NREL National Renewable Energy Laboratory
Innovation for Our Energy Future

Hydrogen Storage Engineering CENTER OF EXCELLENCE

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

2010 DOE Hydrogen Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting

Matthew Thornton, NREL

June 8th 2010

Project ID# ST008

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

Overview

Timeline

HSECoE start date: FY09
HSECoE end date: FY13
Percent complete: 25%

Budget

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

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.

Hydrogen Storage Engineering CENTER OF EXCELLENCE

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 trade-offs 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

Performance, Cost & Energy Analysis

M. Thornton, NREL

Vehicle Requirements (Boundaries & Configurations)

NREL

Ford, GM, PNNL, UTRC

Manufacturing & Cost Analysis

PNNL

NREL, GM, Ford, UTRC

Tank-to-Wheels

NREL

PNNL, UTRC, GM, Ford

Forecourt Requirements

UTRC

Ford, GM

Vehicle Requirements Objectives

- Develop and apply model for evaluating hydrogen storage requirements, performance and cost trade-offs at the vehicle system level.
  - e.g. Range, cost, size, efficiency, mass, performance
- Model application will Identify
  - Relative importance/sensitivity of trade-offs
  - Critical tech targets
  - Pathways to meet GO/NO-GO criteria
  - Important trends
  - Assumptions that are “driving” vehicle design and H2 storage requirements

Accomplishments

Created a Hydrogen Storage Vehicle Model

Generate higher level component models

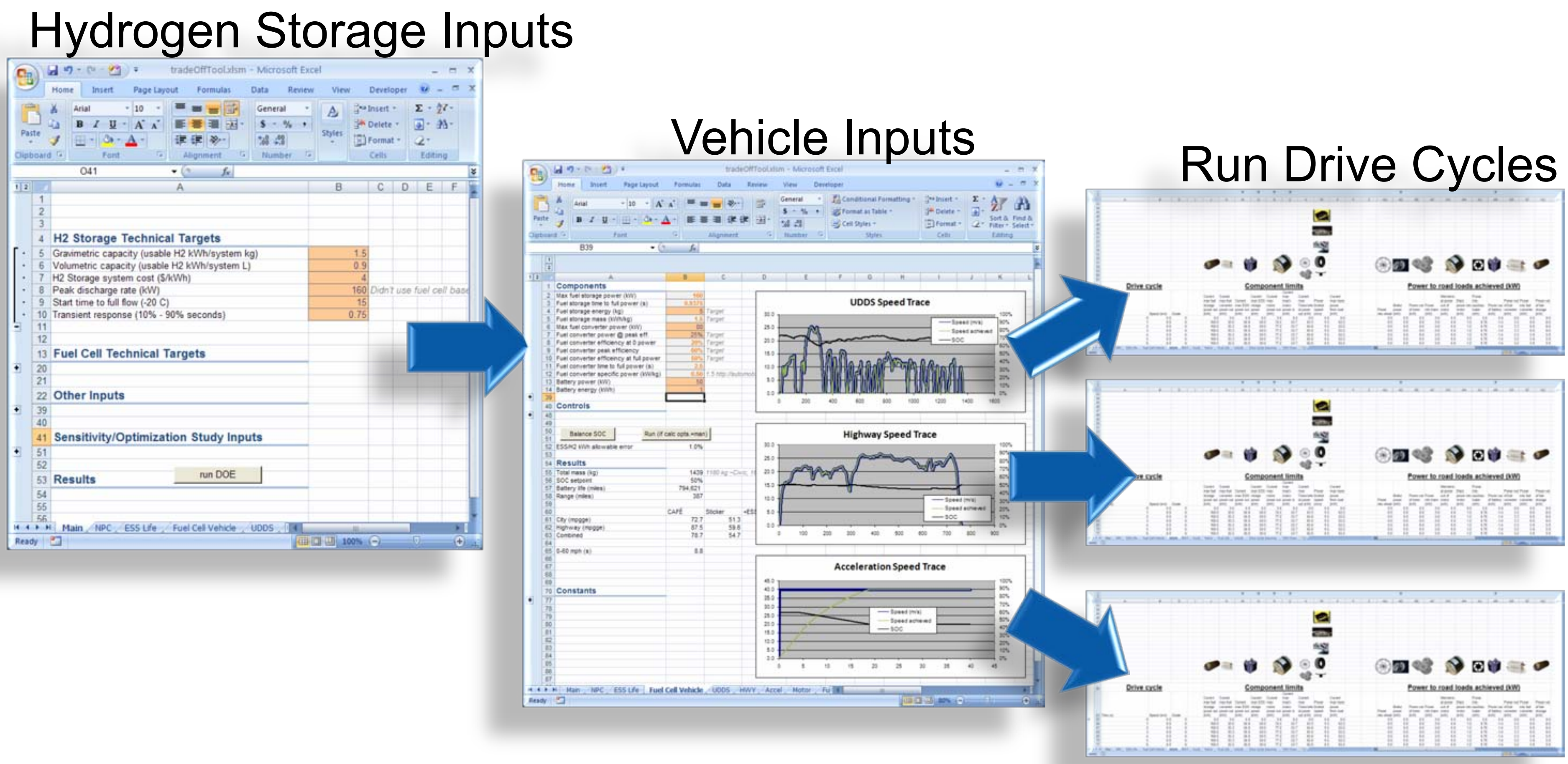
Hydrogen **S**torage **SIM**ulator

Run faster simulations

Advantages

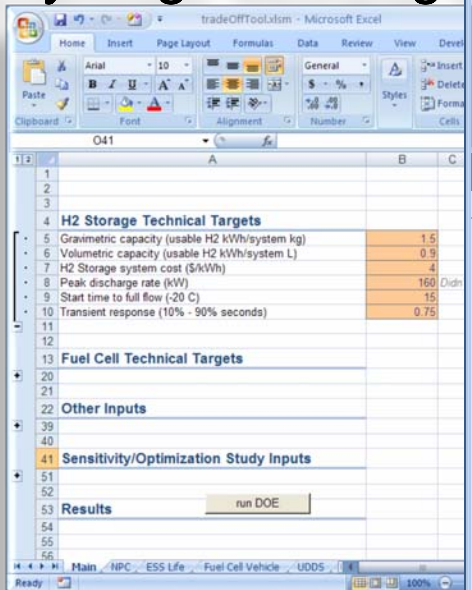
- >10x *faster* allowing for improved trade-off analysis
- Clear representation of technical targets to enhance target analysis

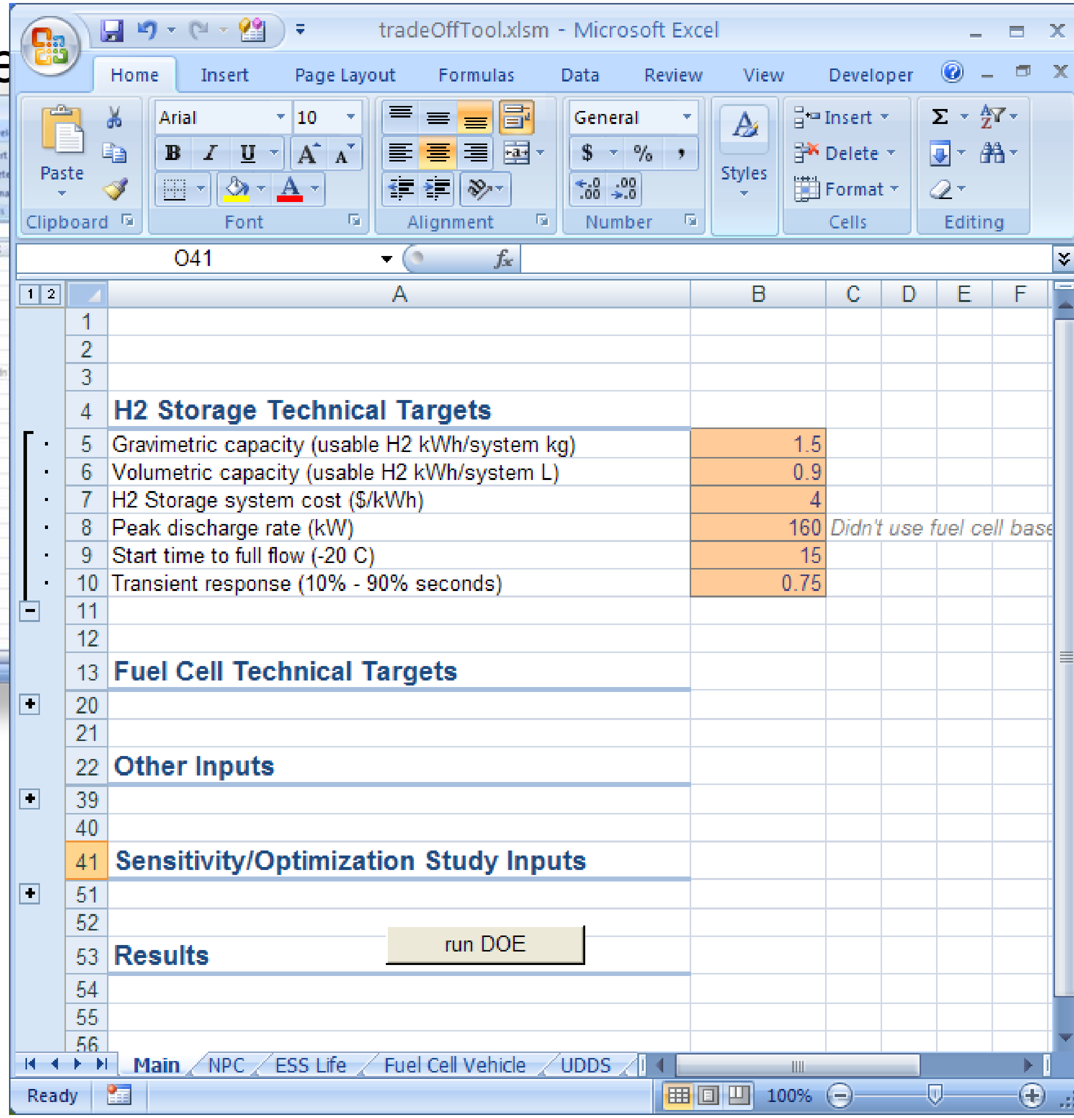
Accomplishments: HSSIM Structure



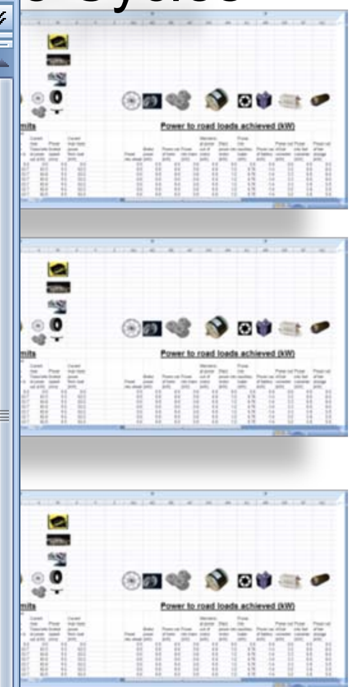
Accomplishments: Hydrogen Storage Inputs

Hydrogen Storage





e Cycles

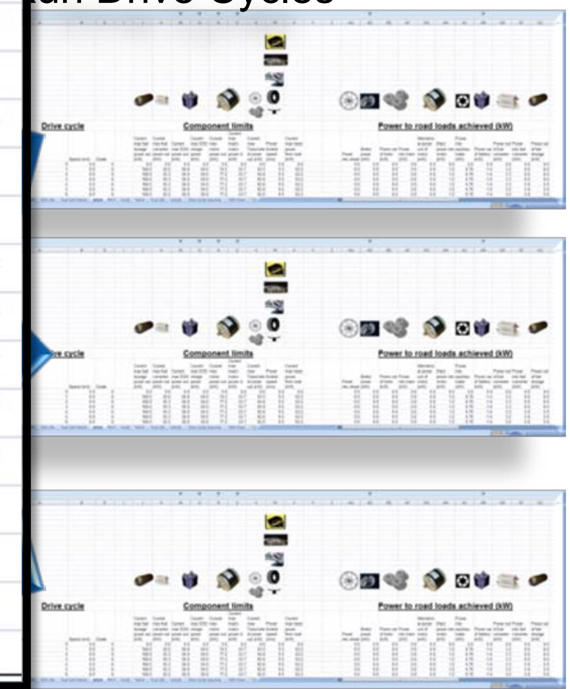


Accomplishments: Vehicle Inputs

Hydrogen Storage Inputs

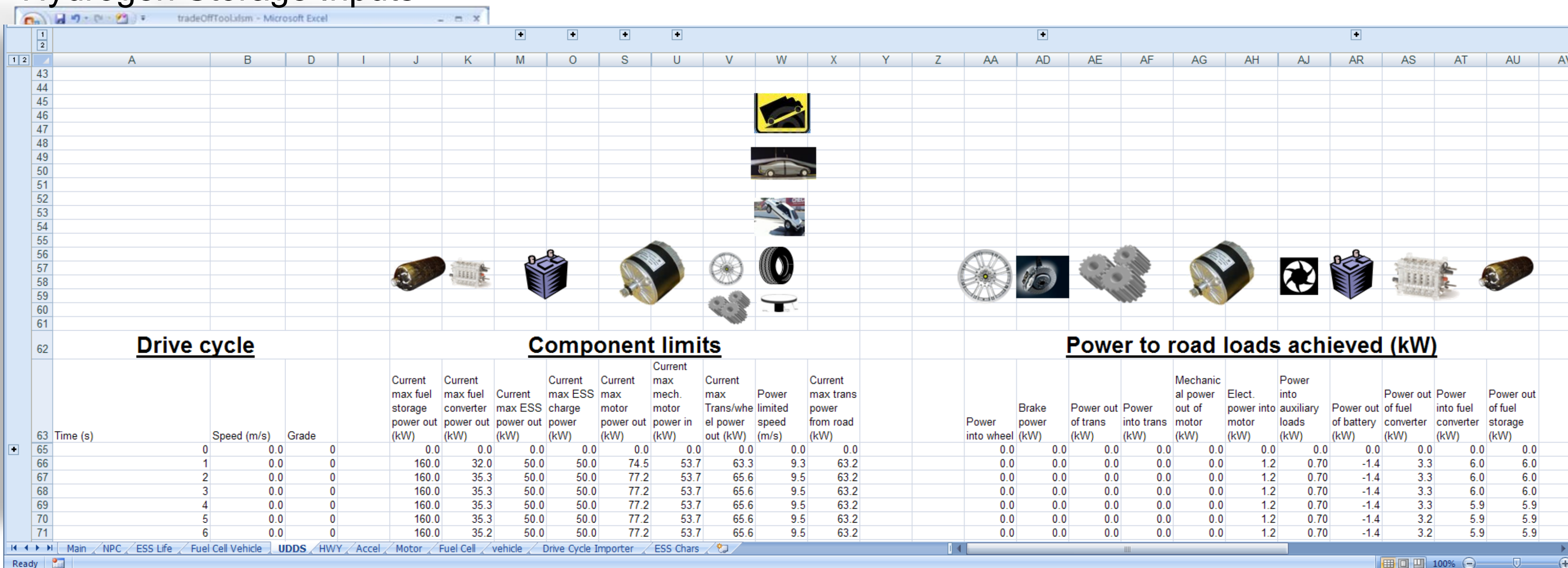
2	**Components**		
3	Max fuel storage power (kW)	160	*Target*
4	Fuel storage time to full power (s)	0.9375	*Target*
5	Fuel storage energy (kg)	3.92	
6	Fuel storage mass (kWh/kg)	1.5	*Target*
7	Max fuel converter power (kW)	100	
8	Fuel converter power @ peak eff.	10%	
9	Fuel converter efficiency at 0 power	20%	*Target*
10	Fuel converter peak efficiency	57%	*Target*
11	Fuel converter efficeincy at full power	50%	*Target*
12	Fuel converter time to full power (s)	1.25	*Target*
13	Fuel converter specific power (kW/kg)	0.65	*Target*
14	Battery power (kW)	30	
15	Battery energy (kWh)	1	
40			
41	**Controls**		

un Drive Cycles



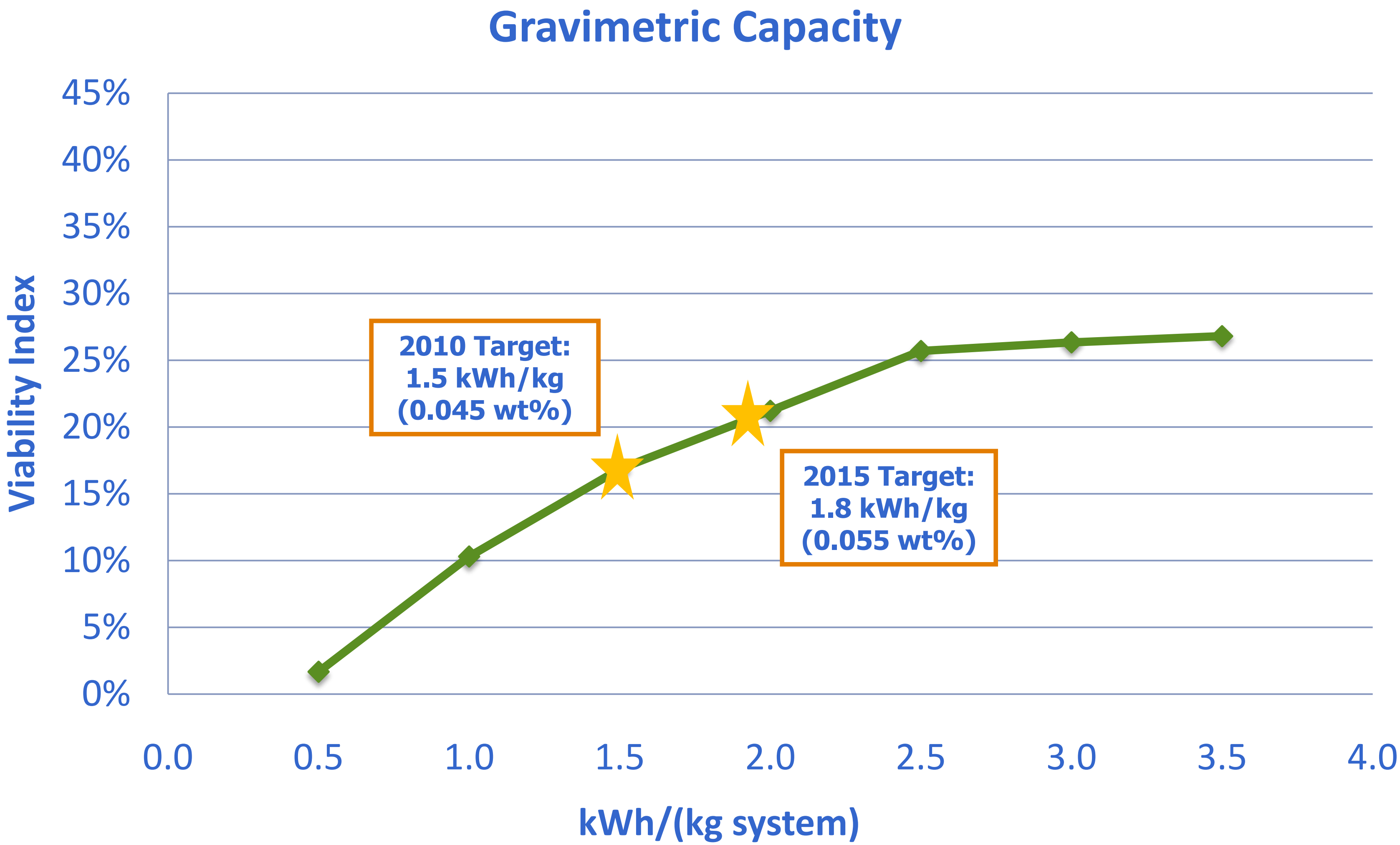
Accomplishments: Vehicle Model

Hydrogen Storage Inputs



Row	Drive cycle			Component limits									Power to road loads achieved (kW)										
63	Time (s)	Speed (m/s)	Grade	Current max fuel storage power out (kW)	Current max fuel converter power out (kW)	Current max ESS power out (kW)	Current max ESS charge power (kW)	Current max motor power out (kW)	Current max mech. motor power in (kW)	Current max Trans/wheel power out (kW)	Power limited speed (m/s)	Current max trans power from road (kW)	Power into wheel	Brake power (kW)	Power out of trans (kW)	Power into trans (kW)	Mechanical power out of motor (kW)	Elect. power into motor (kW)	Power into auxiliary loads (kW)	Power out of battery (kW)	Power out of fuel converter (kW)	Power into fuel converter (kW)	Power out of fuel storage (kW)
65	0	0.0	0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
66	1	0.0	0	160.0	32.0	50.0	50.0	74.5	53.7	63.3	9.3	63.2	0.0	0.0	0.0	0.0	0.0	1.2	0.70	-1.4	3.3	6.0	6.0
67	2	0.0	0	160.0	35.3	50.0	50.0	77.2	53.7	65.6	9.5	63.2	0.0	0.0	0.0	0.0	0.0	1.2	0.70	-1.4	3.3	6.0	6.0
68	3	0.0	0	160.0	35.3	50.0	50.0	77.2	53.7	65.6	9.5	63.2	0.0	0.0	0.0	0.0	0.0	1.2	0.70	-1.4	3.3	6.0	6.0
69	4	0.0	0	160.0	35.3	50.0	50.0	77.2	53.7	65.6	9.5	63.2	0.0	0.0	0.0	0.0	0.0	1.2	0.70	-1.4	3.3	5.9	5.9
70	5	0.0	0	160.0	35.3	50.0	50.0	77.2	53.7	65.6	9.5	63.2	0.0	0.0	0.0	0.0	0.0	1.2	0.70	-1.4	3.2	5.9	5.9
71	6	0.0	0	160.0	35.2	50.0	50.0	77.2	53.7	65.6	9.5	63.2	0.0	0.0	0.0	0.0	0.0	1.2	0.70	-1.4	3.2	5.9	5.9

Accomplishments:
Tech Target Sensitivity Analysis



Milestones

- Meet with OEMs (4/09) Complete
- Develop Models (4/09) Complete
- Obtain key data and validate models (5/09) Complete
- Link/run models/simulations (7/09)
- Obtain preliminary results for base physical storage scenario (9/09)
- Integrate vehicle model with FC/Storage system models for a variety of solid state storage materials (7/10)
- Run simulations to produce results to identify key system trade-offs for input to storage system designs and go/no-go decisions (12/10)

Next Steps

- Linking with other models
  - Need input on what needs to be coupled
  - How (language, time step, etc.)
- Obtain data/models from other teams
  - Fuel cell
  - Hydrogen storage system
  - Forecourt impacts on storage capacity
  - Manufacturing cost

Well to Wheels Analysis Objectives

- Perform hydrogen storage system WTW energy analysis to evaluate GHG impacts with a focus on storage system parameters, vehicle performance and refueling interface sensitivities.
  - Develop vehicle level models and obtain FE figures for overall WTW analysis
  - Obtain data from center partners on fuel interface/dispensing/station energy requirements
  - Obtain key outside data for H2 production and distribution and tank production and CO2e emission factors (GREET, H2A, etc.) and calculate WTV (power plant) efficiencies
  - Link to critical interdependent models and data to obtain final results

Accomplishments

- Created a draft framework to discus modeling approach and integration
- Participated on SSAWG calls and WTW DOE base case discussion
- Provided FE figures and simulation results for FCV and HEV for base case analysis
- Obtained preliminary GHG emissions and WTV efficiency figures for baseline physical storage systems from DOE base case analysis
- Began working with GREET and H2A

Accomplishments

Preliminary Physical Storage GHG Emissions Figure from DOE Base Case Analysis – Draft. Next Steps to Obtain GHG Emissions from Solid State Systems Below

	WTW H2 Cost ($/kg)	WTV Efficiency (%)	WTW GHG (gms/mi)
350 Bar Pipeline	4.29	56.7	208
700 Bar Pipeline	4.76	51.5	224
CcH2 LH Truck	4.89	40.3	296
250 MOF 177	4.89	40.1	297
SAB			
NaAlH4			
AX-21			

Milestones

- Obtain preliminary results for base physical storage scenario (5/10) Complete
- Run Vehicle Simulations for baseline MPG figures(5/10) Complete
- Calculate baseline results for solid state storage scenario (9/10)
- Run analysis to produce results to identify key system trade-offs for input to storage system designs and go/no-go decisions (12/10)

Future Work

- Linking vehicle models and data with WTW model
  - Work with ANL on GREET integration
- Obtain data/models from other teams
  - Fuel cell
  - Hydrogen storage system
  - Forecourt impacts on storage capacity
  - Manufacturing cost

Objectives: Media Engineering Properties

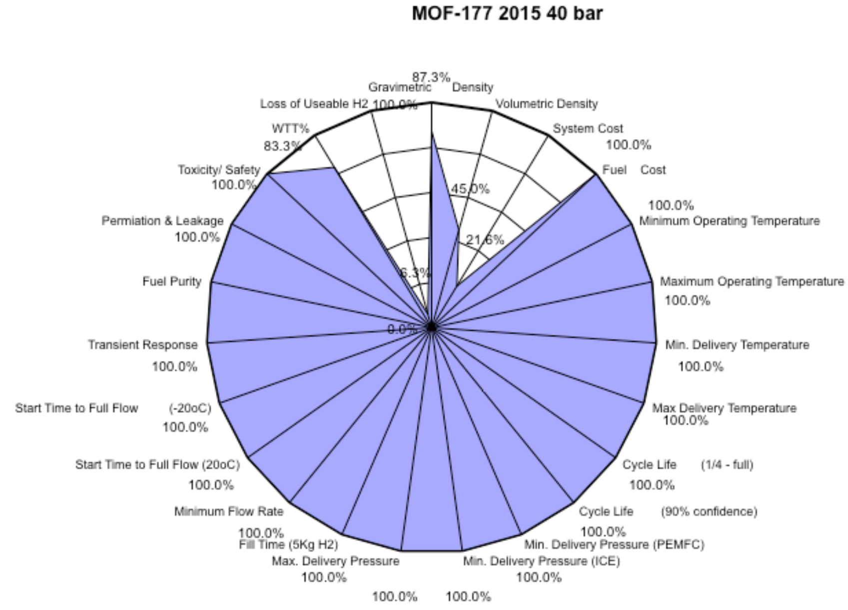
- Work with Hydrogen Storage Center of Excellence and community to identify potential materials for engineering analysis
  - Technology Team Co-lead: Hydrogen Storage Materials Center of Excellence Collaborations, in the Materials Operating Requirements (MOR) Technology Area
- Measure and characterize promising sorption material properties for on-board 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: Media Engineering Properties

- Identified potential materials for analysis that may meet HSECoE goals
  - » Based on earlier analysis, need inexpensive materials with bulk densities >0.7 g/ml
  - » Measuring additional material properties for pyrolized PEEK and Aerogel
  - » Looking at ambient temperature Pt/AC-IRMOF 8, which enables RT storage system
- Identified storage system design guidance needed to help meet DOE storage targets with sorption materials
- Helped define measurement tasks for MOR Adsorbent Team
  - – NREL to generate initial data of selected new materials
  - – Work with HSCoE and other partners to get enough materials and characterization information
    - » Potential kg scale material synthesis. Identify material properties needed for center modeling and engineering activities
    - » Worked with selected HSCoE partners to get gram quantity samples
- Led development of sorbent selection criteria for engineering analysis
- Helped establish tentative agreement among Center of Excellence members that HSECoE and Data Base being established by George Thomas can be and should be virtually the same for sorbent materials.
- Assembled/provided Partner Capabilities document

Accomplishments: Media Engineering Properties

- Initial evaluation of sorbent based system using ANL/TIAX MOF-177 analysis assuming ~250 bar storage
  - Meets HSECoE and DOE 2010 **capacity** targets
  - >4x & 8x from DOE 2010 & 2015 cost targets, respectively
  - Only ~60% and 25% of HSECoE Phase I and II cost goals
  - Also dormancy times are only 12 to 50% of 2010 target
    - This will decrease volumetric capacity and increase costs to fix
- Evaluation based on ANL/TIAX MOF-177 analysis assuming ~40 bar storage
  - Capacity targets now an issue, but close for HSECoE Phase II; could meet with lower storage temp.
  - >2x & 4x from DOE 2010 & 2015 cost targets, respectively
  - Meet and 50% of HSECoE Phase I and II cost goals, respectively
  - Dormancy times must still be worked, but better at 40 bar
    - Will decrease volumetric capacity and increase costs
- Provides guidance for future efforts: e.g.
  - Need improved volumetric via optimized materials
  - Must include system cost and efficiency in analysis



Spider chart showing the degree to which a potential sorbent based system (using MOF-177) might meet DOE 2015 hydrogen storage targets.
This evaluation is very rudimentary and only meant to provide guidance for future work; it is not quantitative.

Accomplishments: Media Engineering Properties

- Performed initial analysis to provide input guidance for sorbent system design
  - Must use integrated sorbent storage system capacity, cost, and efficiency analysis
    - » Must balance performance and cost to meet HSECoE goals and DOE targets
    - » Capacity and performance targets can be met, but only with high system costs and poor system efficiencies
    - » Should consider WTT% and "ownership" costs too, up to now secondary considerations
  - For sorbents, must work on 4 main areas to lower costs (i.e. need to reduce tank costs by >50% and BOP costs by ~75%) to ~$5/kWh needed for the HSECoE goal
    - » Increase vol. capacities by using higher bulk density sorbents; lowers storage P
      - » Use optimized pore size materials with bulk densities >~0.7 g/ml, crystal densities >1g/ml; lowers P
    - » Lower storage pressure: reduces tank costs (~40%) and BOP costs (~75%)
      - » e.g. storage pressures of 50 to 150 bar
    - » Increase delivered H_2 from sorbent; e.g. use larger ΔT swing and lower storage temperature
      - » May need to increase material thermal conductivity to lessen heat exchanger
      - » Balance extra components needed to achieve, i.e. heat exch., cooling costs, insulation
    - » Do analysis on larger systems (i.e. up to 13 kg H_2), reduces all costs 30-50%
  - Suggest we model what "ideal" material properties needed to meet DOE 2015 targets
    - » Provides DOE recommendations on future project selection criteria

Future Work

- To meet DOE 2015 storage targets, “new” sorbent materials must be used
  - Requires detailed and accurate material property measurements of lab (mg) scale samples
    - » Use unique measurement/synthetic capabilities to perform the required high quality measurements to assess selected materials for the system analysts
      - » e.g. using 1-100 mg samples, measure isotherms (P,T), heats, SSAs, pore size, compaction effects, kinetics/diffusion (P,T), bulk density, decomposition, stability (P,T) thermal conductivity, …
  - Requires scale-up synthesis to make sufficient materials
    - » Work with partners to scale selected synthesis to obtain sufficient material for characterization and perhaps scaled system testing
  - Identify with system analysis what material properties most important
    - » e.g. pore size, binding energy, adsorption mechanism, conductivity, density, …
    - » Work with material development partners and sorbent community to obtain/synthesize selected materials

Summary

- Manage HSECoE Performance, Cost and Energy Analysis Technology Area
- Develop and apply model for evaluating hydrogen storage requirements, performance and cost trade-offs at the vehicle system level.
- Perform hydrogen 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