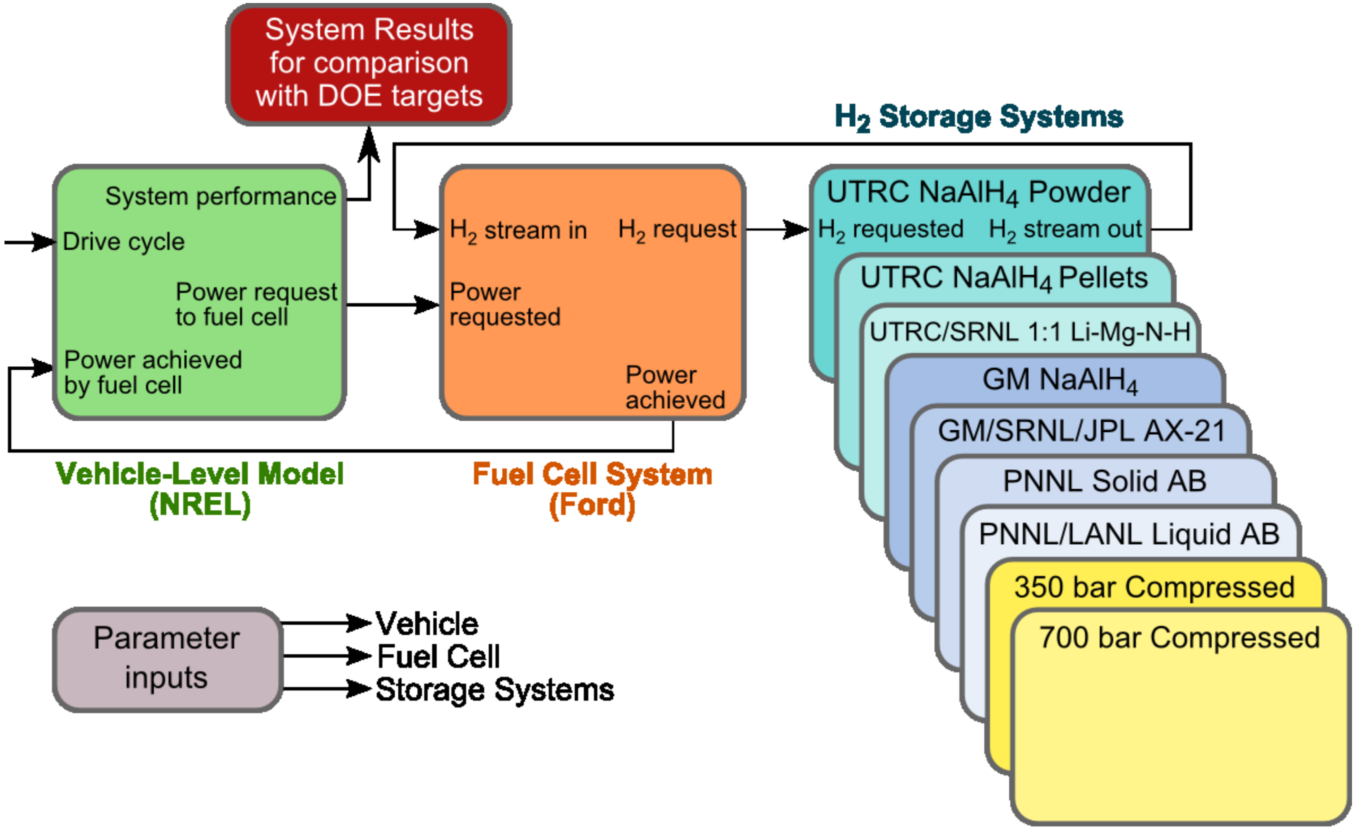
Approach

Provide a common means of system comparison



Approach

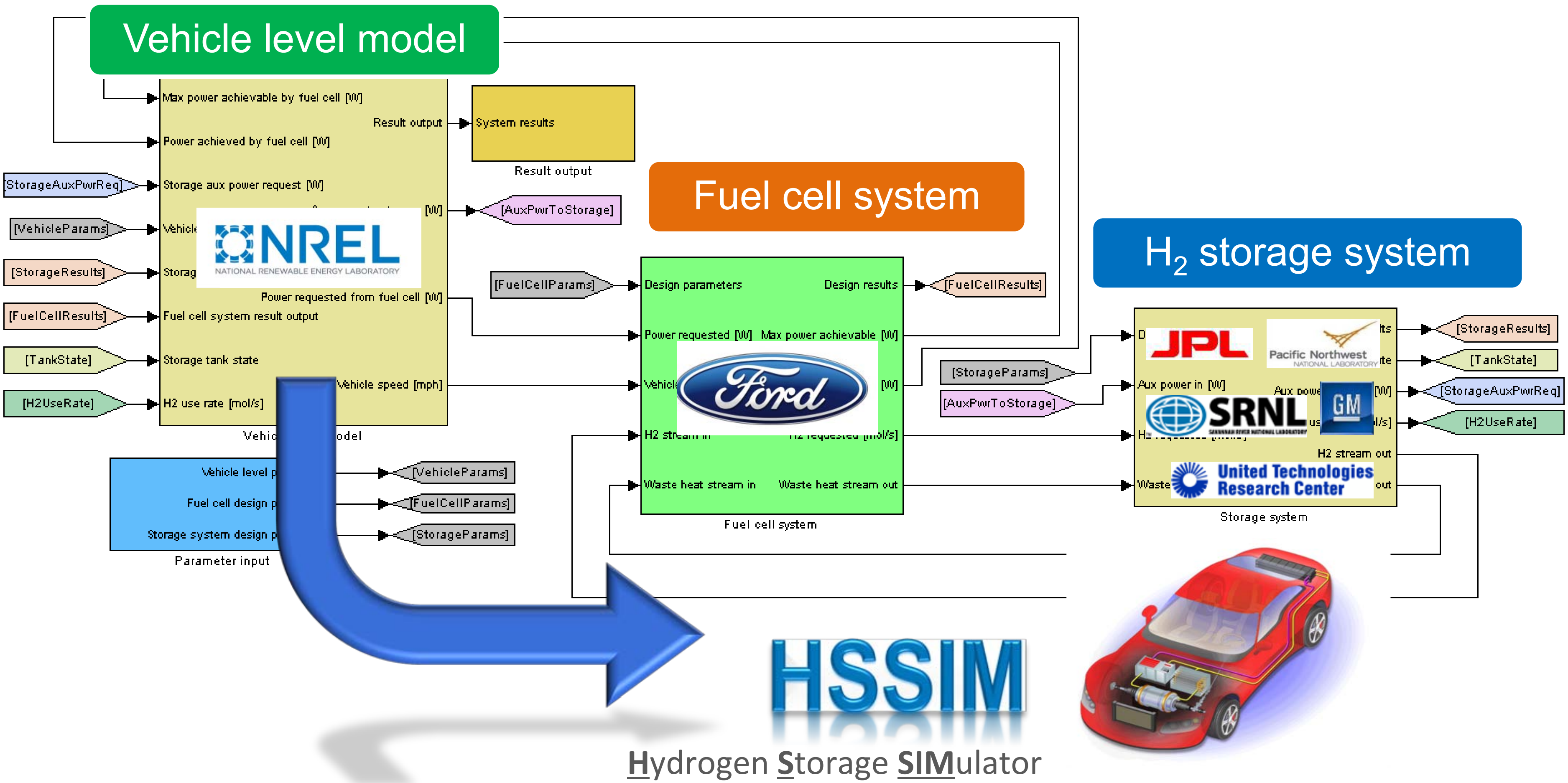
Developed well-defined, high-level interfaces



Slide provided courtesy of José Miguel Pasini UTRC

Integrated Model Framework

Implemented in the MATLAB/Simulink environment



HSSIM (Vehicle Model) Structure

Model Inputs

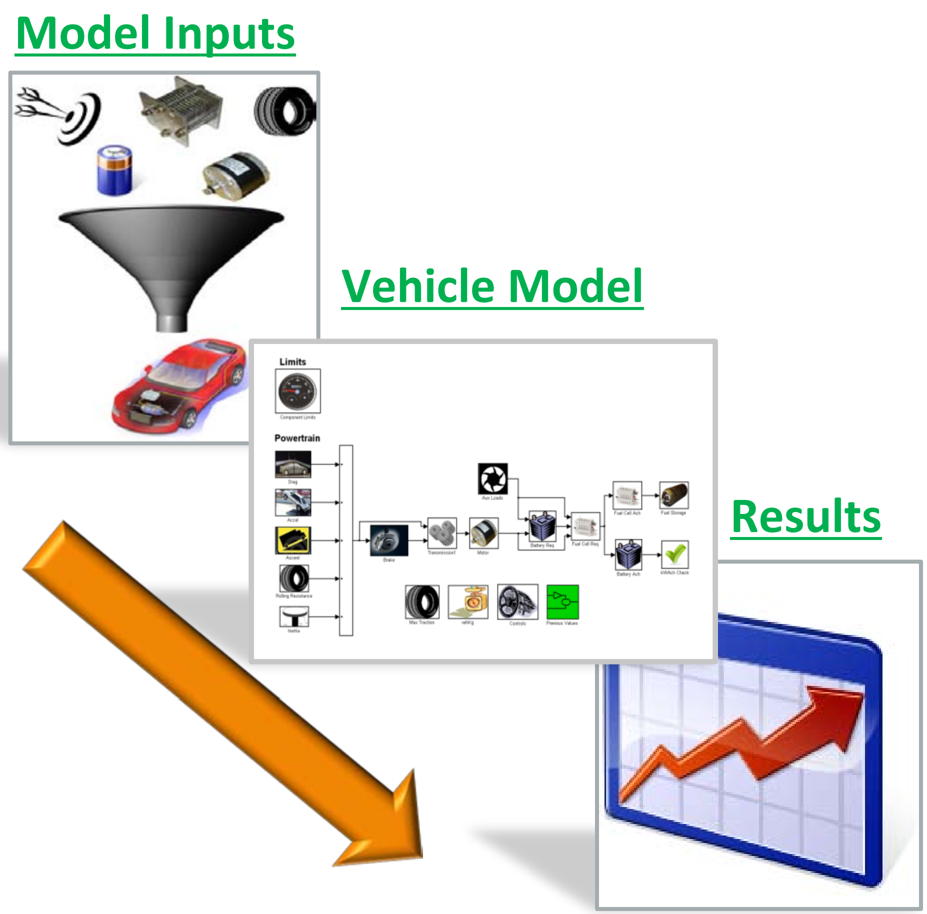
- Vehicle characteristics
- Fuel cell characteristics
- H_2 storage system
- Vehicle level test matrix

Vehicle Model

- Power requirement calculation

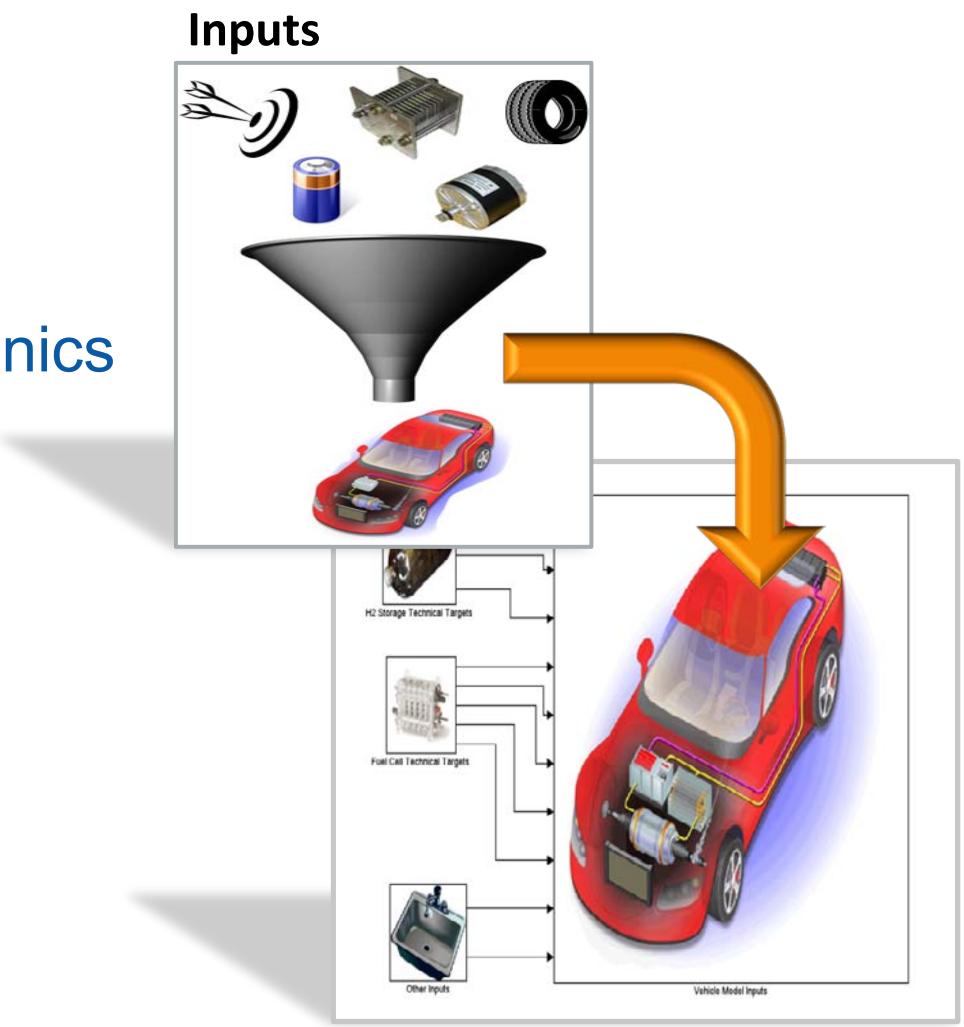
Results

- Fuel economy (mpgge)
- Range (miles)
- Vehicle mass (kg)
- Onboard efficiency (%)
- Vehicle performance



Key Vehicle-Level Components

1. H_2 storage system
2. Fuel cell system
3. Motor and power electronics
4. Energy storage
5. Vehicle attributes



Vehicle Model Components

From the H_2 Storage System

Significant Inputs:

- System mass (kg)
- System volume (l)
- Onboard usable H_2 (kg)
- H_2 total use rate (mol/s)
- Auxiliary power request (kW)
- System cost ($/kWh)

From the Fuel Cell System

Significant Inputs:

- System mass (kg)
- System volume (l)
- Max power achievable (kW)
- H_2 flow received (mol/s)
- Power achieved (kW)
- System cost ($/kWh)

Assumptions

Vehicle

Midsize Car Class (Family Sedan):

Vehicle Attribute	Units	Value
Glider mass[1]	kg	990
Frontal area	m^2	2.2
Drag coefficient	–	0.29
Rolling Resistance	–	0.008
Tires	–	P195/65R15

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

Vehicle Test Schedule

UDDS

Urban Dynamometer Drive Schedule

HWFET

Highway Fuel Economy Cycle

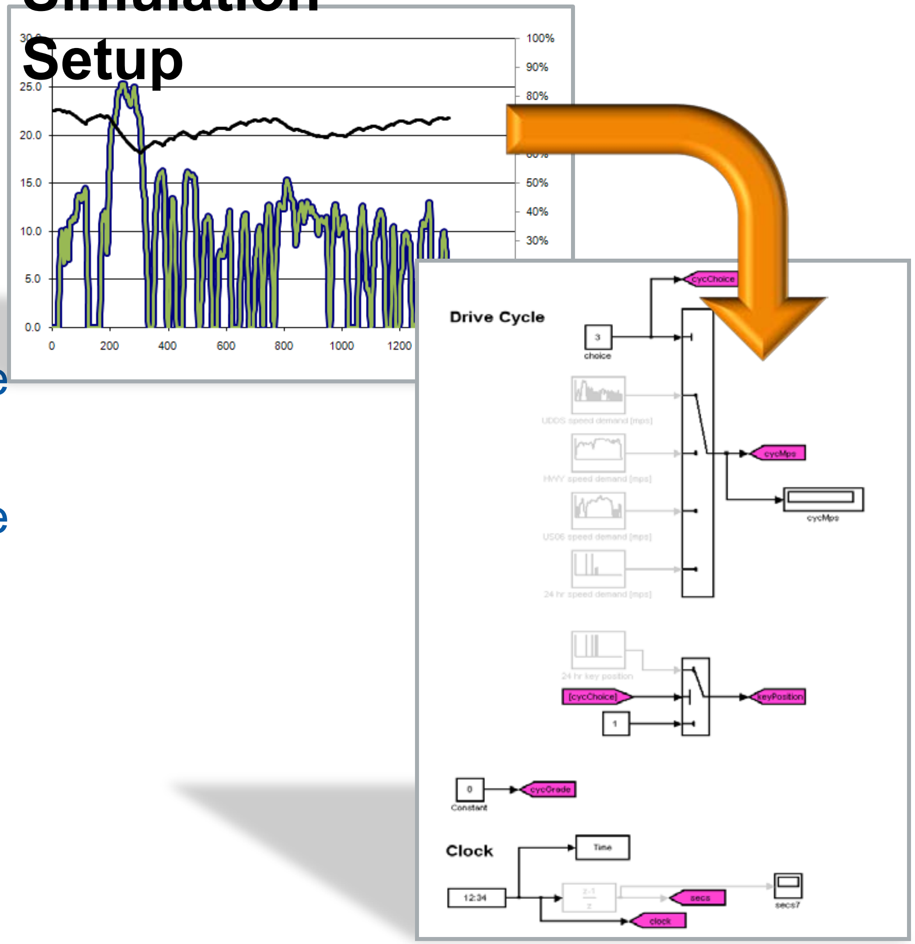
US06

Supplemental Federal Test Procedure

SC03

Supplemental Federal Test Procedure

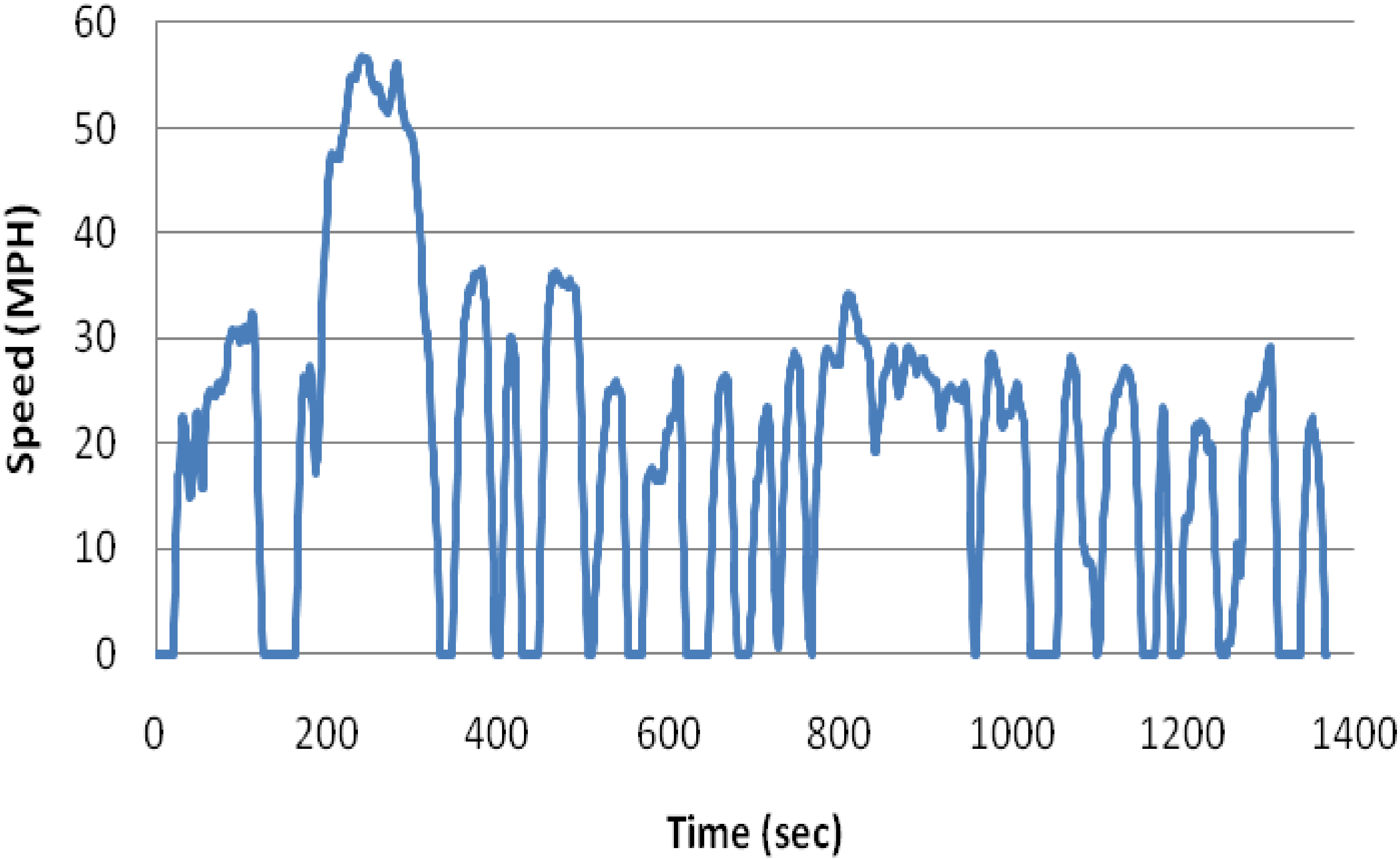
Simulation Setup



Test Matrix – Drive Cycle Used To Test the Systems

Case	Test Schedule	Cycles	Description	Test Temp (°F)	Distance per cycle (miles)	Duration per cycle (minutes)	Top Speed (mph)	Average Speed (mph)	Max. Acc. (mph /sec)	Stops	Idle	Avg. H2 Flow (g/s)*	Peak H2 Flow (g/s)*	Expected Usage
1	**Ambient Drive Cycle** - Repeat the EPA FE cycles from full to empty and adjust for 5 cycle post-2008	UDDS	Low speeds in stop-and-go urban traffic	75 (24 C)	7.5	22.8	56.7	19.6	3.3	17	19%	0.09	0.69	**1. Establish baseline fuel economy (adjust for the 5 cycle based on the average from the cycles) 2. Establish vehicle attributes 3. Utilize for storage sizing**
		HWFET	Free-flow traffic at highway speeds	75 (24 C)	10.26	12.75	60	48.3	3.2	0	0%	0.15	0.56	
2	**Aggressive Drive Cycle** - Repeat from full to empty	US06	Higher speeds; harder acceleration & braking	75 (24 C)	8	9.9	80	48.4	8.46	4	7%	0.20	1.60	**Confirm fast transient response capability – adjust if system does not perform function**
3	**Cold Drive Cycle** - Repeat from full to empty	FTP-75 (cold)	FTP-75 at colder ambient temperature	-4 (-20 C)	11.04	31.2	56	21.1	3.3	23	18%	0.07	0.66	**1. Cold start criteria 2. Confirm cold ambient capability – adjust if system does not perform function**
4	**Hot Drive Cycle** - Repeat from full to empty	SC03	AC use under hot ambient conditions	95 (35 C)	3.6	9.9	54.8	21.2	5.1	5	19%	0.09	0.97	**Confirm hot ambient capability - adjust if system does not perform function**
5	**Dormancy Test**	n/a	Static test to evaluate the stability of the storage system	95 (35 C)	0	31 days	0	0	0	100%	100%			**Confirm loss of useable H2 target**

Test Matrix – Drive Cycle Used To Test the Systems



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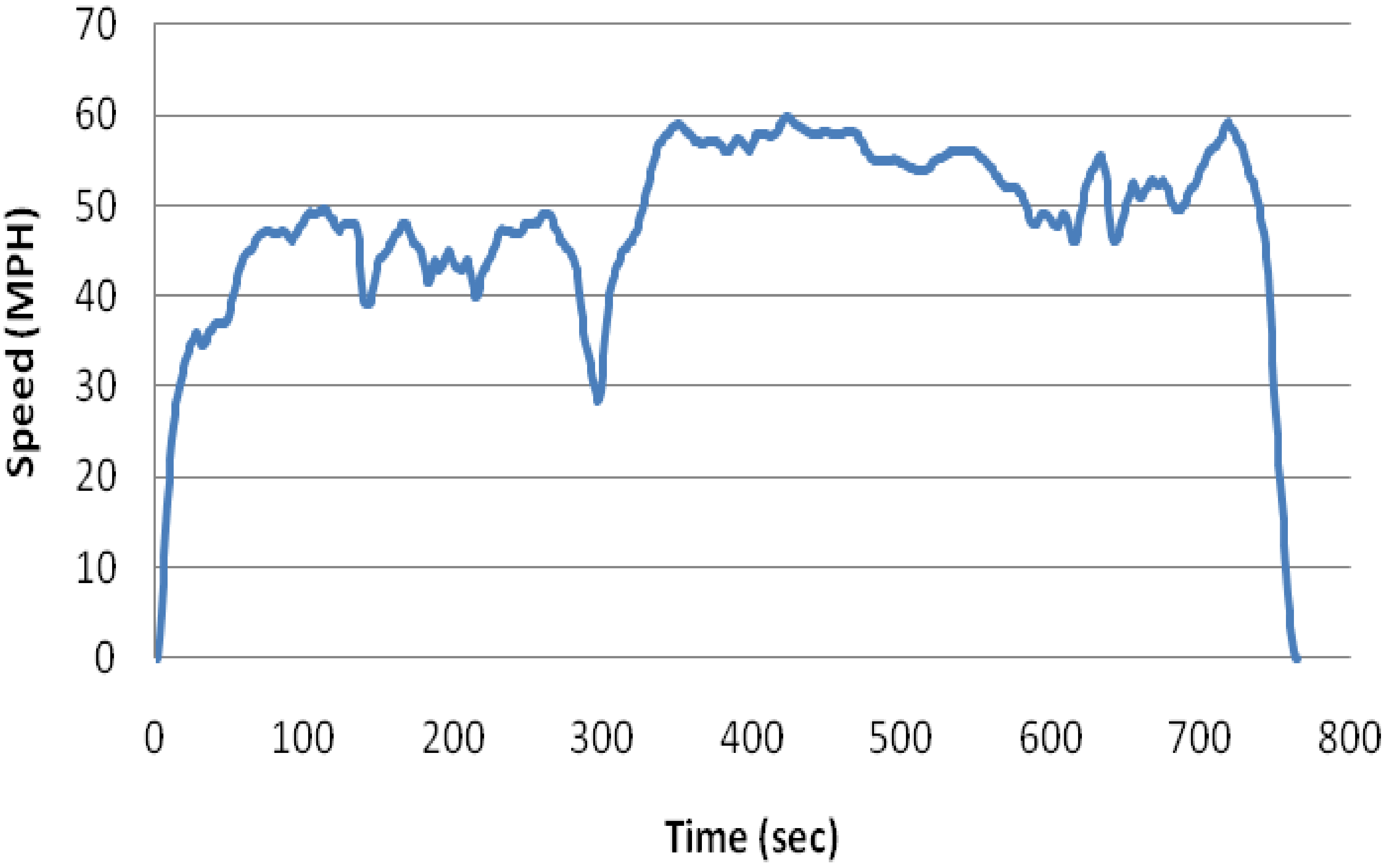

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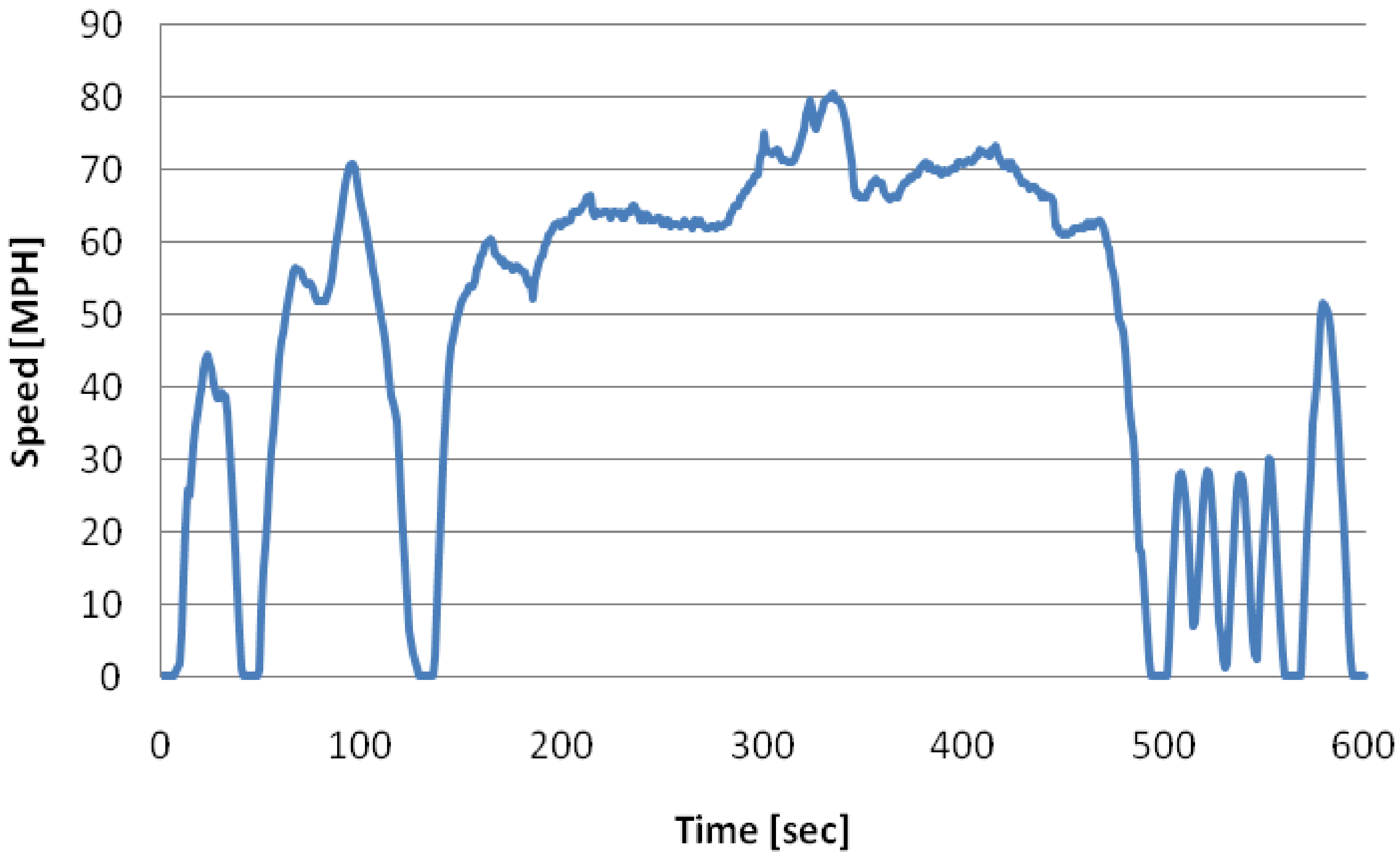
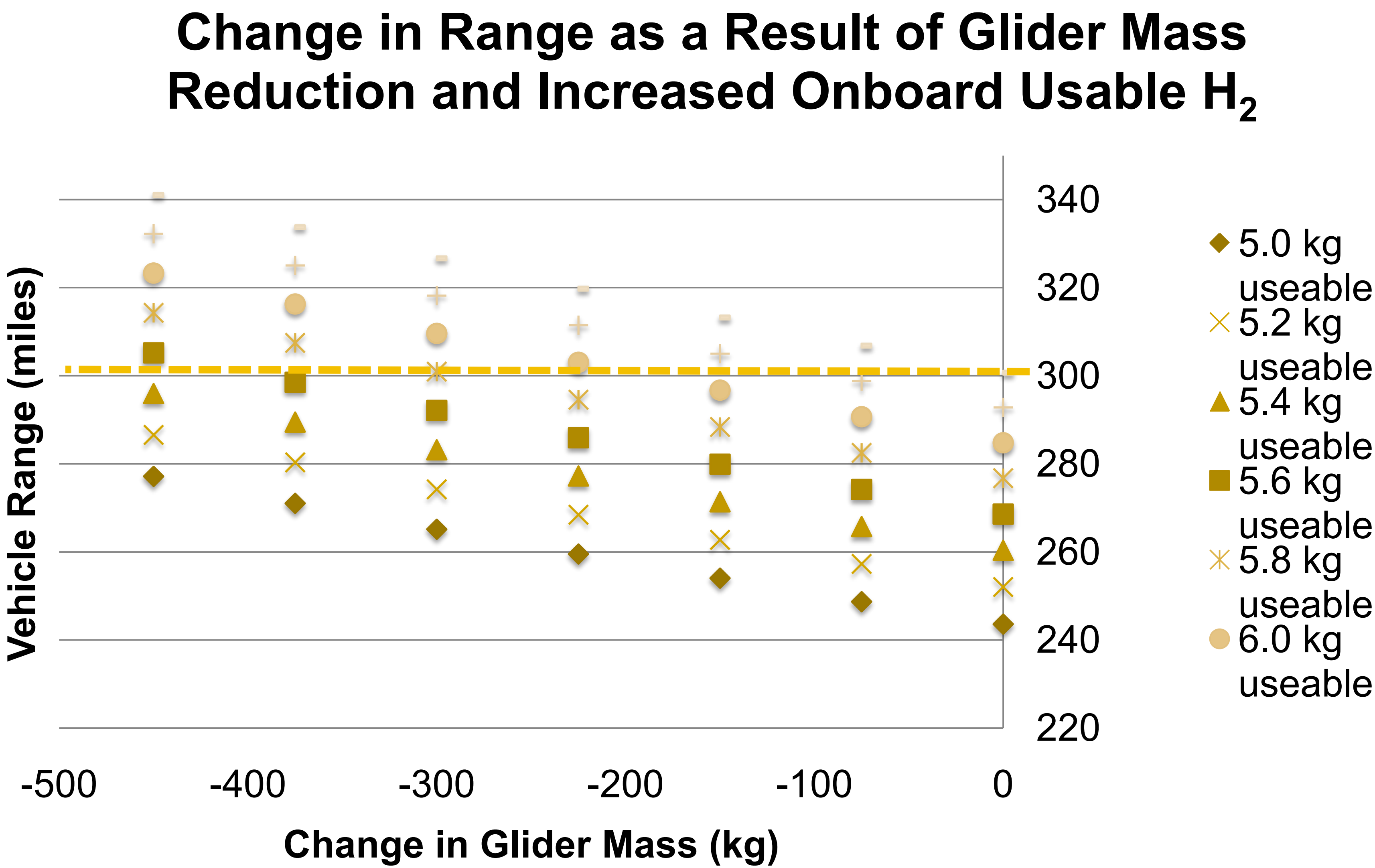


Model Outputs

1. Fuel economy (mpgge)
2. Range (miles)
    - H_2 storage must enable a driving range >300 miles
        - UDDS and HWFET fuel economy values are adjusted and combined based on EPA standards
        - Calculation is based on the combined fuel economy value
3. Vehicle mass (kg)
4. On-board efficiency (%)
5. Drive matrix performance

Results

Model Application – $NaAlH_4$ Example



Results – $NaAlH_4$

Vehicle Test Schedule Results: Reduced glider mass and increased onboard H_2

- Multiple options available to achieve 300 mile range goal
- Must decide which direction to take to achieve most viable vehicle system

Vehicle Results	Units	$NaAlH_4$	$NaAlH_4$	$NaAlH_4$
Usable H_2	kg	5	6.4	5.6
Glider Mass	Kg	900	900	450
Vehicle Mass	kg	1791	1924	1398
UDDS Fuel Economy	mi/kg-H_2	46.6	44.9	52.6
HWFET Fuel Economy	mi/kg-H_2	51.5	49.8	57.0
Combined Fuel Economy	mi/kg-H_2	48.7	47.0	54.5
Range	miles	244	301	305
0 – 60 mph time	sec	10.8	11.3	9.3

Assumptions: 80 kW peak fuel cell power with 20% hybridization and a 100 kW electric motor

Accomplishments: WTW Analysis

- Obtained GHG emissions and WTV efficiency figures for baseline physical storage systems from DOE base case analysis.
- Ran HDSAM to estimate GHG emissions and WTV efficiency figures for solid state storage systems including $NaAlH_4$ and AX21.

Energy and WTW Analysis

Utilize H2A Hydrogen Delivery Scenario Model (HDSAM)

Standardized Excel spreadsheet tool with the same H2A approach to cost, energy efficiency and GHG emissions analysis but more complex

Pre-loaded with current capital costs and utility costs of H2 delivery components – pipelines, tube trailers, LH2 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)

WTW Base 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, LH2, 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)

HDSAM Application – Analysis of Storage System Being Assessed

Information needed for each storage system

- System weight, wt%, density, and volume
- Total and usable H_2 (5.6 kg)
- Venting rate and dormancy time
- System T and P at full and ¼ tank
- Energy used to release H_2
- System cost
- Cooling load at refueling station
- Fill time/rate
- Fuel economy (from HSSIM)

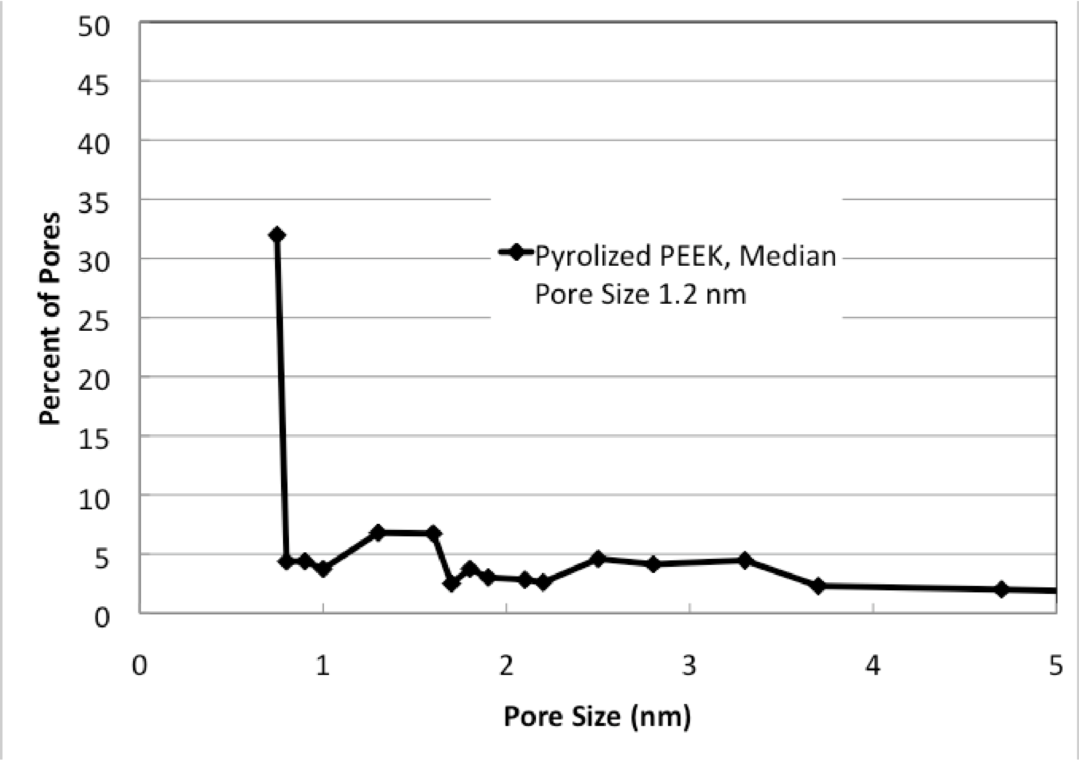
Accomplishments: WTW Analysis

Preliminary Physical Storage GHG Emissions Figure from DOE Base Case Analysis and Solid State Systems from HSECoE Analysis

	WTW H_2 Cost ($/kg)	WTV Efficiency (%)	WTW GHG (gms/mi)
350 Bar Pipeline	4.26	56.7	197
700 Bar Pipeline	4.71	54.4	208
CcH_2 LH Truck	4.80	42.7	279
250 MOF 177	4.80	42.7	279
200 AX-21	4.81	42.5	373
NaAlH4	7.32	44.1	198
Liquid AB			
MOF-5			
TiCr(Mn)H2			

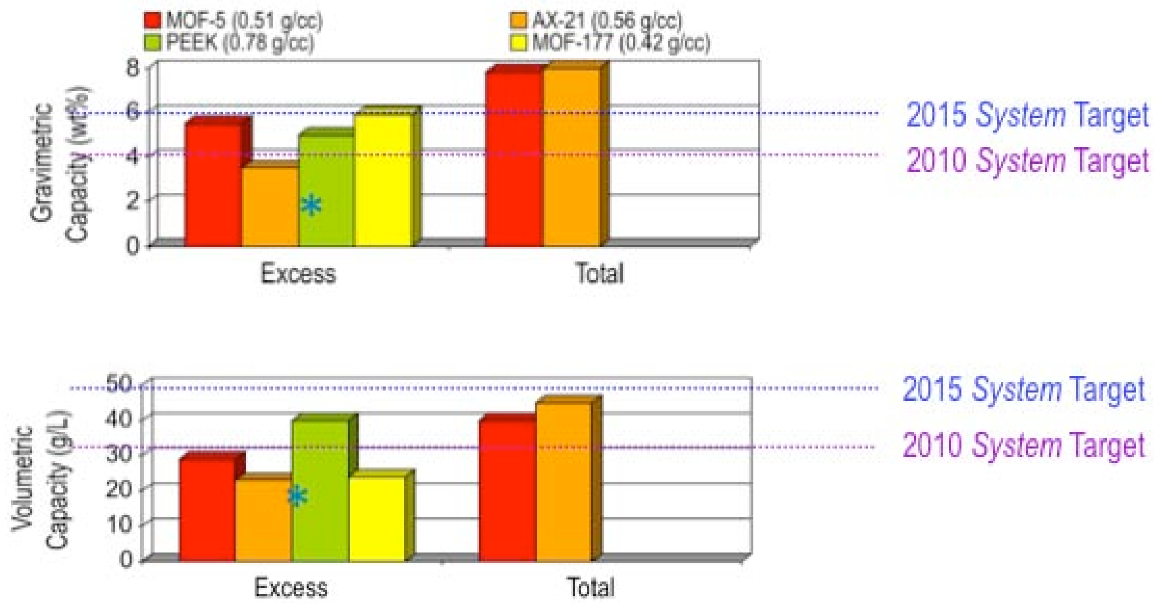
Accomplishments – Media Engineering Properties

- **NREL demonstrated that materials with optimized pore structures/sizes can have excellent volumetric capacities**
  - NREL has adjusted processing to produce pyrolyzed polyether ether ketone (PEEK) materials with a median pore diameter of ~1.2 nm and ~3000 m2/g.



Accomplishments – Media Engineering Properties

- **NREL demonstrated that materials with optimized pore structures/sizes can have excellent volumetric capacities**
  - **This material has the potential to meet DOE 2015 system targets for both gravimetric and volumetric hydrogen storage capacities at~80 K storage temperatures. This is due to the ability of these optimized materials to have demonstrated specific surface areas over 3000 m2/g and bulk densities over 0.7 g/ml.**



Comparative Summary: Materials-based hydrogen uptake for different compacted sorbents being evaluated by the HSECoE

* **PEEK data based on pellet in press vessel (i.e. freestanding pellet not yet obtained)**

- **Values taken at max. excess uptake which corresponds to pressures of 60, 30, 40, and 50 bar for MOF-5, AC, PEEK, MOF-177 respectively; T = 77 K.**
- **AC and PEEK data taken from Aug. 2010 Sorbent SA Meeting slides.**
- **MOF-177 data from R. Zacharia et al, J. Mater. Chem. 2010, 20, 2145.**

Milestones

- Recommend materials for future H_2 storage system analyses by the HSECoE Complete (3/11)
- Evaluate various storage system impact on vehicle performance, cost and viability (9/11) Complete
- Evaluate various storage system efficiencies (energy inputs, GHG emissions and well to power plant efficiency) 50% Complete (9/11)
- Provide HSECoE appropriate engineering properties on recommended materials for future H_2 storage system analysis 50% Complete (9/11)

Next Steps

- Continue to run simulations to:
  - Refine storage systems sizing
  - Evaluate progress toward tech targets
- Run HDSAM to evaluate (liquid AB, MOF-5, and $TiCr(Mn)H_2$:
  - Well-to-power plant efficiency
  - GHG
  - H_2 cost
- Looking at ambient temperature PEEK and Pt/AC-IRMOF 8, which enables RT storage system

Summary

- Manage HSECoE performance, cost, and energy analysis technology area.
- Develop and apply model for evaluating H_2 storage requirements, performance, and cost tradeoffs at the vehicle system level.
- Perform H_2 storage system WTW energy analysis to evaluate GHG impacts with a focus on storage system parameters, vehicle performance, and refueling interface sensitivities.
- Assist center in the identification and characterization of sorbent materials that have the potential for meeting DOE technical targets as an onboard systems.