



Evaluation of Protected Metal Hydride Slurries in a H₂ Mini- Grid

**Hydrogen Technical Analysis
Phase II Work in Progress**

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TIAX, LLC
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The hydrogen “Energy Station” concept has been proposed by DOE and others to facilitate the development of a hydrogen fuel infrastructure.

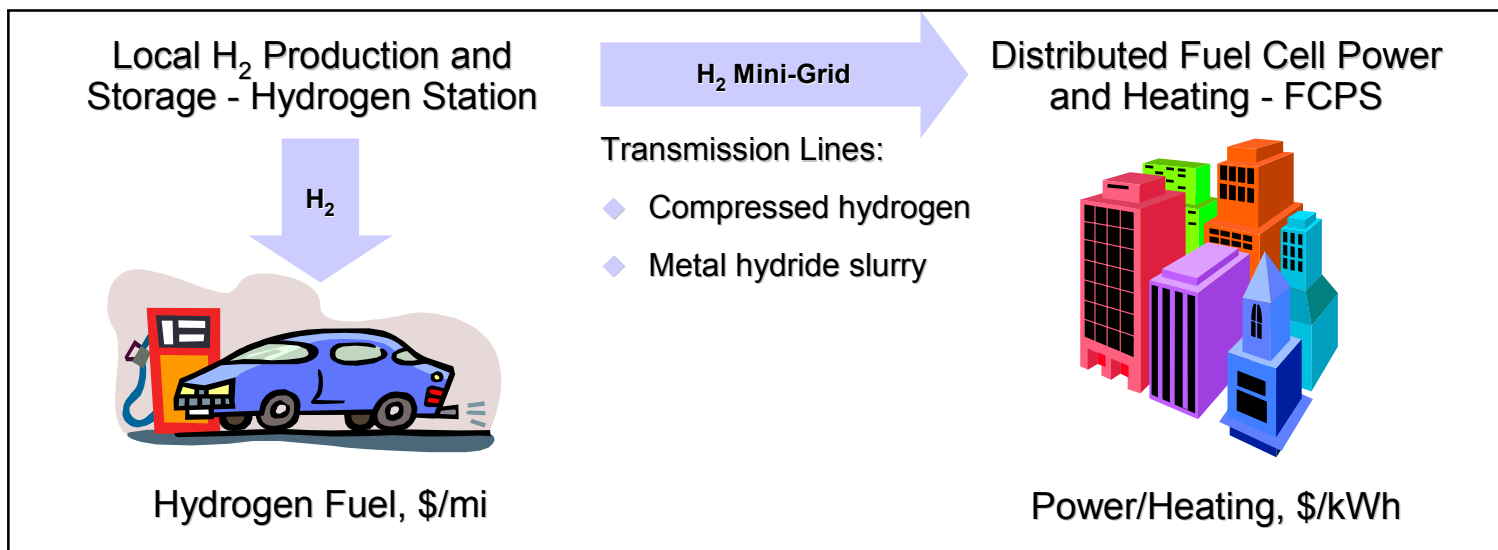
- ◆ Hydrogen is produced for stationary PEM fuel cell power systems (FCPS) and for fueling fuel cell vehicles (FCVs) at a hydrogen station
- ◆ Provides economies-of-scale and high utilization for hydrogen (H₂) production and storage equipment
- ◆ Opportunity for early revenue by supplying reliable power
- ◆ Helps solve “chicken and egg” problem for FCV/H₂ infrastructure

In addition, the Energy Station concept improves the commercialization of FCPS by lowering technical/economic risk compared to reformat-FCPS.

- ◆ Reduces risk of stack impurities poisoning
- ◆ Improves stack anode utilization
- ◆ Improves efficiency and reduces technical risk and cost of H₂ production
 - A single, larger reformer can operate base-loaded with H₂ storage
- ◆ Central hydrogen storage replaces need for battery
- ◆ Synergies with transportation developments

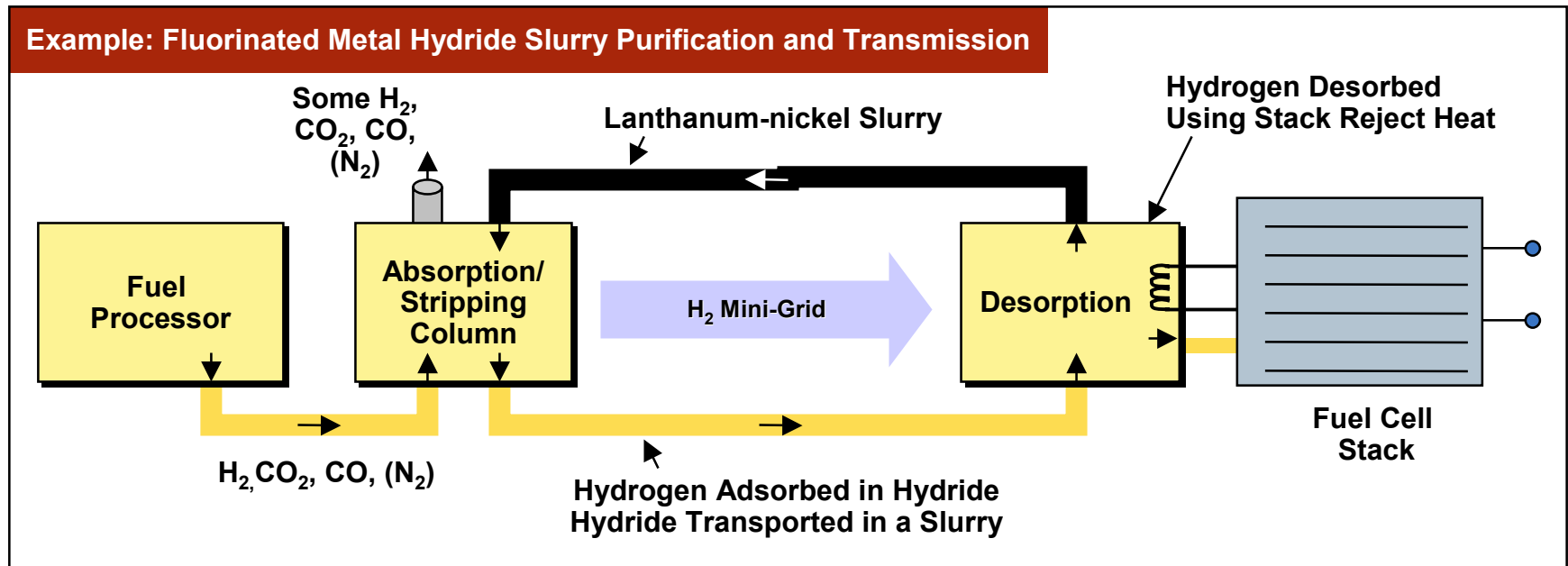
Distributed FCPS utilizing a H₂ Mini-Grid can provide all the benefits of a Hydrogen Energy Station and also provide cogen to buildings.

- ◆ Reduced technical risk and cost compared to distributed reformate-FCPS (see Energy Station Concept discussion)
- ◆ Fuel cell waste heat can be used for hot water or space heating in buildings (i.e. “cogen”)
- ◆ Distributed FCPS utilizing a H₂ Mini-Grid are quiet and emissions free



However, the perceived safety of hydrogen transmission is a major barrier to it's implementation, especially in commercial/residential areas.

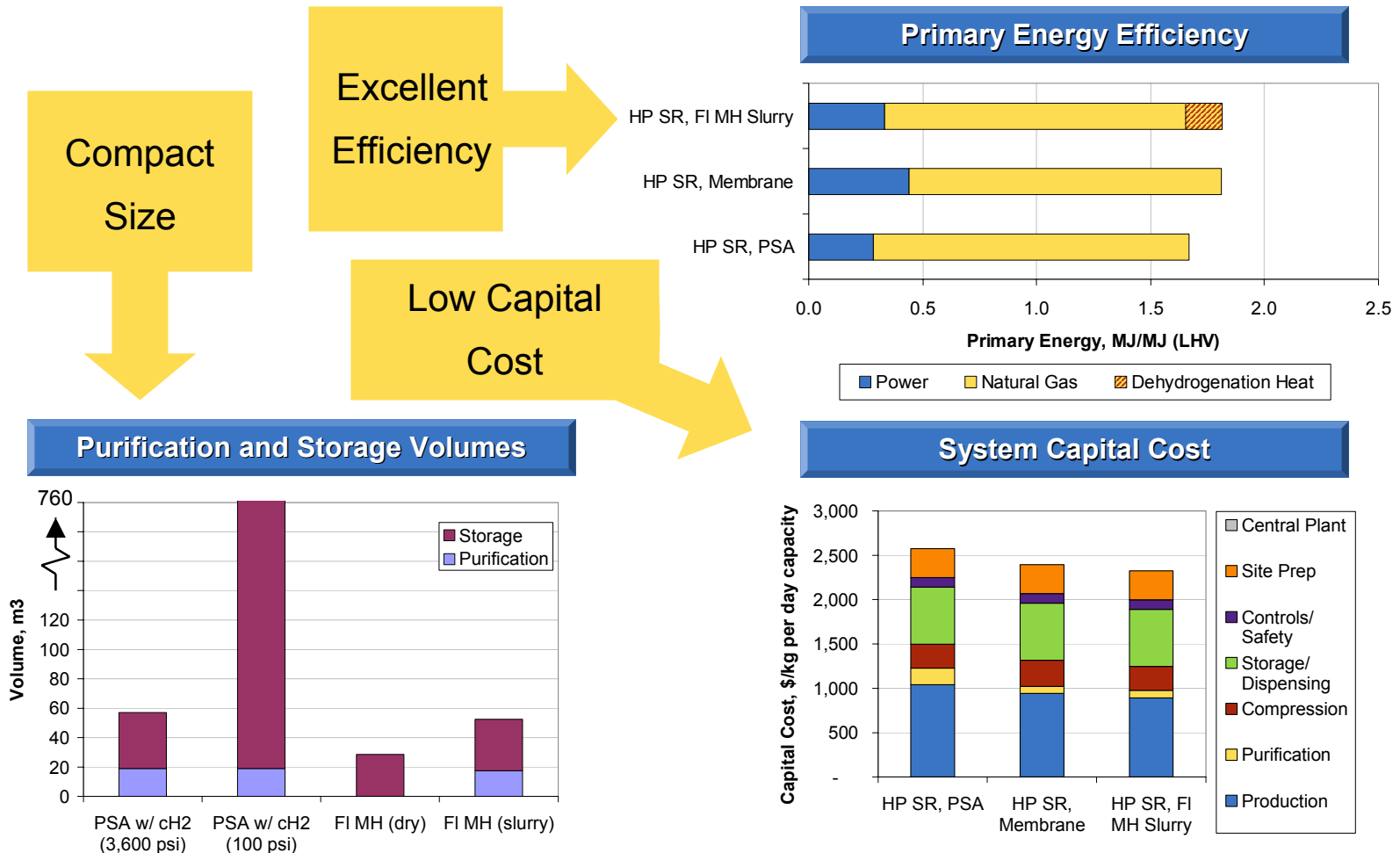
Metal hydride (MH) slurries are safer and are potentially more efficient and cheaper than compressed gas hydrogen (cH_2) transmission in pipelines.



Potential Advantages:

- ◆ Safer than cH_2 storage/transmission - reduced permitting and right-of-way costs
- ◆ Excellent efficiency if dehydrogenation heat can be supplied by waste heat (e.g. fuel cell)
- ◆ Requires less space than low pressure cH_2 storage/transmission
- ◆ Convenient method of combined purification, storage, and transmission
- ◆ Protected (i.e. fluorinated) MH slurries can purify reformat streams at low cost

In Phase I, we identified fluorinated metal hydride (FI MH) slurries as having potential to provide benefits as a purification and storage media.



Legend: HP SR = high pressure (10 atm) steam reformer, Membrane = Zr-Ni metal membrane, PSA = pressure swing adsorption, LHV = lower heating value

Before FI MH can be used for H₂ purification, further development will be required to prove its feasibility and optimize its implementation.

- ◆ Current MH have low tolerance to impurities typically found in reformat streams, especially oxygen and carbon monoxide
- ◆ Fluorinated (or in some other way protected) metal hydrides should be able to demonstrate high tolerance to impurities
 - Researchers in Japan have shown a fluorinated surface layer will protect the MH from multiple impurities

Compound	Impurity Threshold, vol		Comment	Reference
	Fluorinated	Untreated		
Carbon Monoxide	<100 ppm	<10 ppm	Was shown by applying a particular fluorination method	Japan Metals and Chemicals
	<3000 ppm			Kogakuin University ¹
Carbon Dioxide	< 20%	<100 ppm		Kogakuin University ¹ and Japan Metals and Chemicals
Oxygen	< 20%	<10 ppm	During MH storage: no surface oxidation was found after 15 day exposure to air	X.-L. Wang, S. Suda ²

¹ Personal communication with Pr. S. Suda of Kogakuin University

² Stability and Tolerance to Impurities of the Fluorinated Surface go Hydrogen-Absorbing Alloys, Journal of Alloys and Compounds 227 (1995) 58-62.

The purpose of Phase II is to evaluate the feasibility of using FI MH slurries for purification and transmission in a H₂ Mini-Grid concept.

- ◆ Assess the viability of using fluorinated (or otherwise treated) metal hydrides for the purification of carbon monoxide-containing hydrogen streams
 - Using computational modeling to help fully characterize the limitations of fluorination and identify alternative technologies
- ◆ Assess the attractiveness and viability of using fluorinated metal hydride slurries in a hydrogen distribution system (H₂ Mini-Grid)
 - Including both vehicle refueling stations and building combined heat and power systems
- ◆ Establish research and development (R&D) objectives for the development of hydrogen distribution systems using fluorinated metal hydrides
 - Identify key barriers and possible development paths
 - Contingent on a positive outcome from above

In Task 1, we will analyze the potential cost and performance of H₂ Mini-Grid concepts for integrated fueling and power systems.

Subtasks to Task 1: System Analysis

Subtask 1: Evaluate metal hydride slurry purification, storage and dispensing apparatus for Integrated Systems (fueling and power)

Subtask 2: Develop hydrogen fueling system designs

Subtask 3: Develop fuel cell power system designs

Subtask 4: Determine cost of electricity (COE), hydrogen costs, energy use, and GHG* and other emissions for H₂ Mini-Grid concepts and stand-alone systems

Subtask 5: Reporting

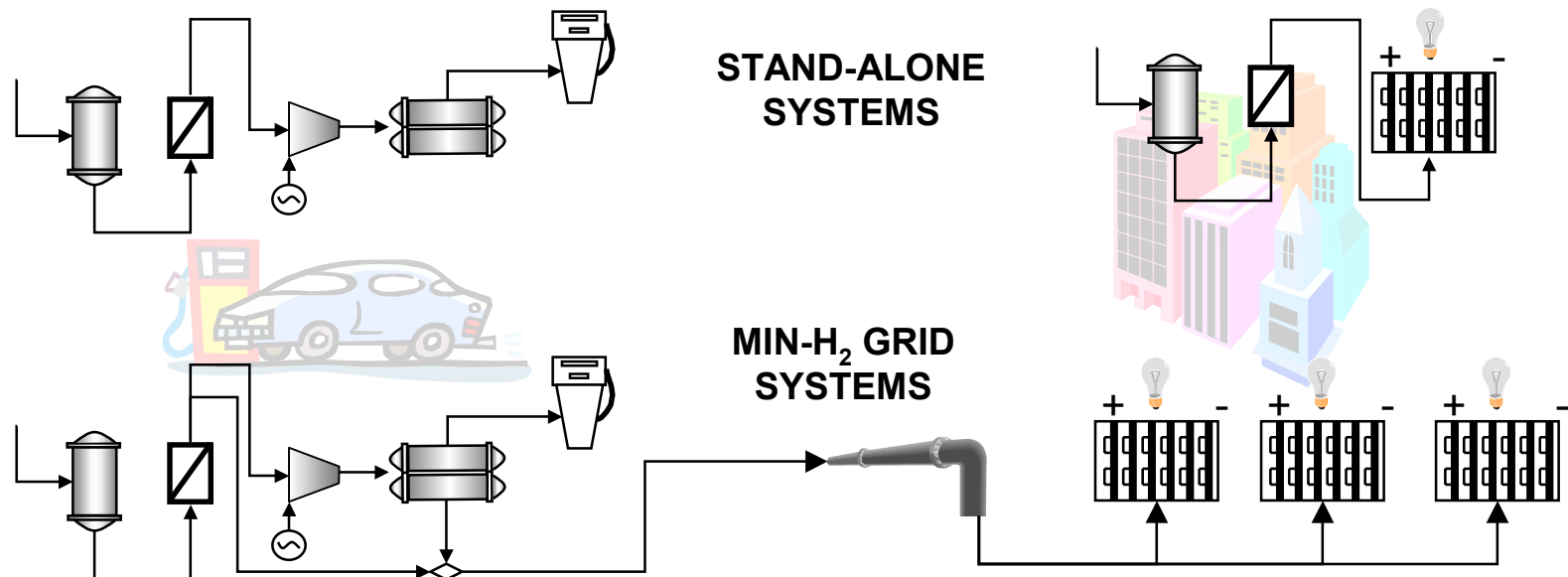
* GHG = green house gases (CO₂, CH₄, etc.)

We will investigate local hydrogen production for fueling direct-H₂ FCVs and distributed FCPS.

- ◆ <1,000 kg/day H₂ fueling capacity for compressed gas hydrogen (cH₂) FCVs
 - On-site hydrogen production via 10 atm steam reformer
 - ↳ Highest overall efficiency of the four reformer types investigated in Phase I
 - ↳ Renewables-based production is also a promising application for the H₂ Mini-Grid
 - On-site hydrogen storage via compressed gas or MH slurry
- ◆ <100 kWe PEM FCPS serving commercial and residential buildings
 - Various building load profiles - heat and power demands
 - Power and co-gen heating (conventional and high temperature PEM)
 - Grid connected for high utilization (note: load-following is possible for direct-H₂ FCPS)
 - Base-loaded during peak hours - reduces demand charges
 - Turned off when power demand drops below FCPS design power - simplest, doesn't cut into utilities' base-load and compete with cheap off-peak grid power
 - Hydrogen storage at fueling station also acts as a reliability enhancer for the FCPS

We will evaluate a number of H₂ Mini-Grid configurations and compare them to stand-alone FCPS.

- ◆ PSA with high pressure cH₂ storage and low pressure cH₂ transmission
- ◆ FI MH slurry purification and transmission and high pressure cH₂ storage
- ◆ FI MH slurry purification, transmission, and storage
- ◆ Stand-alone: (1) Reformate-FCPS and (2) distributed reformate production with FI MH slurry purification/storage



In Task 2, we will perform a molecular-level theoretical evaluation of the long-term feasibility of fluorinated metal hydride purification.

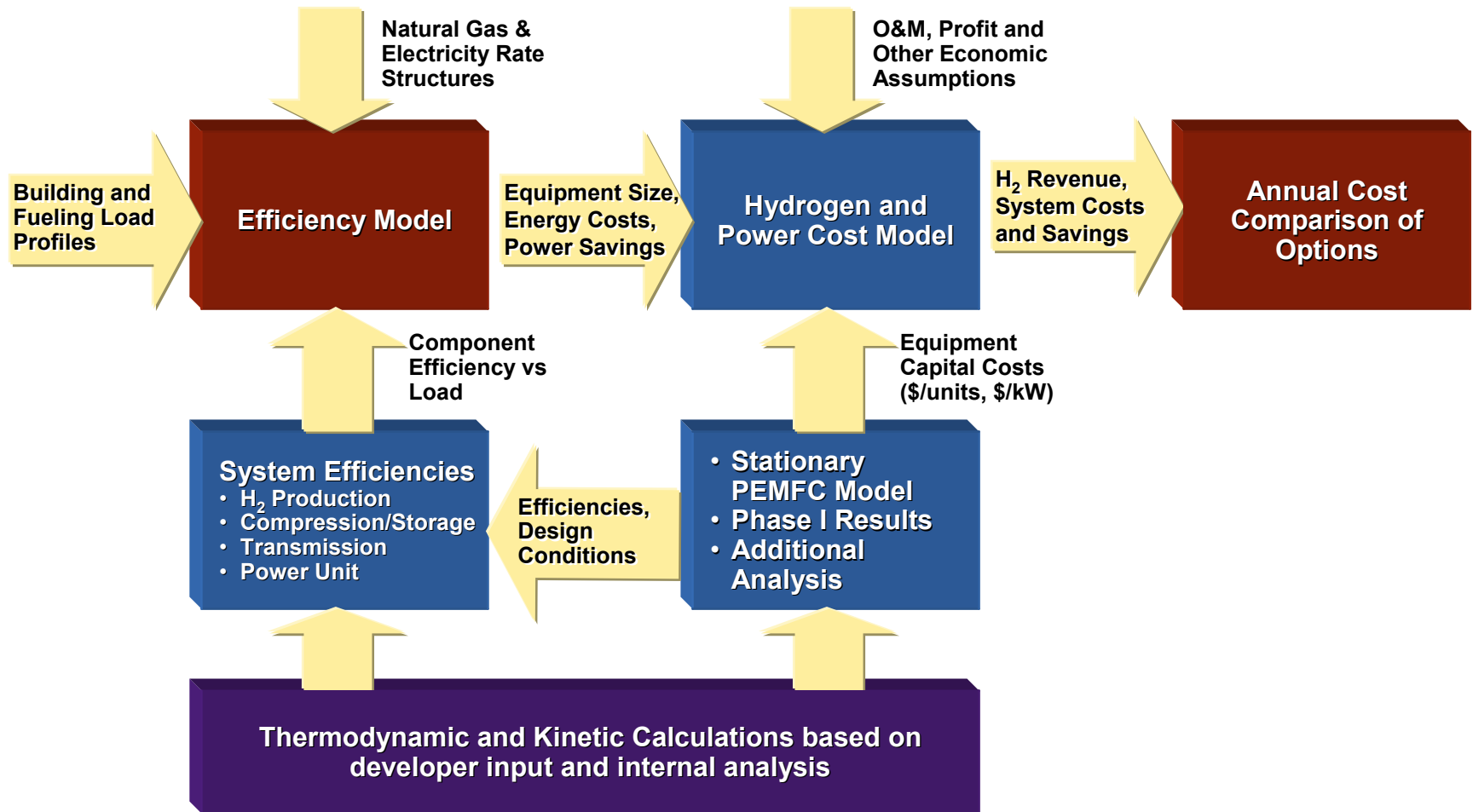
- ◆ Use first principles and quantum modeling to understand the underlying microscopic mechanism of a fluorinated metal alloy (e.g. La-Ni-Al)
- ◆ Test two main hypotheses:
 - Fluorination reduces the binding energy of undesired molecular species (e.g. O₂ and CO)
 - Diffusion barrier created by the fluorinated surface is much lower for hydrogen molecules than for undesired molecules
- ◆ Generate a general model for surface protection of metal hydrides
- ◆ Formulate general principles for protection techniques based on the general model
- ◆ Search for alternative protection methods or compounds that are even more effective in a practical application

We originally proposed to perform experimental tests to determine FI MH properties and performance, but this contract did not support lab-based R&D.

To date, we have constructed efficiency and cost models for the overall analysis and are in the process of refining the model inputs.

- ◆ An efficiency model has been developed
 - Inputs: building hourly electric and heat load profiles for the entire year, thermodynamic model results (e.g. efficiencies, cogen potential) for the FCPS and H₂ station
 - Outputs: grid power, natural gas, and FCPS hydrogen demands; GHG and other emissions
- ◆ Detailed cost calculations are being determined
 - Inputs: efficiency model results, capital cost inputs, utility rates for grid power and natural gas
 - Outputs: annual costs (electric energy and demand, natural gas, and capital cost charges)
- ◆ Preliminary design of a cH₂ Mini-Grid has been determined
 - Based on a combination of current natural gas and hydrogen distribution practices

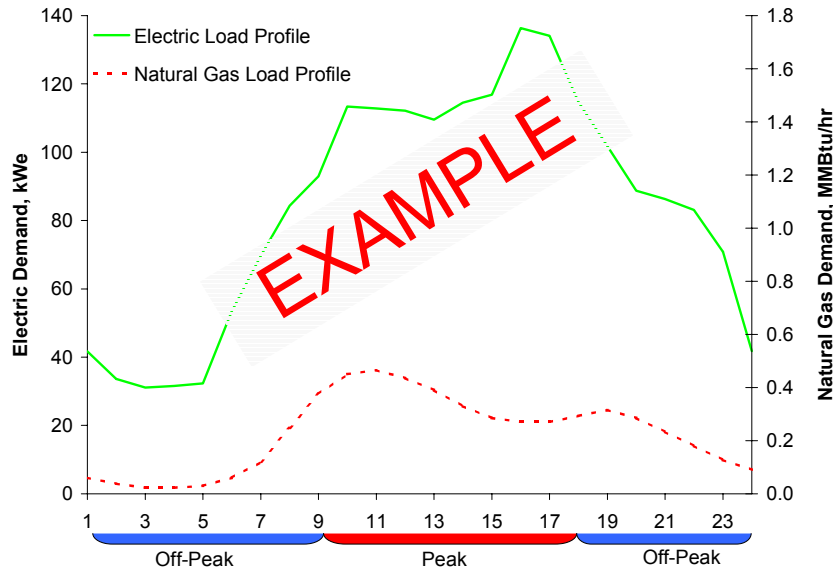
Efficiency and cost models are the backbone of the analysis to determine overall annual system costs and savings.



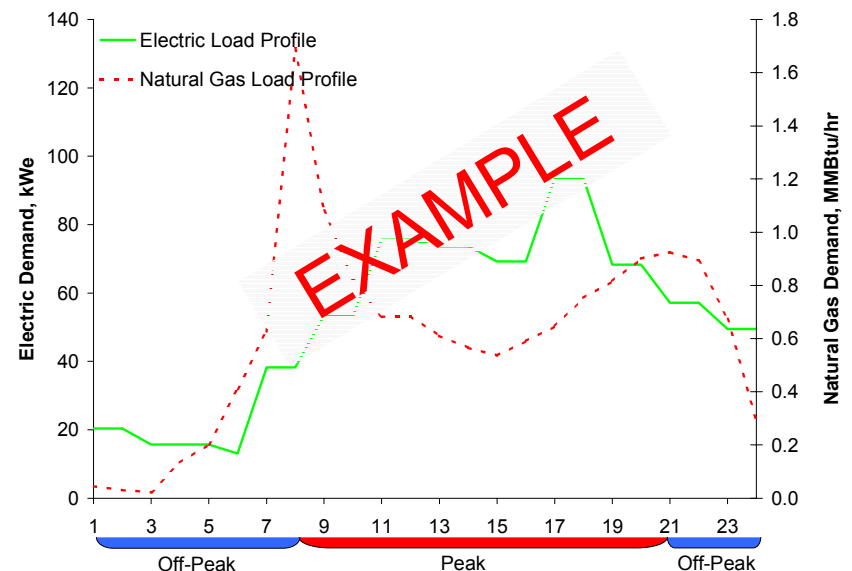
Hourly electric and heat load profiles for residential and commercial buildings have been generated for a typical meteorological year (TMY).

- ◆ Using EnergyPlus software
- ◆ Load profiles are used in the efficiency model to calculate:
 - FCPS operating times (turns on when the building demand exceeds design power)
 - Grid and FCPS monthly energy and peak power demands from the building
 - Cogen use (only when fuel cell is on and building heat is needed)

July 1 Profile for Multi-family residence in NYC



Jan 1 Profile for Multi-family residence in NYC



We constructed thermodynamic models to evaluate system parameters that can effect system efficiency and FCPS cogen capabilities.

- ◆ Using HYSYS process modeling software
- ◆ Thermodynamic results are used in the efficiency model to calculate:
 - Hydrogen (or natural gas) demand and cogen potential from the FCPS
 - Natural gas and power demand from the hydrogen station
- ◆ Models for both the FCPS and hydrogen station have been developed

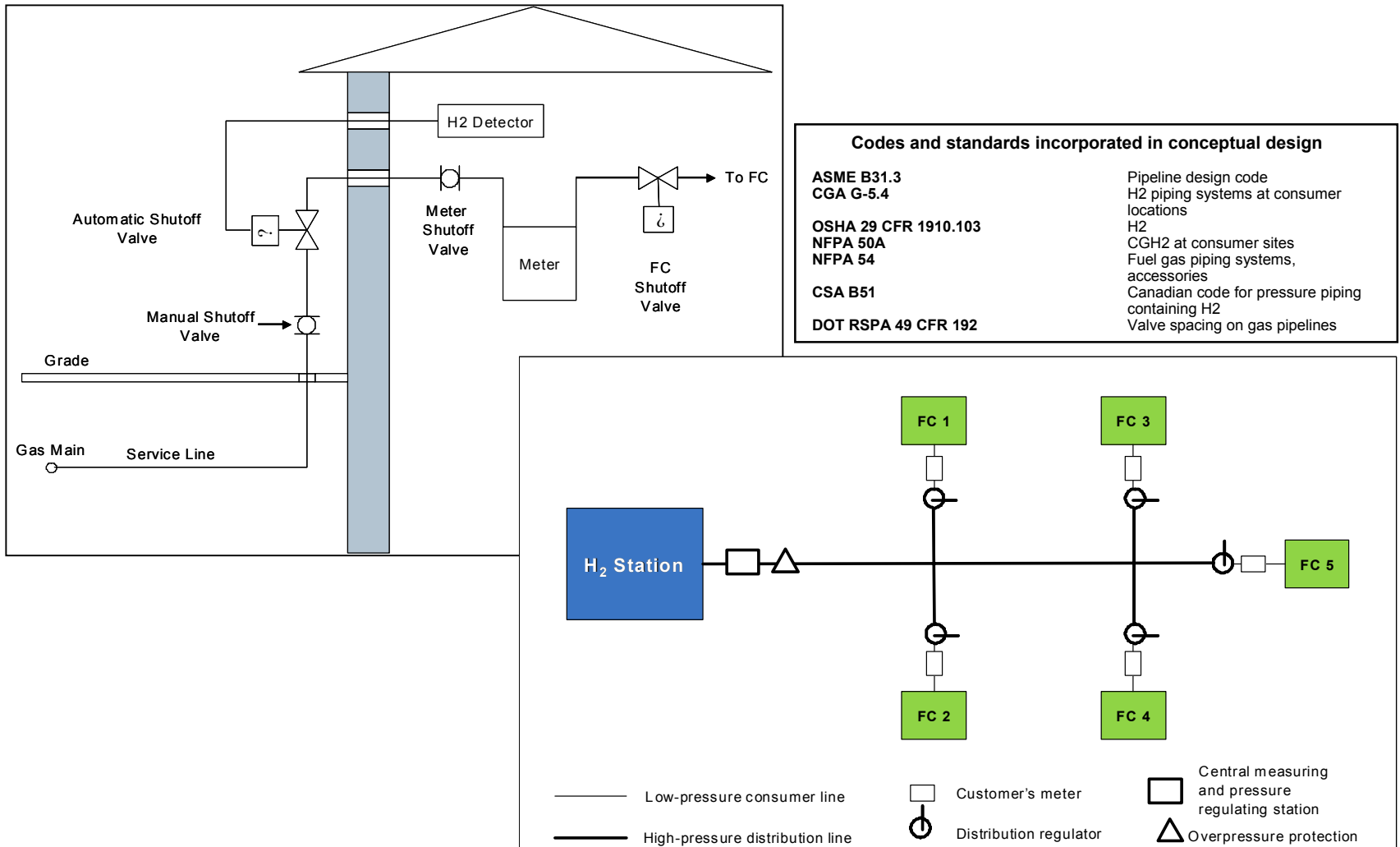
FCPS Parameters	Base Case	Low Temp.	Low Voltage	Low H ₂ Util.	High Press.
Temperature, °C	80	70	80	80	80
Design Voltage, V	0.70	0.70	0.63	0.70	0.70
Hydrogen Utilization, %	95		95	88	95
Pressure, atm	1.2		1.2	1.2	1.5
Preliminary Results					
Cogen Capability ¹ , kWth/kWe	0.68	0.81	0.87	0.87	0.87
System Efficiency ² , % (LHV)	49	49	44	45	48

EXAMPLE

¹ Cogen is reduced by humidification requirements.

² Includes 95% power electronics (i.e. inverter) efficiency, 95% hydrogen utilization, and parasitic loads.

U.S. Gas Pipeline Code, NFPA, and industry experts were consulted for the design of hydrogen gas delivery systems to consumer sites.

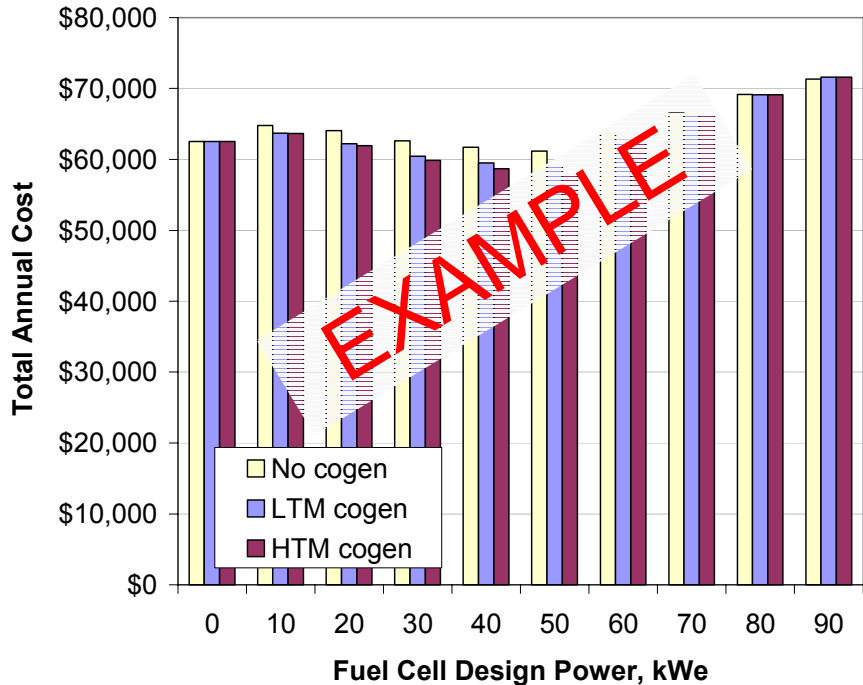


Annual costs will be determined once capital costs have been estimated (work in progress).

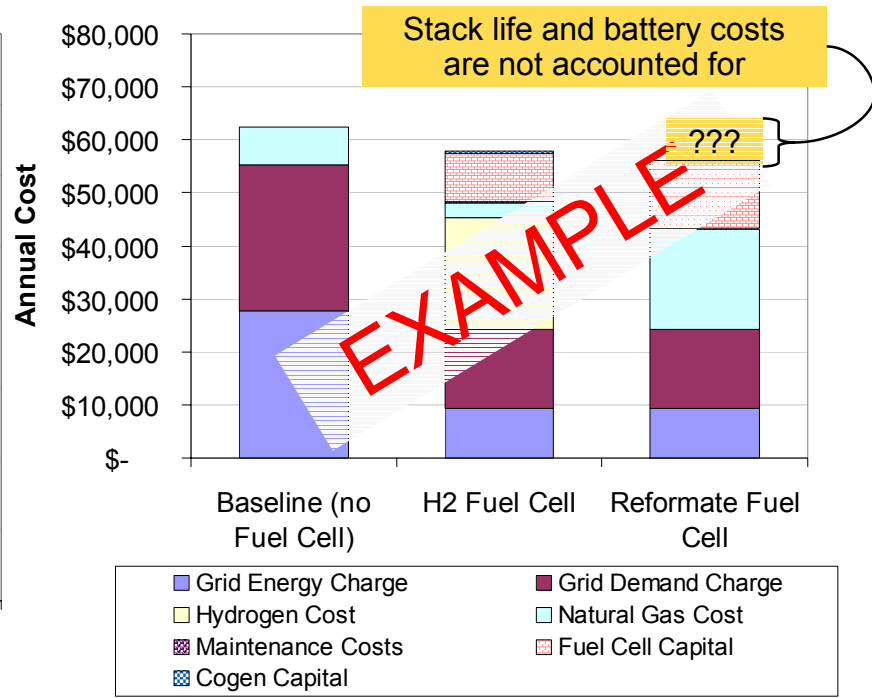
- ◆ Capital costs for the hydrogen station (production, compression, and storage equipment)
 - We are updating capital costs, scaling factors, and progress ratios
 - Based on detailed vendor quotes and internal analyses from Phase I
 - ↳ Phase I analysis assumed 100s units per year production volumes
- ◆ Hydrogen transmission cost
 - System designs have been conceptualized
 - We are estimating capital costs based on vendor quotes and additional cost assessments
 - “Right-of-way” costs dominate in most cases
- ◆ Capital costs for distributed FCPS
 - We are constructing a cost model that will automatically scale costs according to the user supplied production volume and rated power assumptions
 - Based on previous stationary PEMFC cost model

For this presentation, examples of annual costs have been generated based on assumptions for hydrogen and capital costs.

Direct-H₂ FCPS Ownership Cost



FCPS Ownership Cost Comparison



Key Assumptions:
 50 kW FCPS with high temperature membrane (HTM); capital costs = \$916/kW Direct H₂ and \$1,253/kW Reformate-FCPS; H₂ = \$1.00/kg

Using the cost model, design power and various other model inputs can be optimized to reduce total annual cost or GHG emissions.

At the end of Task 1, we will be able to assess the attractiveness and viability of using fluorinated metal hydride slurries in a H₂ Mini-Grid.

- ◆ Investigate performance of MH slurries and H₂ Mini-Grid systems:
 - Cost: hydrogen, power/heating, annual
 - Environment: energy use, GHG and other emissions
 - Other benefits: technical risk, reliability enhancement, and others
- ◆ Comparison to baseline and other systems:
 - Integrated hydrogen station concept Vs. stand-alone hydrogen station
 - MH slurry Vs. cH₂ transmission
 - FCPS (with and without cogen) Vs. conventional grid power and natural gas heating
 - FCPS utilizing a H₂ Mini-Grid Vs. stand-alone FCPS (hydrogen and reformat-based)

At the end of Task 2, we will be able to assess the long-term viability of using fluorinated (or otherwise treated) MHs for hydrogen purification.

- ◆ Establish selectivity of CO/H₂ separation based on energy surface calculation for transport through the layer
- ◆ Determine viability of fluorinated hydrides
- ◆ Develop and test hypothesis for optimization of barrier layer
- ◆ Establish R&D objectives for MH slurries based on Task 1 and 2 results
 - Identify key barriers and possible development paths
 - Contingent on a positive outcome from above