Thermodynamic, Economic, and Environmental Modeling of Hydrogen (H_2) Co-Production Integrated with Stationary Fuel Cell Systems (FCS)

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Overview

Timeline

- Project start date: Jan 2009
- Project end date: Sept 2010
- Percent complete: 12%

Budget

- Total project funding
  - 100% DOE funded
- Funding received in FY08:
  - $5K Sandia NL
- Expenditures for FY09 (to-date):
  - $56K Sandia NL
  - $11K UC Irvine
  - $1K other contracts
- Total available funding for FY09:
  - $163K shared by all parties

Barriers

- Barriers addressed
  - A. Future Market Behavior [developing economic & thermodynamic models of advanced H_2 -FCS to describe future H_2 supply]
  - B. Stove-piped/Siloed Analytical Capability [building cross-disciplinary engineering & business models; teaming with national labs (TSPI team) to jointly integrate H_2 -FCS into models]
  - D. Suite of Models and Tools [improving models with optimization, thermodynamic analyses of theoretical limits, novel FCS design and control]

Partners

- Interactions/ collaborations:
  - UC Irvine [H_2 separation thermodynamic models]
  - Transportation and Stationary Power Integration (TSPI) team: SNL, NREL, LANL, ORNL, BNL, ANL [jointly integrating H_2 co-production models]
  - Fuel Cell Energy, Inc. [MCFC expertise]
  - Technology Management, Inc. [SOFC expertise]
  - Fuels Pathways Integration Technology Team (FPITT): SNL, NREL, ANL, LLNL [developing models]; ExxonMobil, Shell, ConocoPhillips, Chevron [evaluating models]

Relevance

Hydrogen Co-Production Integrated with Stationary Fuel Cell Systems (H_2-FCS) can provide H_2 with lower costs, fuel use, & emissions than other H_2 supply chains.

H_2-FCS Concept:

- A conventional distributed fuel cell system can provide clean electricity and recoverable heat to nearby buildings. This system can be re-designed to also provide excess hydrogen (H_2) for supplying H_2 vehicles or industry (merchant H_2).
- H_2-FCS can provide H_2 with lower costs, fuel use, & emissions.

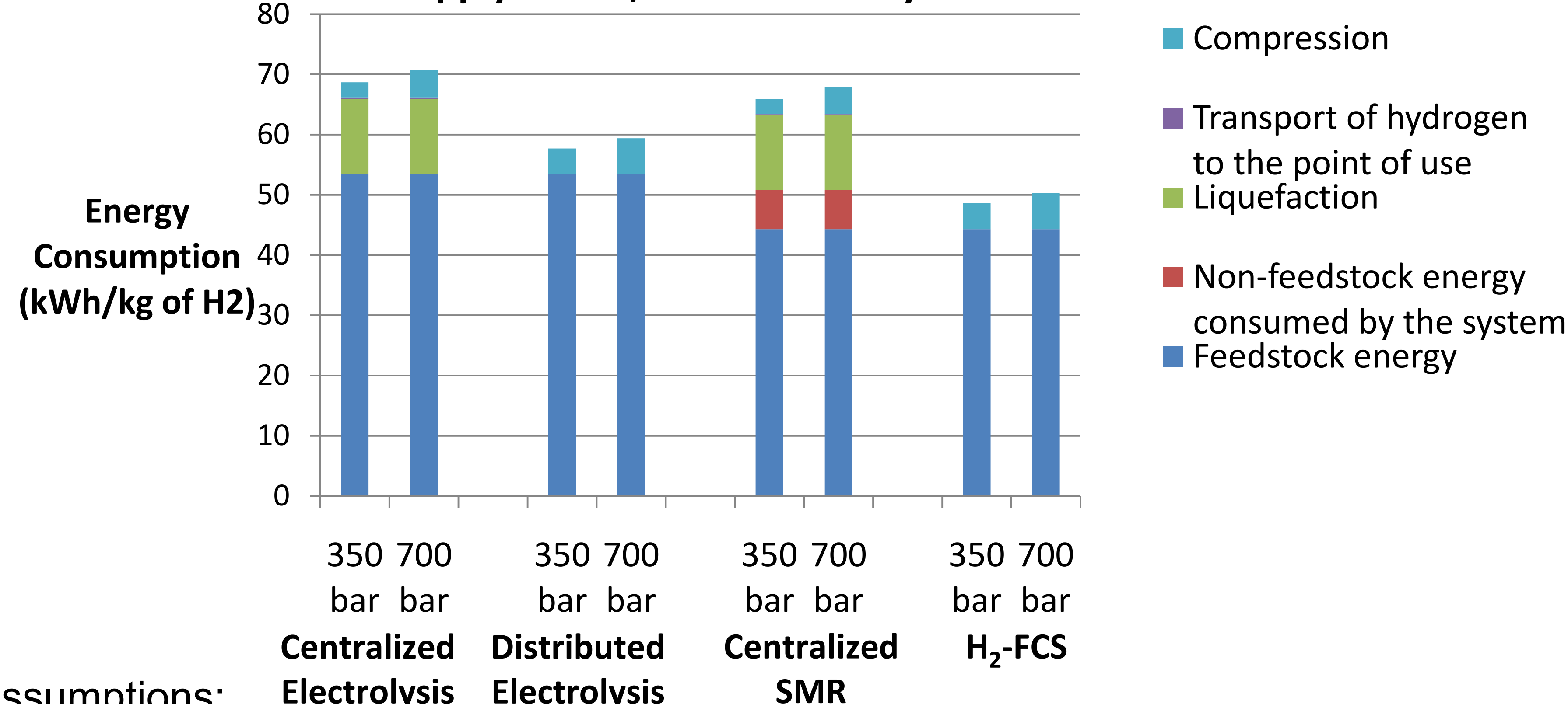
Advantages of this Approach:

- H_2-FCS can supply H_2 locally, without the added H_2 transport infrastructure and related capital costs, energy use, and emissions seen with centralized production.
- H_2-FCS can supply H_2 in response to H_2 demand, and as a H_2 vehicle fleet grows. When H_2 demand is low, H_2-FCS can sell more electricity and heat instead, and thereby retain high system capacity utilization and lower costs.
- H_2-FCS can address the “chicken-or-egg” problem associated with a lack of H_2 refueling stations for initial H_2 fleets.
- H_2-FCS can improve fuel security by relying on local, widely-available feedstock.
- H_2-FCS can make H_2 with less additional fuel than distributed steam methane reforming (SMR) by reusing high temperature fuel cell waste heat to warm the endothermic steam reforming process to make excess H_2.
- Synergistic benefits include that a lower fuel utilization increases overall efficiency (i.e., higher Nernst Voltage, lower mass transport losses, lower cooling requirement and associated air blower parasitic load.)
- Less energy is needed to make and to transport H_2 to vehicles using H_2-FCS compared with centralized electrolysis, distributed electrolysis, or centralized SMR.

Relevance

H_2-FCS consumes less energy to make and to transport H_2 compared with other H_2 supply chains.

Energy requirements for providing H_2 to refuel vehicles via various supply chains, based on life cycle assessment



<u>Assumptions:</u>

- Centralized electrolysis plant is located in Palm Springs, CA. 100% of electricity used is wind power. H_2 is transported by diesel-fueled truck to Los Angeles (LA).
- Distributed electrolyzer is located at fueling station & consumes100% wind power.
- Steam methane reforming (SMR) plant is located in Long Beach, CA; H_2 is transported by a diesel-fueled truck to LA.

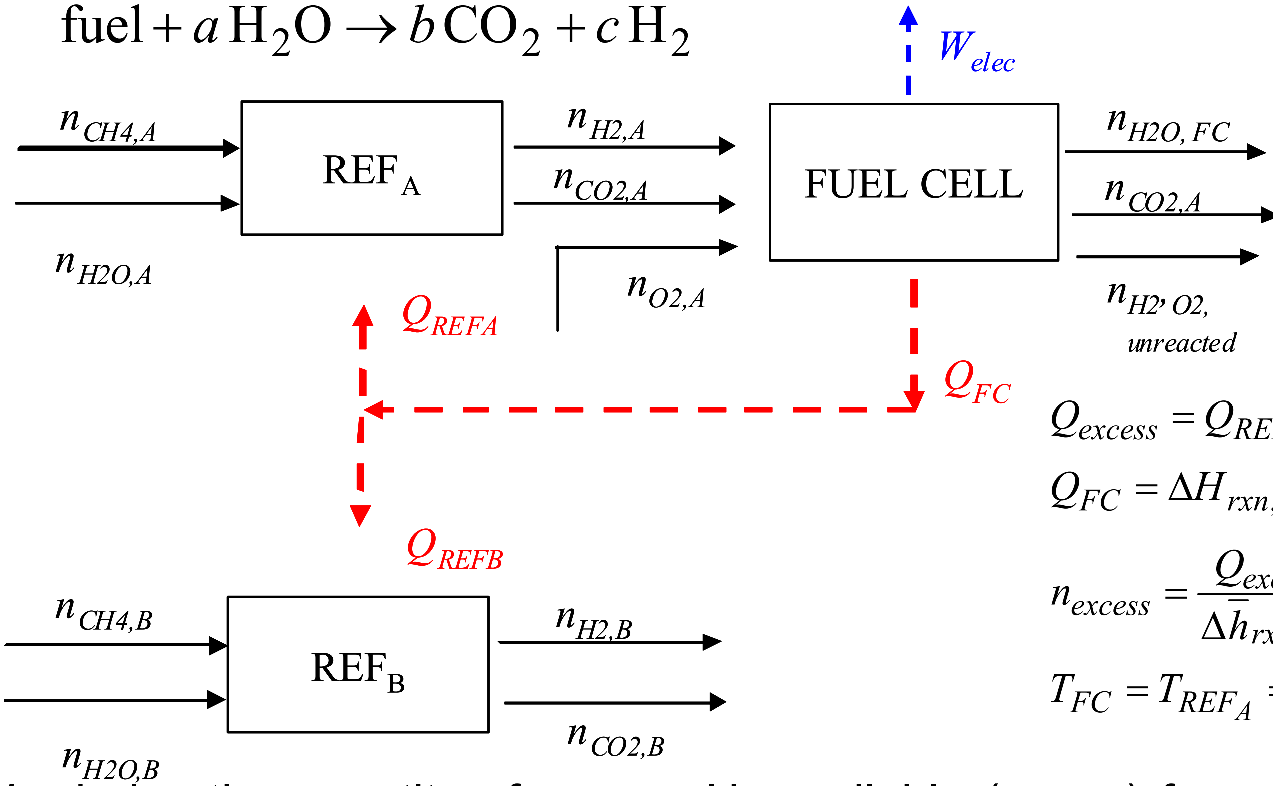
Relevance – Project Objectives

We analyze the potential for H_2 co-production within high temperature stationary fuel cell systems (H_2-FCS) and identify novel designs with minimum 1) CO_2 and 2) cost.

#	Objectives	#	Progress Notes	Comments	Percent Complete
1	Develop novel H_2-FCS designs that release low greenhouse gas emissions.	1.1	We derive the theoretical limit of excess H_2 from fuel cell electrochemical waste heat alone, without added feedstock fuel use or CO_2 emissions.	We developed analytical and chemical engineering process flow sheet models to show that an idealized 1 megawatt electric fuel cell operating between 800 and 1000ºC could make ~150 to 450 kg H_2 /day, without added fuel use or CO_2 emissions.	12%
		1.2	We identify optimal cycle designs for thermally integrating the hydrogen separation unit (HSU) & the fuel cell, to reuse anode-off gas waste heat, consume less work, & increase H_2 yield with no added fuel or CO_2.	We built chemical engineering process flow sheet models to identify an optimal HSU cycle design that meets pressure swing absorption (PSA) unit inlet requirements, recovers 73% of available anode-off gas waste heat, consumes 11% of gross electricity, & increases H_2 yield by 132%, without any added feedstock fuel use or CO_2 emissions. Our approach minimizes fuel consumption and CO_2 emissions by re-using available waste heat and minimizing losses.	12%
		1.3	We show minimum CO_2 emissions for designs with our approach using heat & H_2 load following, operating at any electrical output.	We advanced optimization models that show that, for a given set of assumptions, the designs with the lowest CO_2 emissions tended to combine a) electrical and thermal networking, b) a variable heat-to-electric power ratio, c) a variable H_2-to-heat ratio, d) first load following heat demand as the primary control, and e) then load following H_2 demand as the secondary control.	12%
2	Develop novel H_2-FCS designs with low H_2 production cost.	2.1	We show that cost optimization favors designs operating at maximum electrical output, with heat & H_2 load following.	We advanced optimization models that show that, for the assumptions and options investigated, the designs with the lowest energy costs tended to combine a) electrical and thermal networking, b) a variable heat-to-electric power ratio, c) a variable H_2-to-heat ratio, with d) maximum electrical output, e) heat load following, and e) H_2 load following.	12%

We reduce energy to make H_2 by using fuel cell heat for endothermic reforming. We derive the theoretical limit of excess H_2 from electrochemical waste heat alone.

$$\text{fuel} + a\,H_2O \rightarrow b\,CO_2 + c\,H_2$$



$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O$$

$$\text{SOFC} : O^{2-}\ \text{carrier}$$

$$\text{MCFC} : CO_3^{2-}\ \text{carrier}$$

$$Q_{excess} = Q_{REF_B} = Q_{FC} - Q_{REF_A}$$

$$Q_{FC} = \Delta H_{rxn,fc} - W_{elec}$$

$$n_{excess} = \frac{Q_{excess}}{\Delta \bar{h}_{rxn,sr}} = \frac{\left(\Delta H_{rxn,fc} - W_{elec}\right) - Q_{REF_A}}{\Delta \bar{h}_{rxn,sr}}$$

$$T_{FC} = T_{REF_A} = T_{REF_B}$$

We derive the quantity of excess H_2 available (n_{excess}) from electrochemical waste heat (Q_{FC}). The steam reforming reactions can provide H_2 (A) for the fuel cell's anode or (B) for excess H_2 production. For benchmarking a H_2 co-producing system against a standard system, we analytically separate the two processes – (A) and (B) -- in two "virtually" separate steam reformers – REF$_A$ and REF$_B$. REF$_A$ produces enough H_2 for the fuel cell to provide electric power. REF$_B$ produces excess H_2 (for vehicles, etc.)

We model SOFC polarization from 600 to 1000°C.

$$W_{elec} = n_e F V$$

$$V = V^{ideal} - \eta_{act} - \eta_{ohm} - \eta_{conc}$$

$$\eta_{ohm} = i \times \left(R_{anode} + R_{cathode} + R_{IC} + R_{electrolyte}\right)$$

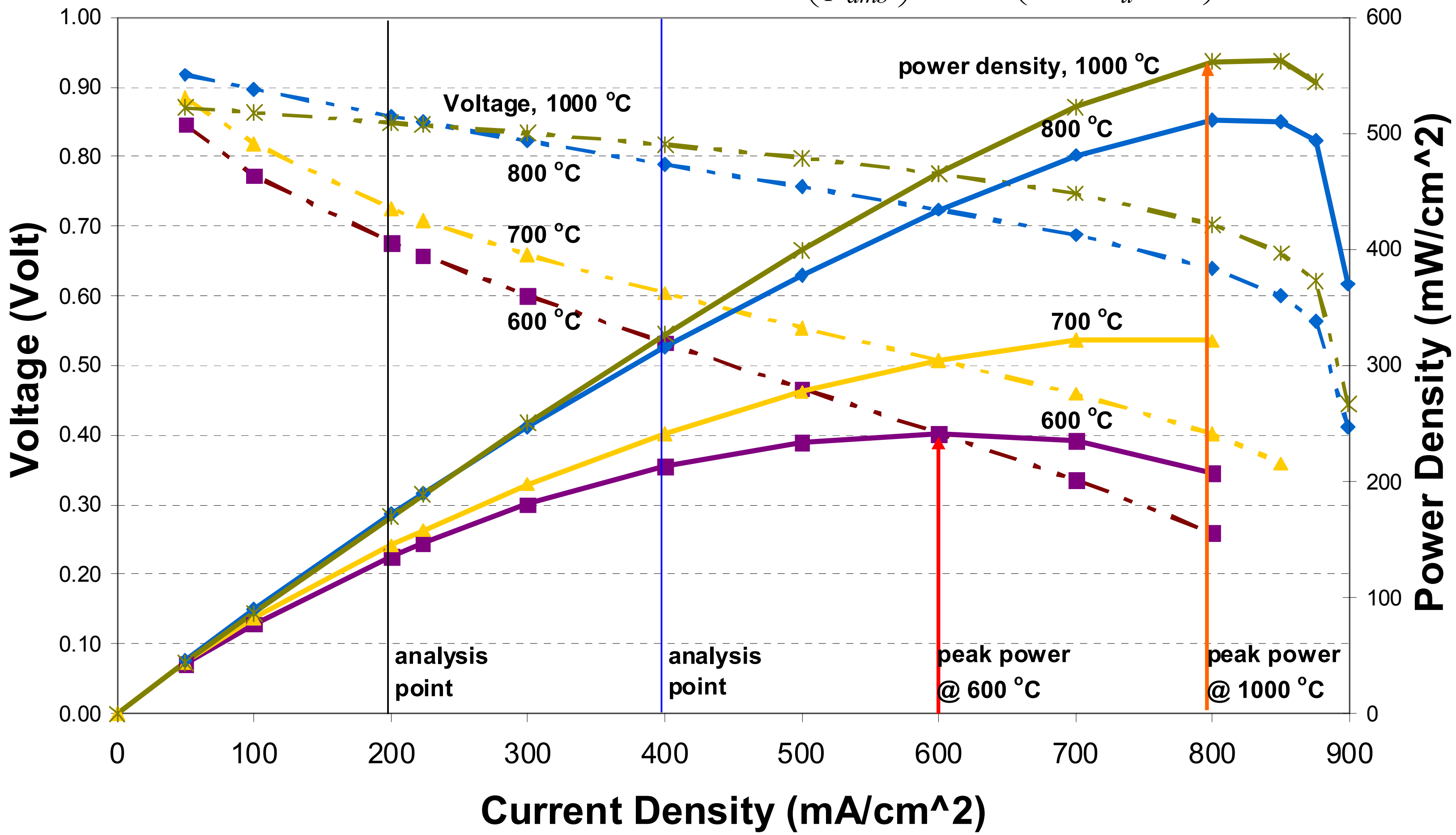
$$\eta_{conc} = -\frac{R_u T_{out}}{n_e F} \ln\left(1 - \frac{j}{j_L}\right)$$

$$\eta_{act} = \frac{R_u T_{out}}{n_e F} \sinh^{-1}\left(\frac{j}{2 j_{o,*}}\right)$$

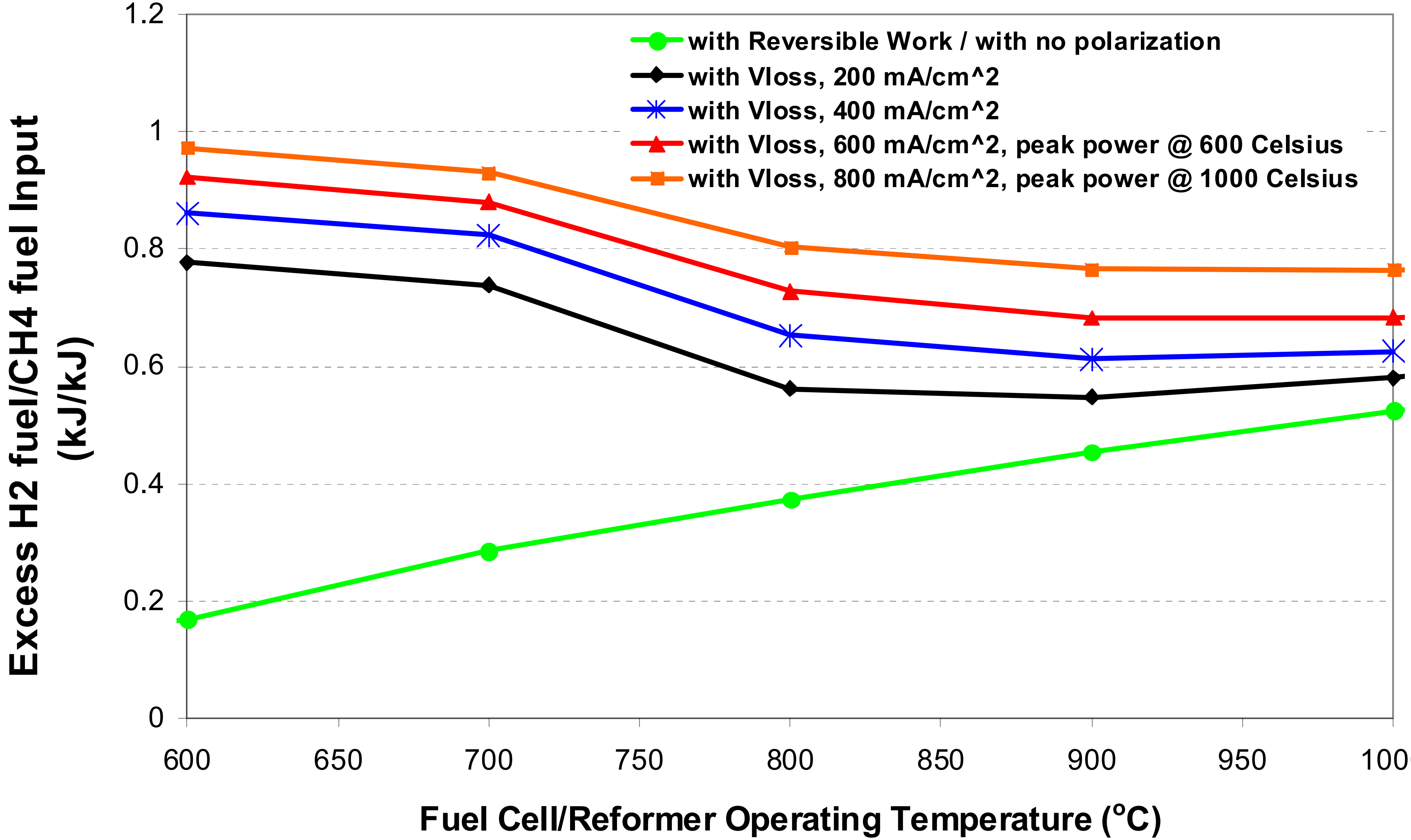
$$j_{o,anode} = \gamma_{anode} \left(\frac{p_{H_2}}{p_{amb}}\right)\left(\frac{p_{H_2O}}{p_{amb}}\right) \exp\left(-\frac{E_{act,anode}}{R_u T}\right)$$

$$j_{o,cathode} = \gamma_{cathode} \left(\frac{p_{O_2}}{p_{amb}}\right)^{0.25} \exp\left(-\frac{E_{act,cathode}}{R_u T}\right)$$

Includes constants published by Shaffer, B., M. Hunsuck, and J. Brouwer, 2008.

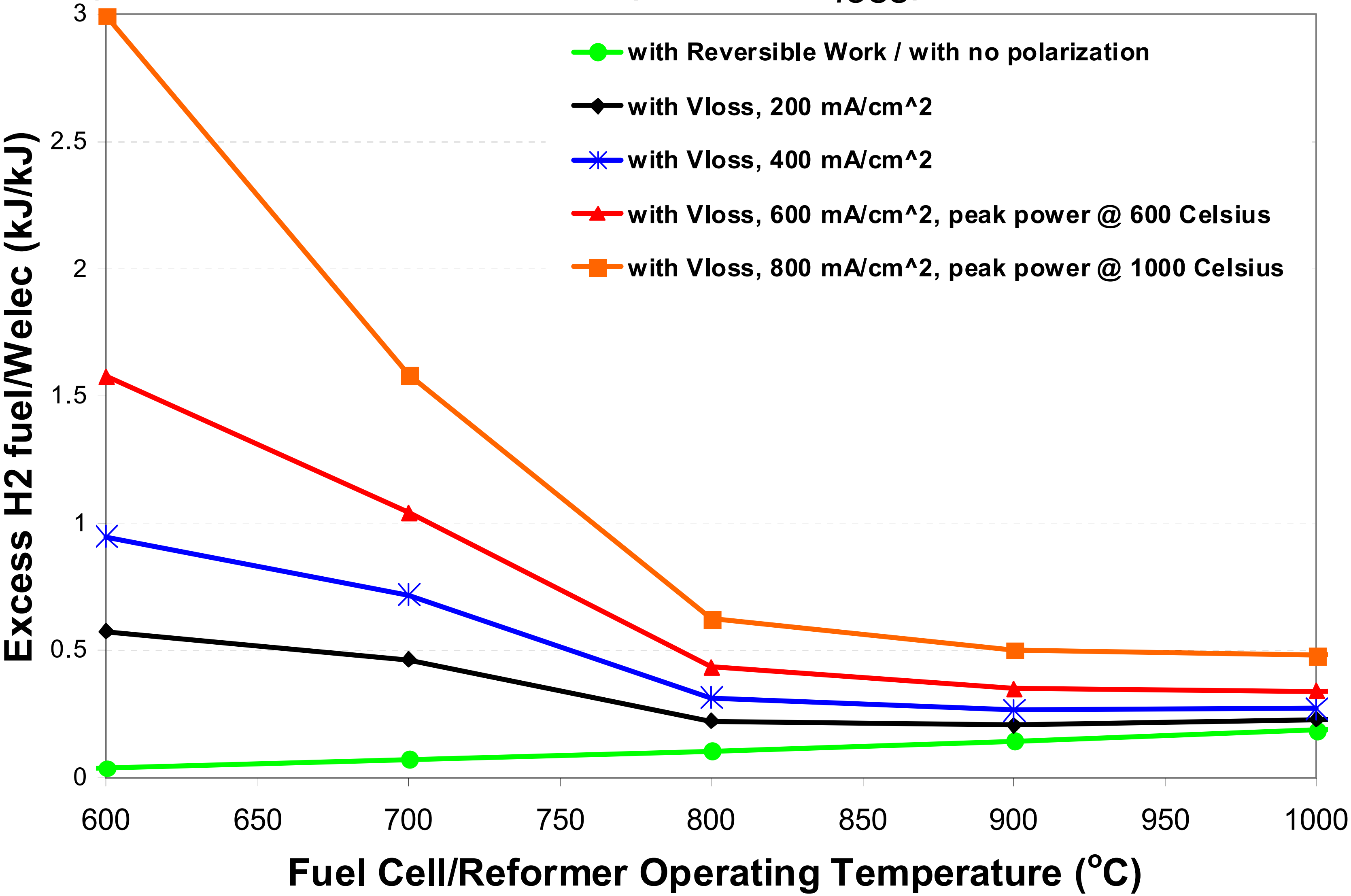


Excess H_2 per unit of fuel input increases with increased irreversible work (i.e., with increased polarization).



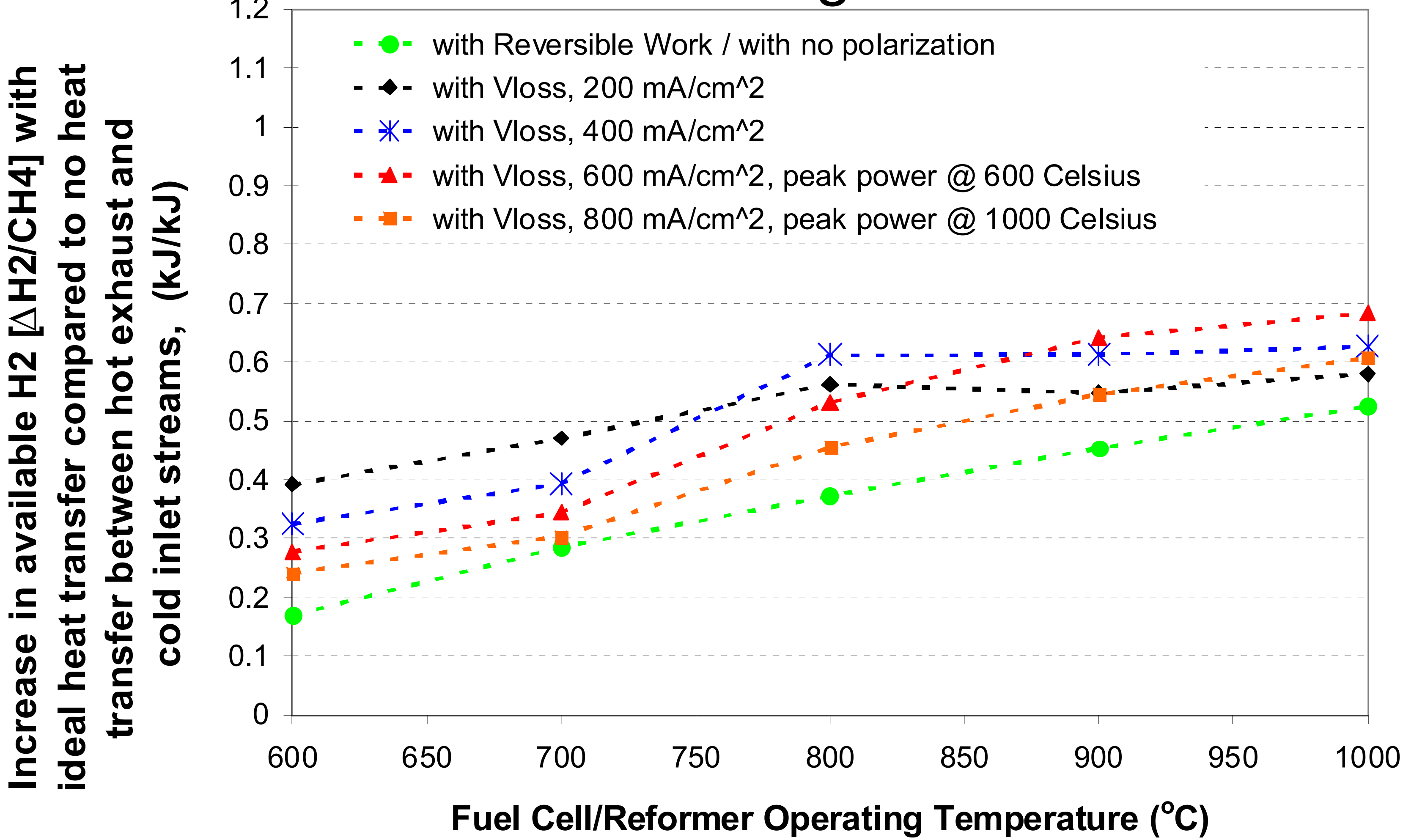
For reversible electrical work, the y-axis ratio increases with increasing temperature. For irreversible work, it decreases with increasing temperature. [SOFC polarization model supplies voltage losses (V_{loss}) at even current density increments (200 mA/cm^2).]

Excess H_2 per unit of electrical work (W_{elec}) increases with higher irreversibilities (more V_{loss}).



This trend occurs to a greater extent as temperature decreases, because as the temperature decreases in the range of 600-1000C, the polarization increases.

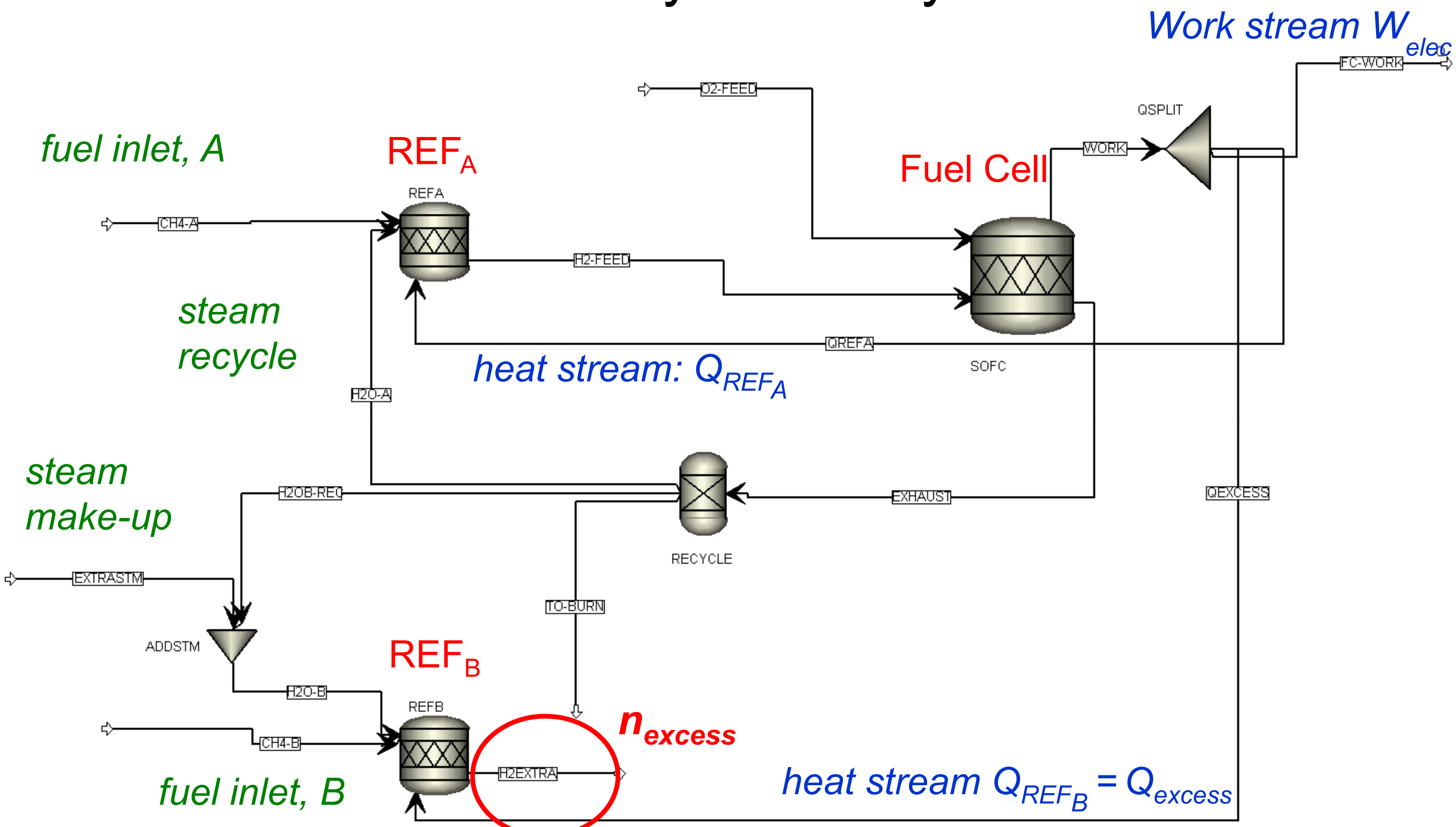
Excess H_2 is greater with more internal reuse of heat between hot outlet and cold inlet gases.



Excess H_2 is greater with (A) ideal heat transfer between hot fuel cell system exhaust gases (CO_2, H_2O, H_2) and cold inlet gases (O_2, CH_4, H_2O) compared with (B) no heat transfer between hot exhaust and cold inlet streams. Excess H_2 depends upon the efficiency of heat exchange in preheating anode and cathode inlet gases.

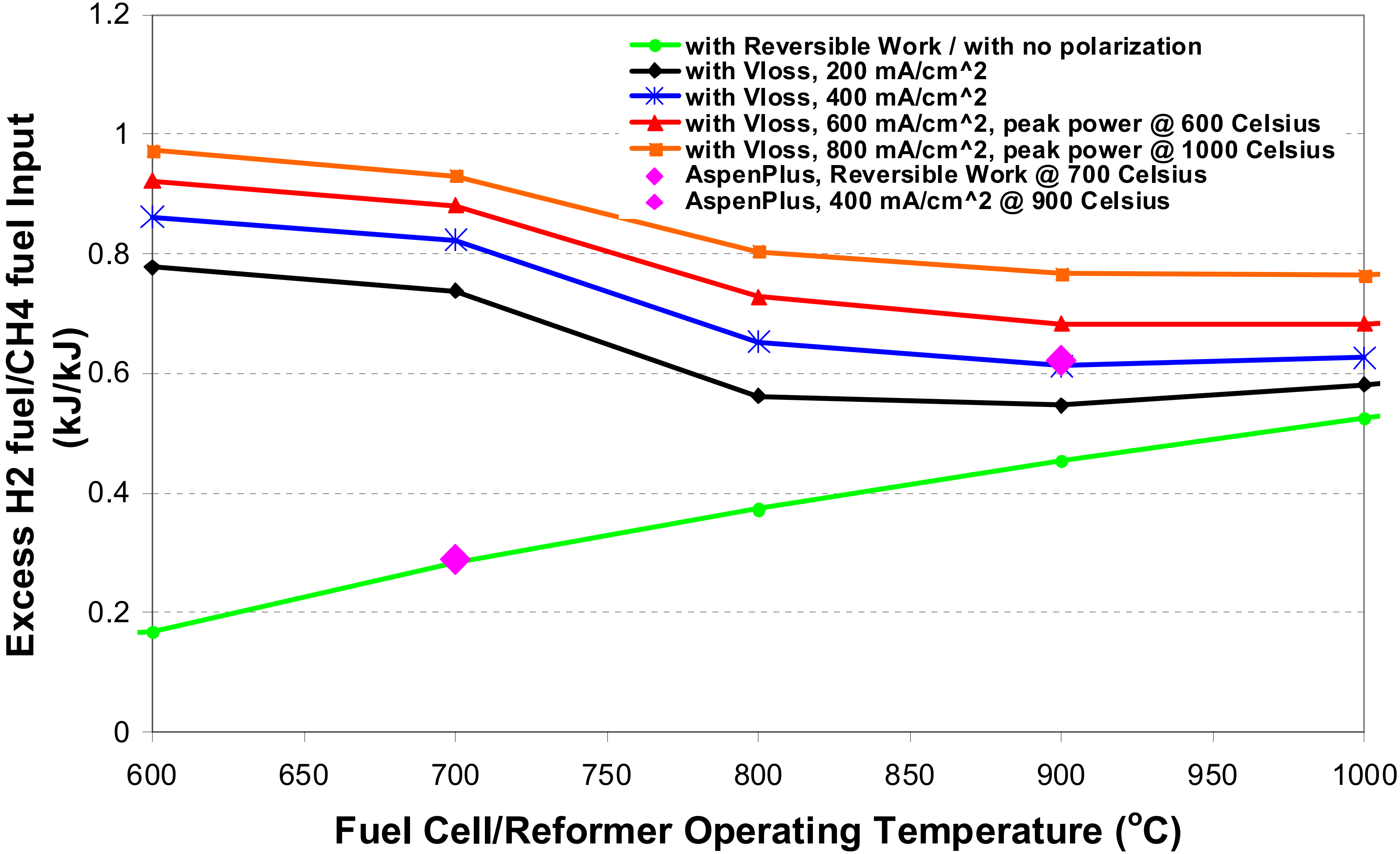
Approach; Objective 1.1

Our AspenPlus™ chemical engineering process flowsheet simulations verify our analytical models.



AspenPlus™ model emulates schematic of analytical model with REF_A and REF_B distinction, ideal heat transfer, high fuel and oxidant utilization within fuel cell, and reuse of fuel cell electrochemical waste heat alone. It calculates excess H_2 available (n_{excess}).

Our AspenPlus^{TM} model results agree with our analytical model calculations.



Results concur for reversible and non-reversible work, for different polarization levels (V_{loss}), and for different operating temperatures.

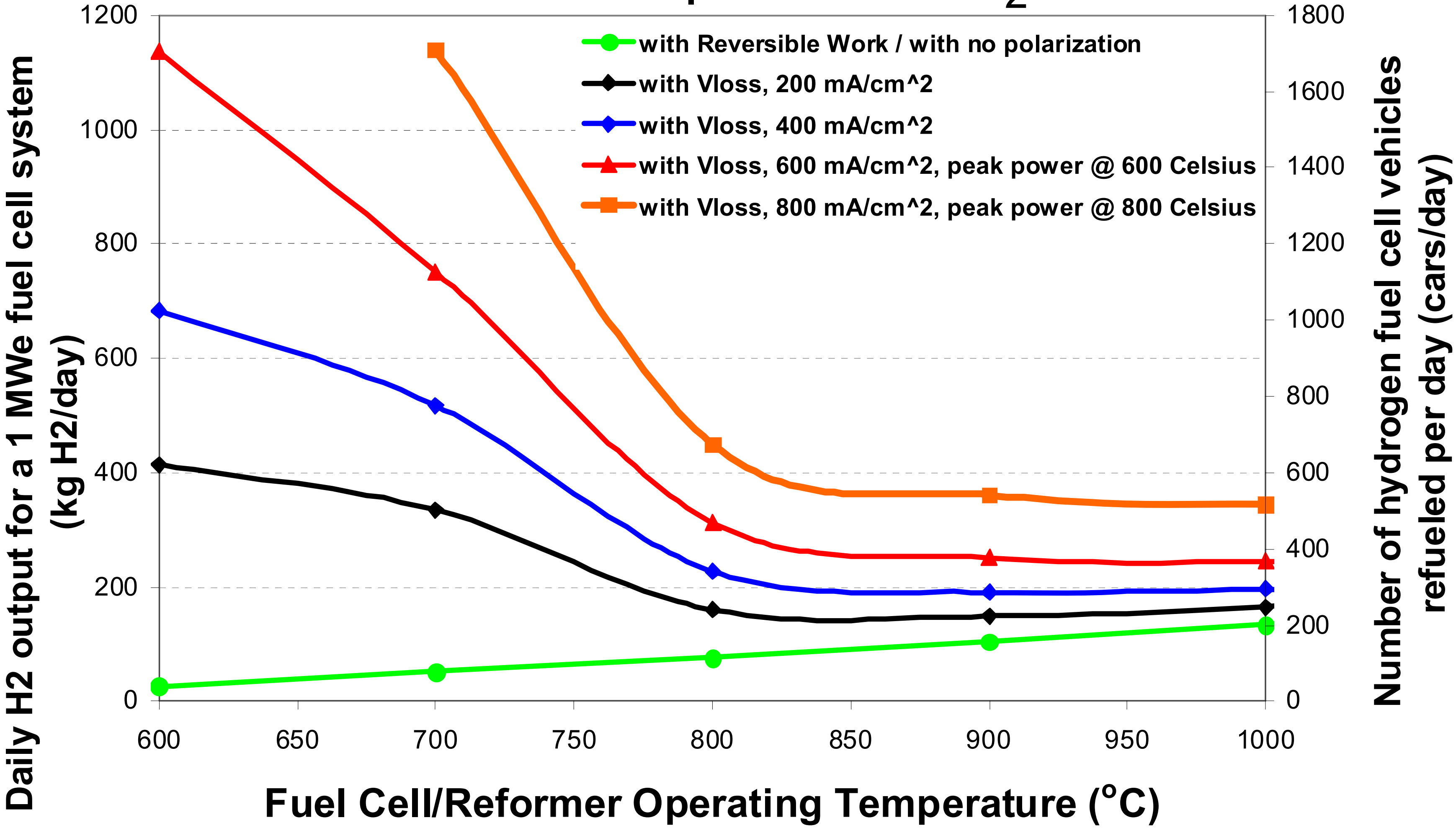
AspenPlus™ model fluid stream table shows results for excess H_2 moles from REF_B, and excess H_2/CH_4, which agree with analytical model.

n_{excess} Excess H_2 fuel/CH_4 fuel input (kJ/kJ)

	CH4-A	CH4-B	H2-FEED	H2EXTRA	H2O-A	H2O-B	H2OB-REC
Mole Flow (kmol/hr)							
CH4	0.25	0.22	0	0	0	0	0
H2O	0	0	0	0.56	0.5	1	0.5
CO	0	0	0	0	0	0	0
CO2	0	0	0.25	0.22	0	0	0
H2	0	0	1	0.874	0	0	0
O2	0	0	0	0	0	0	0
N2	0	0	0	0	0	0	0
Total Flow kmol/hr	0.25	0.22	1.25	1.66	0.5	1	0.5
total Flow kg/hr	4.01	3.51	13.02	21.52	9.01	18.02	9.01
Total Flow cum/hr	24.38	21.31	121.94	161.47	48.77	97.54	48.77
Temperature, K	1173.15	1173.15	1173.29	1173.15	1173.15	1173.15	1173.15
Pressure, bar	1	1	1	1	1	1	1
Vapor Frac	1	1	1	1	1	1	1
Liquid Frac	0	0	0	0	0	0	0
Molar Enthalpy, kJ/kmol	-22855.56	-22855.56	-49352.94	-103436.06	-208462.8	-208462.8	-208462.8
Mass Enthalpy, kJ/kg	-1424.9102	-1432.5422	-4738.1855	-7978.8039	-11568.4129	-11568.4129	-11568.4129
Enthalpy Flow, kW	1.5872	1.3967	17.1364	47.6955	28.9532	57.9063	28.9532
Excess H2 fuel/total CH4 fuel Input	0	0	0	0.62175	0	0	0
Molar Entropy, J/mol-K	-6.65256	-6.65256	49.9988	40.50112	6.40152	6.40152	6.40152
Mass Entropy, J/gm-K	-0.4184	-0.4184	4.8116	3.09616	0.37656	0.37656	0.37656
Molar Density, kmol/cum	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Mass Density, kg/cum	0.16	0.16	0.11	0.13	0.18	0.18	0.18
Average MW	16.04	16.04	10.41	13	18.02	18.02	18.02

Table shows example data for a power density of 400 mA/cm^2 and a fuel cell/reformer operating temperature of 900 ^oC

A 1 megawatt electric (MWe) fuel cell operating between 800 and 1000ºC could make ~150 to 450 kg H_2 /day without added fuel consumption or CO_2 emissions.



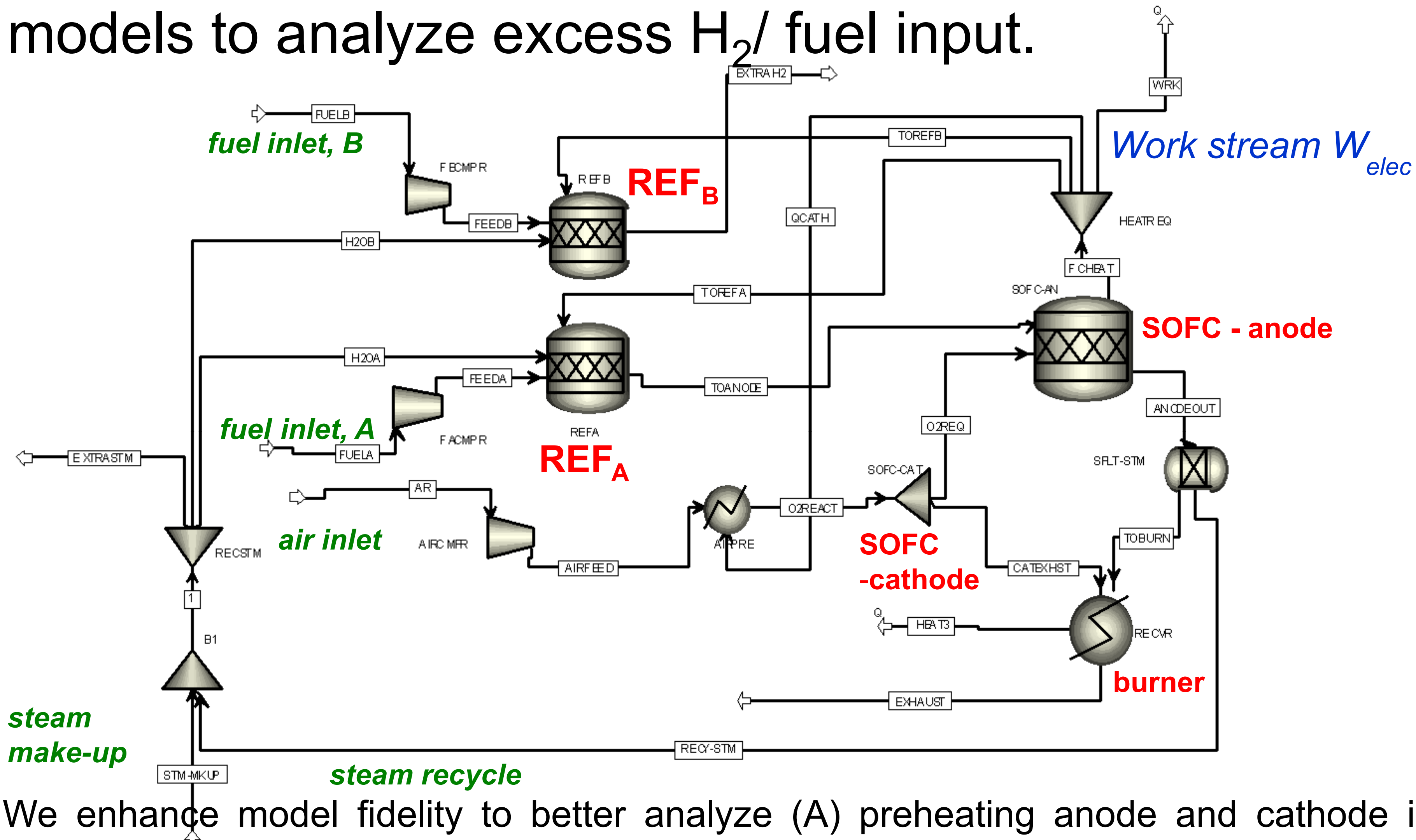
This equates to fueling between ~ 220 and 660 H_2 fuel cell cars per day.

Based on a fuel economy of 60 miles/kg H_2 [1] and an average annual mileage of 15,000.

[1] http://www.fueleconomy.gov/feg/fcv_sbs.shtml

Technical Accomplishments and Progress; Objective 1.1

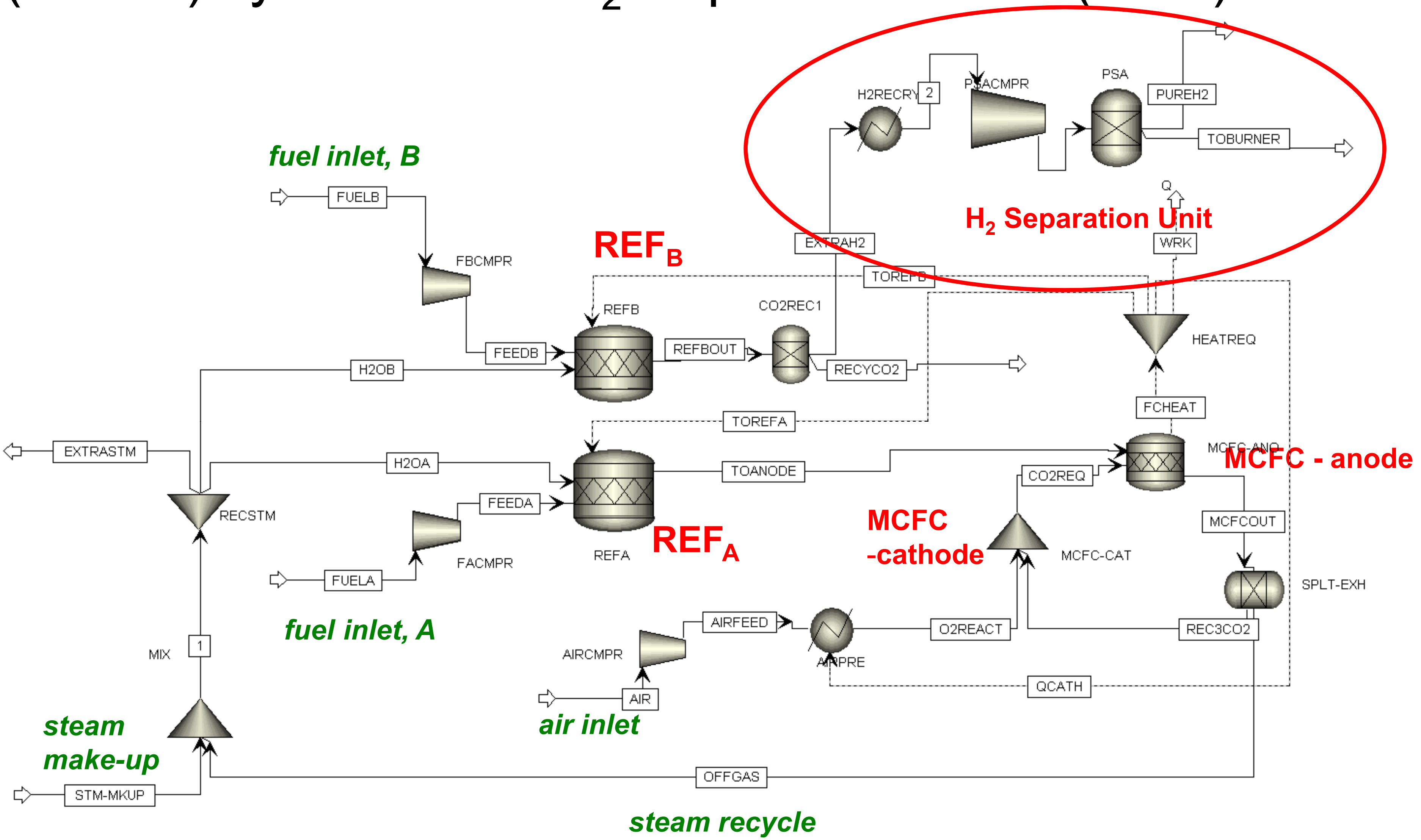
We introduce increasing complexity into AspenPlus™ models to analyze excess H_2/ fuel input.



We enhance model fidelity to better analyze (A) preheating anode and cathode inlet gases, (B) reduced air compressor parasitic power for fuel cell stack cooling, (C) lower anodic fuel and cathode O_2 utilization rates, (D) ancillary loads (pumps, etc.), (E) heat exchanger loop designs, (F) recycle streams, (G) external and internal reforming, (H) thermodynamic cycle designs, and (I) operating conditions (steam-to-carbon ratio, etc.)

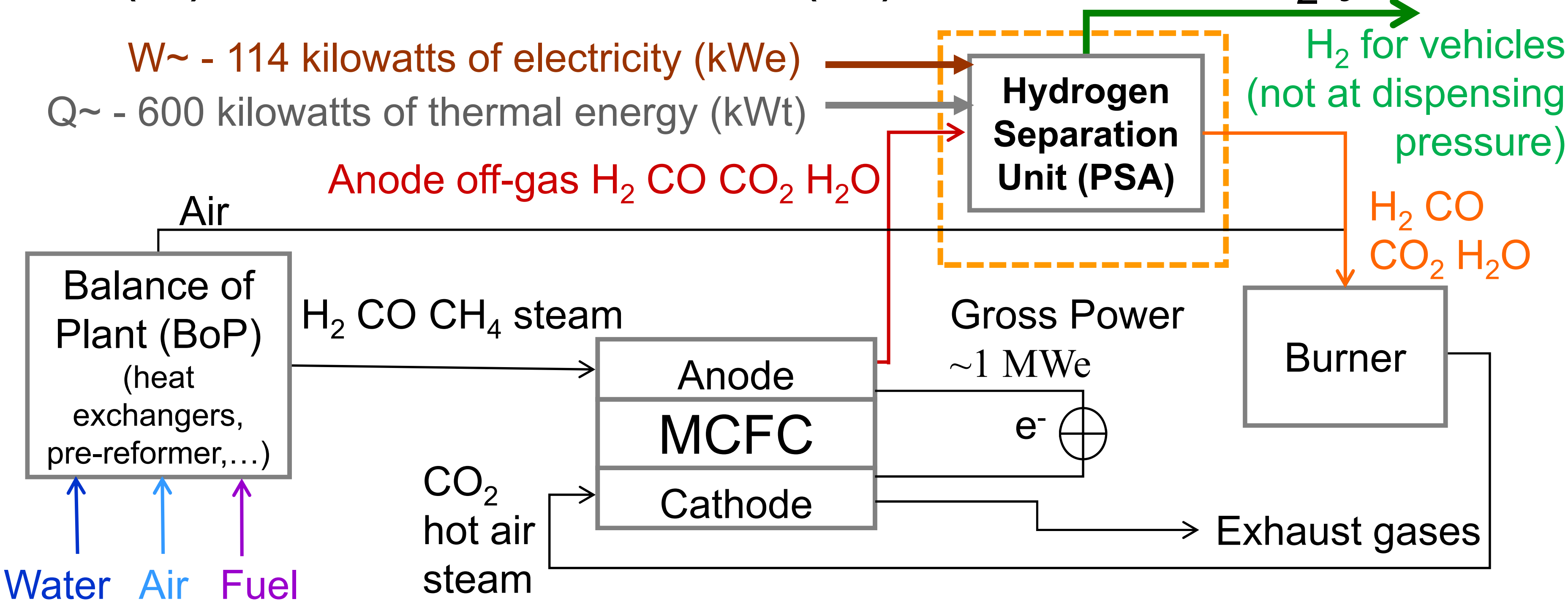
Approach; Objective 1.2

We model the integration of Molten Carbonate Fuel Cell (MCFC) systems with H_2 Separation Units (HSU).



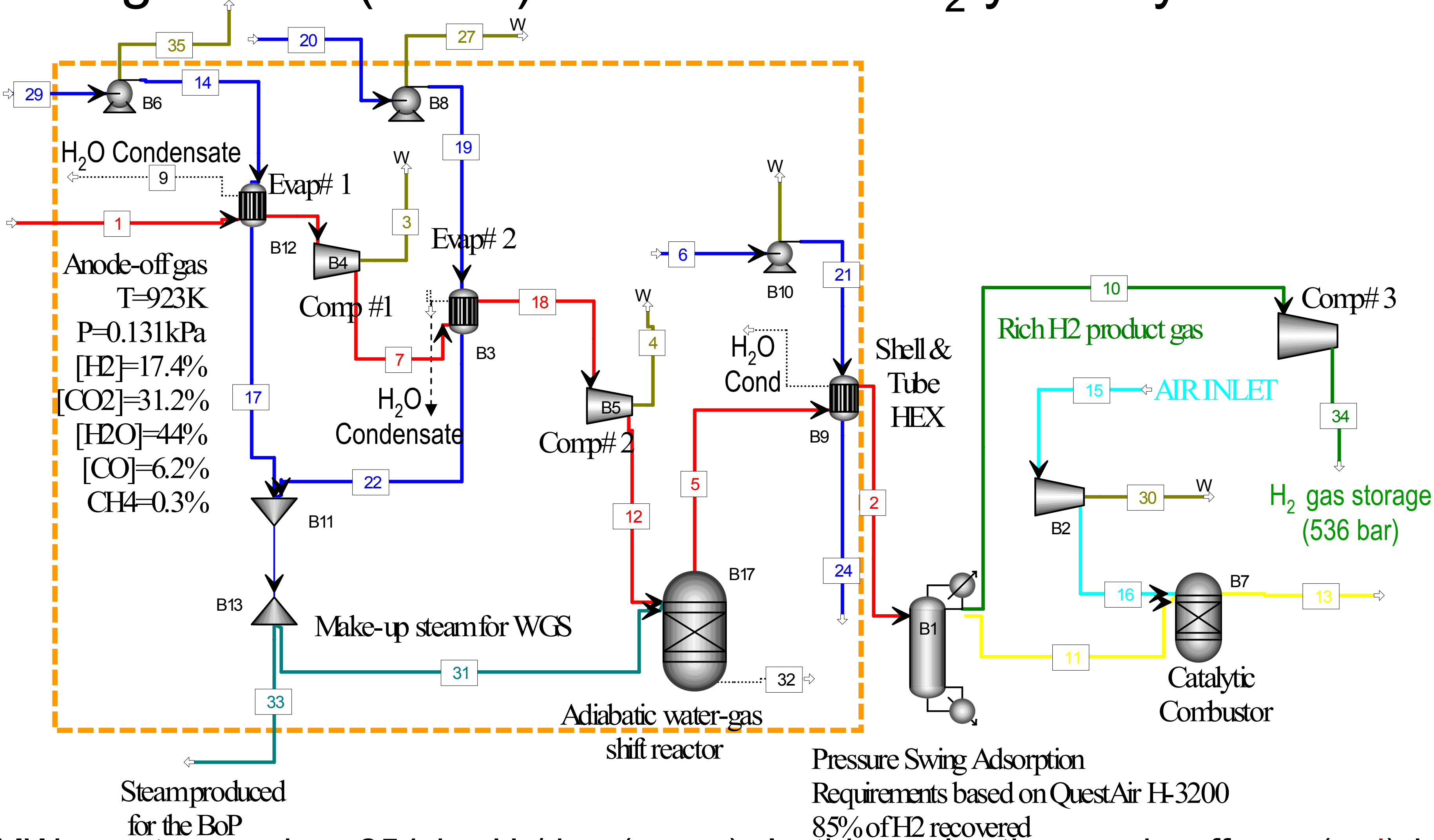
The HSU uses Pressure Swing Absorption (PSA) beds, based on 80% H_2 recovery and QuestAir H-3200 specifications. The 1 MWe MCFC operates with 60% H_2 utilization.

We evaluate cycle design configurations for thermally integrating HSU & fuel cell, with these goals: achieve required inlet temperature & pressure for PSA, reuse all heat (*Q*), consume less work (*W*), & increase H_2 yield.



H_2 yield for vehicle fueling (shown in green) increases when less anode off-gas H_2 (red) is burned for internal heat generation (orange). Heat from H_2 combustion can be displaced by internal reuse of available heat. The anode off-gas (red) must be cooled and compressed to reach the required PSA inlet temperature (~323 K) and pressure (~20 bar). We evaluate configurations where this available heat warms incoming water (blue), air (light blue), & fuel (purple), and displaces H_2 combustion at the burner (orange).

We identify HSU cycle designs with heat recovery & water gas shift (WGS) that increase H_2 yield by 132%.



1 MWe system makes 254 kg H_2/day (green). In this cycle, the anode off-gas (red) is cooled & compressed in series twice, cooled again, undergoes WGS to convert CO to H_2, & is cooled again before the PSA. Recovered heat makes BoP required steam (blue).

This HSU design recovers 73% of the available thermal energy, with a compressor load of 11% of gross power.

Heat Recovery Devices

Heat Exchanger	Heat Recovered (kWt)
Evaporator #1	207
Evaporator #2	178
Post-WGS Heat Exchanger	51
Total	**436**

Compression Work Devices

Compressor	Outlet Pressure (bar)	Work Required (kW)	Comment
1	4	69	for PSA inlet
2	22	45	for PSA inlet
Subtotal		**114**	
3	537	32	for H_2 storage
Total		**146**	

The anode off-gas has 600 kilowatts of thermal energy (kWt) available to recover between the anode outlet and the PSA inlet temperatures. The HSU cycle design shown here recovers 436 kWt of this heat (73%), which provides 91% of system-wide required steam. It requires 114 kW of compressor work (~11% of gross electric power) from compressors 1 & 2 to reach the required PSA inlet pressure (~21 bar.) This HSU design reduces compressor work by lowering compressor inlet gas temperatures. The H_2 delivery sub-system needs an additional 32 kW of compressor work to pressurize H_2 up to 537 bar for H_2 storage, to later dispense H_2 at 350 bar to vehicles. Total compressor load for the HSU and H_2 storage is about 15% of gross electric power.

The marginal increase in H_2 yield due to 1) displaced H_2 combustion alone is 102% (Case 2); 2) WGS alone is 15% (Case 3); & 3) both combined is 132% (Case 4.)

1 MWe Molten Carbonate Fuel Cell	CASE 1	CASE 2	CASE 3	CASE 4
H2 Co-production	**Yes**	**Yes**	**Yes**	**Yes**
Heat Recovery from the Hydrogen Separation Unit (HSU)	**No**	**Yes**	**No**	**Yes**
Water-Gas Shift	**No**	**No**	**Yes**	**Yes**
Fuel in @60% Utilization Factor [kgmol/s]	0.00312	0.00312	0.00312	0.00312
Methane LHV [kJ/kgmol]	800,800	800,800	800,800	800,800
Ein [kW]	2,500	2,500	2,500	2,500
Generated Gross Power [kW]	1000	1000	1000	1000
Thermal energy penalty to reach PSA levels [kW]	600	600	600	600
Heat recovered from HSU by steam production [kW]	0	435	0	435
Hydrogen potential before PSA [kgmol/s]	0.00151	0.00151	0.00173	0.00173
Hydrogen produced [kgmol/s]	0.00063	0.00128	0.00073	0.00147
Hydrogen potential before PSA [kg/s]	0.00302	0.00302	0.00346	0.00346
Hydrogen produced [kg/s]	0.00127	0.00257	0.00145	0.00294
Hydrogen produced [kg/h]	4.56624	9.2412	5.23152	10.5876
Hydrogen Produced [kg/day]	**109.59**	**221.78**	**125.56**	**254.10**
Marginal increase in H2 compared with base case (kg H2/day)	**Basecase**	**112.19**	**15.96**	**144.51**
H_2 production increase (reference CASE 1: NO heat recv; NO WGS)	**Basecase**	**102%**	**15%**	**132%**

Without any HSU heat recovery (Case 1), the fuel cell system has a deficit of 123 kWt of required heat for the BoP. Heat released from the exothermic anodic reactions is consumed by reforming extra fuel. Consequently, to supply this deficit of heat, anode off-gas H_2 is burned, and H_2 yield for merchant H_2 or vehicles is only 110 kg H_2/day.

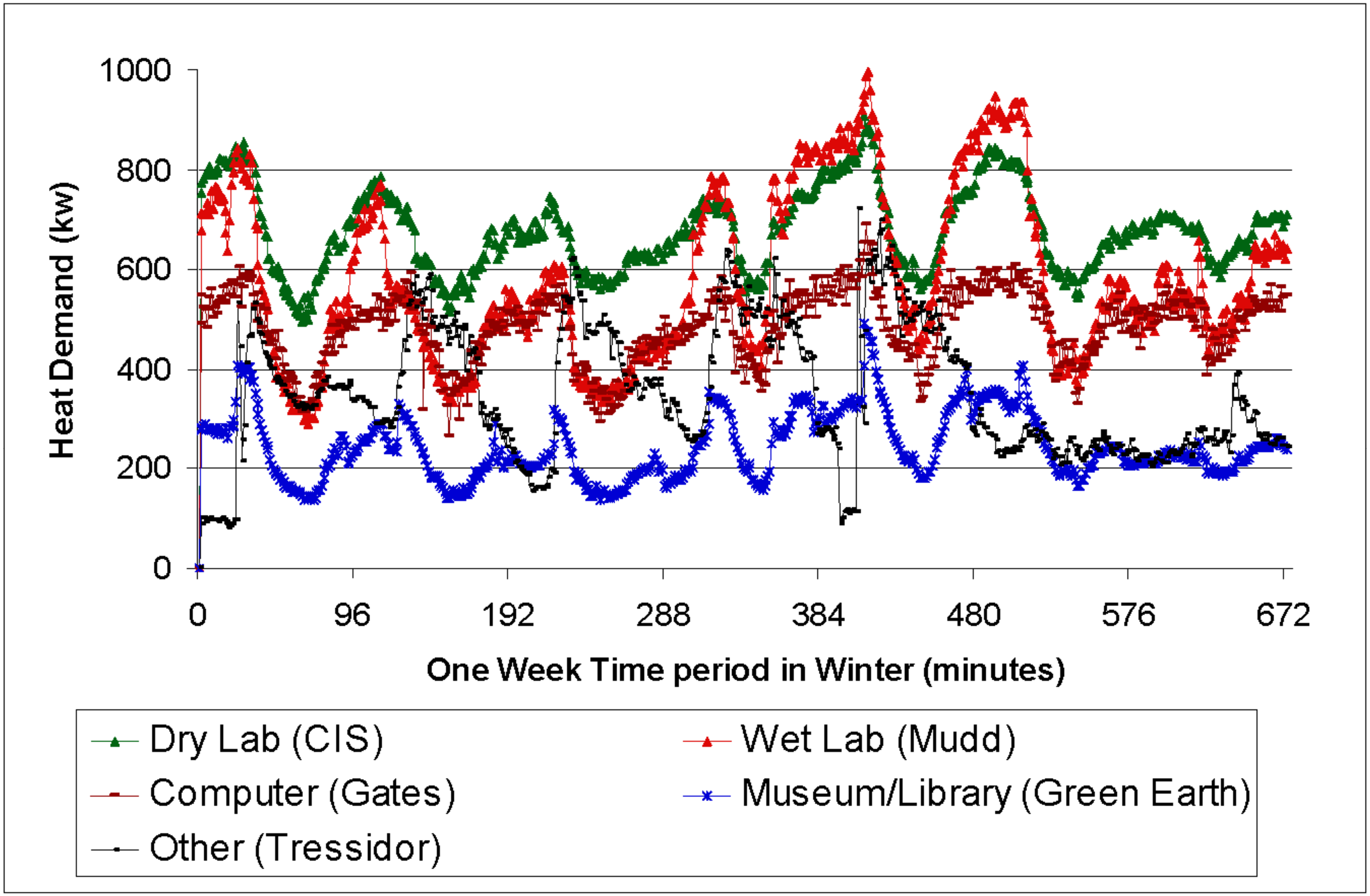
Case 4 meets PSA inlet needs, recovers 73% of heat, uses 11% of electricity, & increases H_2 yield by 132%.

Thermodynamic Characteristic of Stream	Aspen[TM] Flowsheet Fluid Stream Name and Number: HSU IN Anode-off gas	WGS IN	WGS OUT	PSA IN	PSA OUT	Burner OUT / Cathode Inlet Gas
	1	12	5	2	10	13
Mole Flow kgmol/sec						
O_2	0	0	0	0	0.00E+00	0.00279
H_2O	0.003894	0.00046	0.000244	3.50E-05	0	0.00036
CO	0.000541	0.000541	0.000325	0.000325	0	0
CO_2	0.002715	0.002715	0.002931	0.002931	0	0.00328
H_2	0.001518	0.001518	0.001734	0.001734	1.47E-03	0
CH_4	3.25E-05	3.25E-05	3.25E-05	3.25E-05	0	0
N_2	0	0	0	0	0	0.01185
Mole Fraction						
O_2	0	0	0	0	0	0.15267
H_2O	0.44755	0.087298	0.046295	0.006912	0	0.01968
CO	0.06216	0.102695	0.061692	0.064239	0	0
CO_2	0.31205	0.515538	0.55654	0.579522	0	0.17976
H_2	0.17451	0.288308	0.329311	0.342909	1	0
CH_4	0.00373	0.006162	0.006162	0.006417	0	0
N_2	0	0	0	0	0	0.64787
Total Flow kgmol/sec	0.0087	0.005266	0.005266	0.005057	0.001474	0.01829
Total Flow kg/sec	0.208354	0.14649	0.14649	0.142728	0.002971	0.57251
Temperature K	923.15	606.4986	527.5944	323.0022	333.0022	640.54
Pressure N/sqm	106799.8	2221836	2152888	2152888	2118414	101283
Vapor Frac	1	1	1	1	1	1
Liquid Frac	0	0	0	0	0	0
Enthalpy J/kgmol	-2.1E+08	-2.2E+08	-2.3E+08	-2.4E+08	1006438	-64421960
Enthalpy J/kg	-8948283	-8071116	-8240865	-8390823	499254.7	-2058156.6
Enthalpy Watt	-1864412	-1182339	-1207206	-1197605	1483.524	-1178320.3

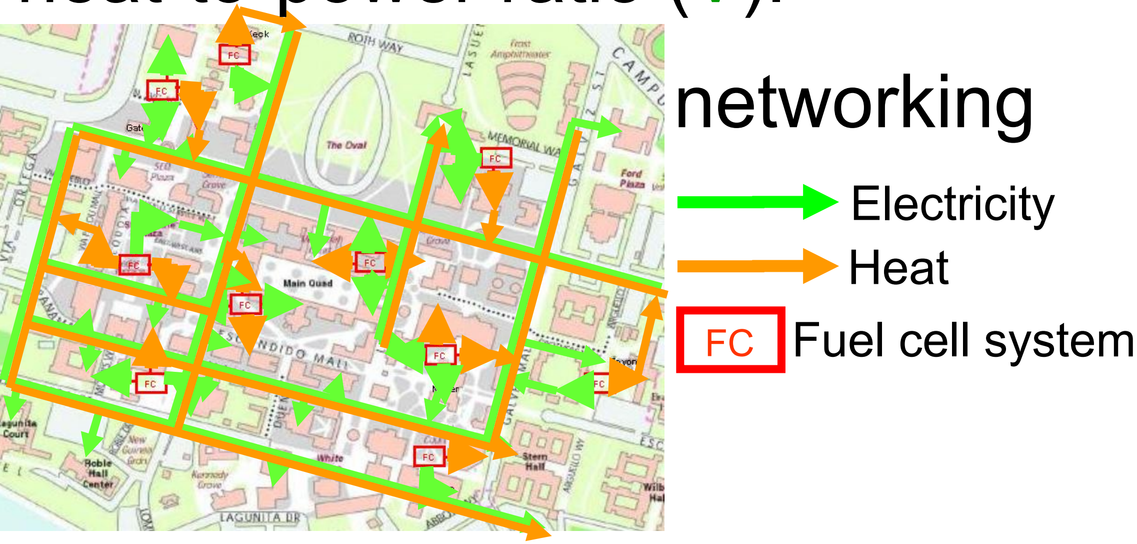
We model the economics and environmental impacts of H_2-FCS using novel operating strategies. The model

- Examines novel operating strategies not common in commercial industry
  - Novel approaches include thermal and electrical networking (N); variable heat-to-power ratio (V); variable heat-to-H_2 ratio (Y); and H_2, electricity, or heat load following (P,E, or H).
- Optimizes the percentage installation of H_2-FCS for
  - minimum CO_2 emissions, or
  - maximum combined energy cost savings both for building owners in using both electricity and heat and for H_2 consumers (H_2 vehicle owners, merchant H_2, etc.) in using H_2 compared with competing technologies.
- Optimizes FCS installation for
  - a particular location
  - climatic region
  - building load curves
  - FCS type, and
  - competitive environment.
- Shows trade-offs amongst competing goals:
  - cost savings to building owners and H_2 consumers, CO_2 reductions, FCS installed capacity and manufacturer sales.

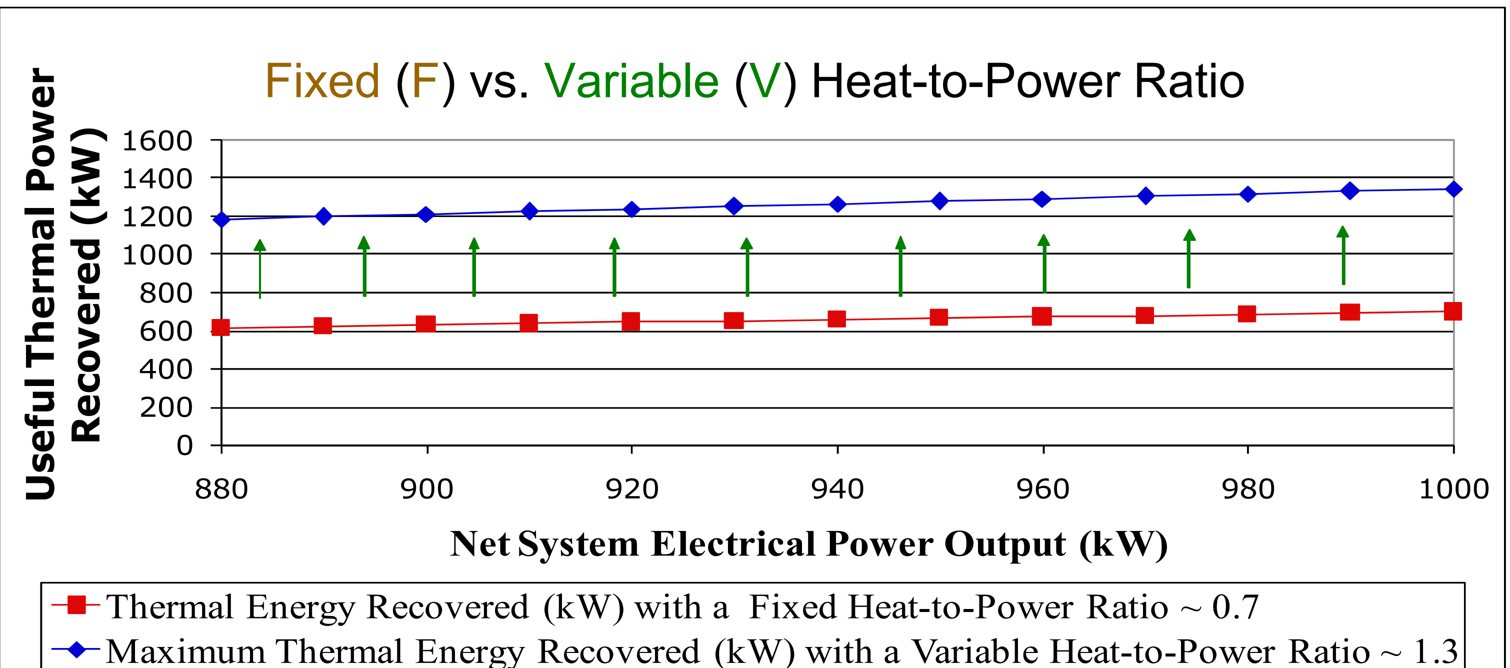
Model tests H_2-FCS against demand data for electricity & steam measured in real-time from 20 buildings & for projected vehicular H_2 demand, each hour in a year.



Novel approaches include networking (N) and variable heat-to-power ratio (V).



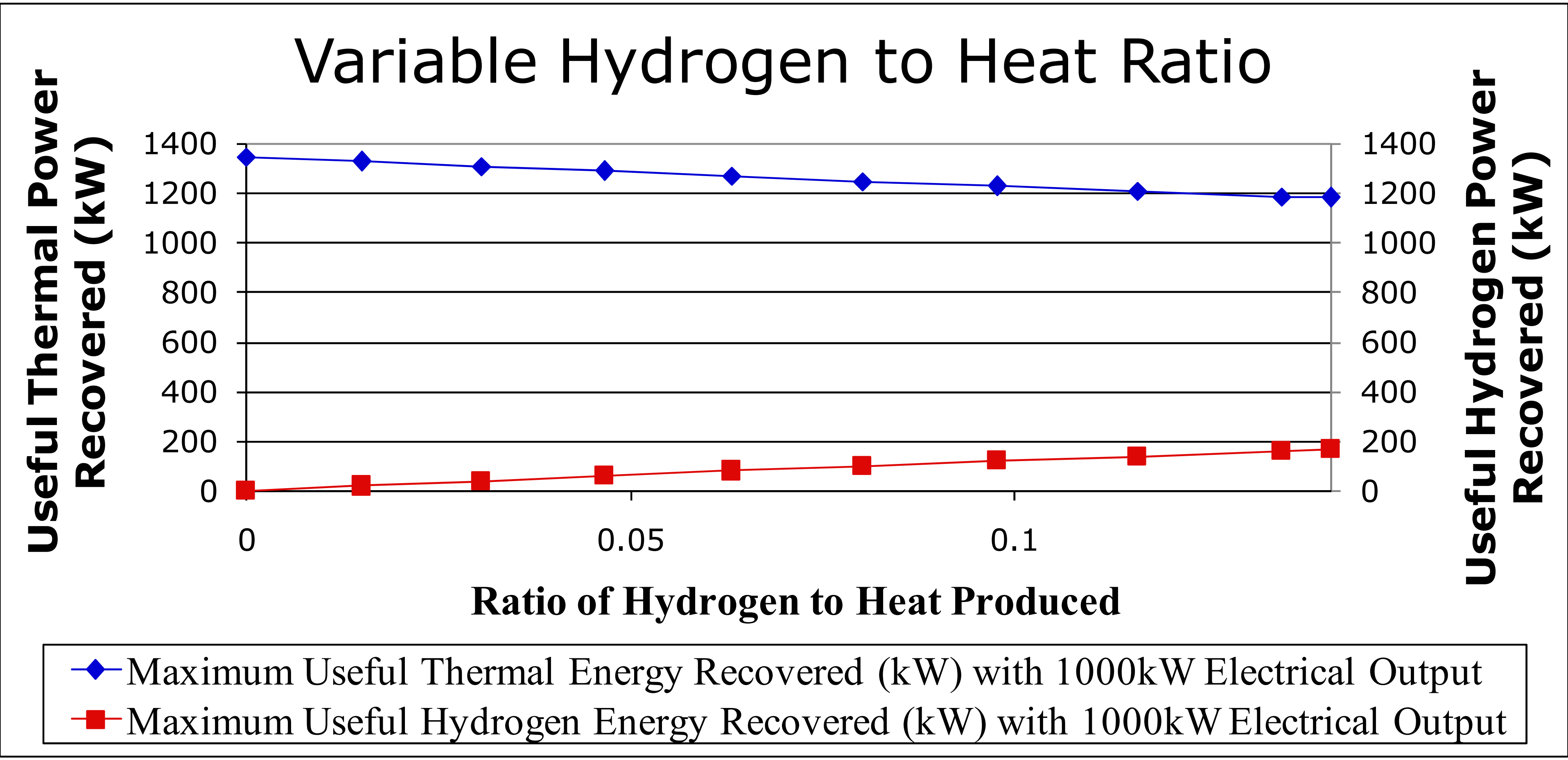
Networks have energy distribution channels. Fuel cells can convey excess heat or electricity into the distribution grid to reach other buildings, and sell back electricity to the grid. Transmission Loss: Electrical ~0%, Thermal ~8%.



Variable heat-to-power ratio increases system operating range.

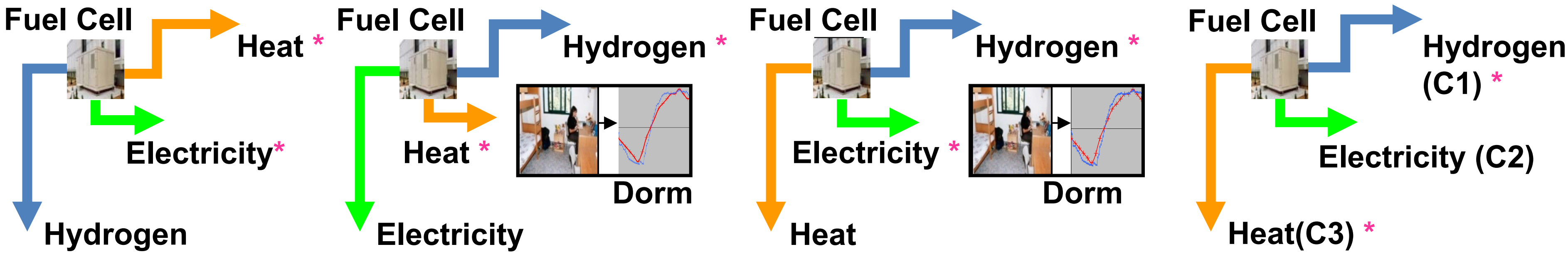
Approach; Objectives 1.3 & 2.1

Novel approaches include variable heat-to-H_2 ratio (Y).



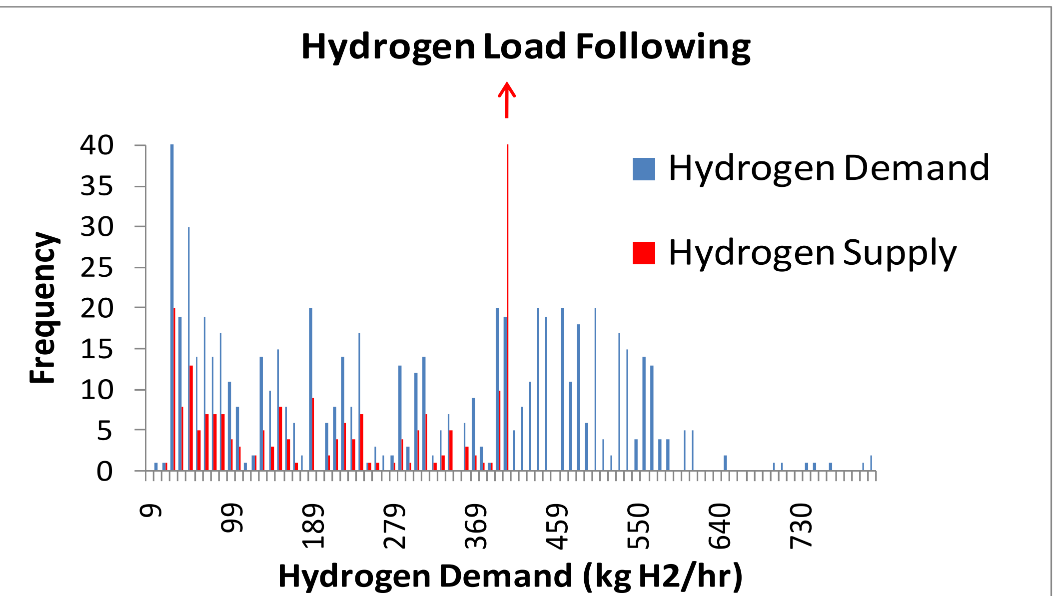
A FCS with a variable heat-to-hydrogen ratio can convert thermal energy into H_2 energy over a certain range of ratios. This ratio reflects the conversion efficiency of using FCS waste heat to warm endothermic steam reforming reactions to make H_2. Each 1 kW of FCS waste heat can make up to 1 kW of H_2 energy (ideal heat transfer).

Novel approaches also include H_2, electricity, or heat load following; in contrast to no load following



H_2 Following (P) Electricity Following (E) Heat Following (H) No Load Following – at Electrical Maximum (EX)

Note: * distinguishes byproducts



Histogram of H_2 demand and supply under load following conditions

Load following the electrical demand results in byproduct heat, and vice versa. No load following is output independent of demand, generally constant. Load following is physically constrained by the system's energy output range and ramp rate.

Approach; Objectives 1.3 & 2.1

Model investigates 13 novel operating strategies.

Strategy	Electrically and Thermally Networked (N) or Stand Alone (S)?	Variable Heat-to-Power Ratio (V), Fixed Heat-to-Power Ratio (F)?	Variable Heat-to-Hydrogen Ratio (Y)	Primary Control: Electricity Power Load Following (E), Heat Load Following (H), Hydrogen Load Following (P), or No Electricity Load Following (EX)?	Secondary Control: Electricity Power Load Following (E), Heat Load Following (H), Hydrogen Load Following (P), No Heat Load Following (HN, HX), or No Electricity Load Following (EN, EX)?	Tertiary Control: Electricity Power Load Following (E), Heat Load Following (H), Hydrogen Load Following (P), No Heat Load Following (HN, HX), or No Electricity Load Following (EN, EX)?
i	N	F	Y	E	HN	P
ii	N	V	Y	E	P	HX
iii	N	F	Y	EX	HN	P
iv	N	V	Y	EX	P	HX
v	N	V	Y	H	P	EN
vi	N	V	Y	H	P	E
vii	N	V	Y	E	H	P
viii	N	V	Y	H	P	EX
ix	N	V	Y	EX	H	P
x	N	V	Y	EX	P	H
xi	N	V	Y	P	H	EN
xii	N	V	Y	P	H	EX
xiii	N	V	Y	P	H	E

Strategies i to xiii are all electrically and thermally networked (N), with a variable heat-to-H_2 ratio. A number of novel operating strategies are investigated with primary, secondary and tertiary controls for H_2, electricity, and heat load following. Most FCS are now installed as [SFEXHN].

Approach; Objectives 1.3 & 2.1

Model tests FCS against competing H_2 generators. FCS waste heat is reused for steam reforming to H_2.

- The model optimizes for the minimum total electricity, heating, and H_2 yearly costs by altering the installed fuel cell system capacity.
- The total yearly costs include, but are not limited to, the fuel cell system capital, maintenance, and fueling costs and the competing generators' electricity, heating, and H_2 costs.
- All demand not supplied by fuel cells is purchased from the competing generators.
- A fuel cell system load following controls will match the hourly demand if it is within the physical constraints of the system.
- Results are compared to a base case of no fuel cells installed. In the base case, all energy demands are supplied by competing electricity, heat, and H_2 generators.
- H_2 production is included in the fuel cell system operation in a manner similar to steam methane reforming (SMR). Waste heat from the high temperature fuel cell system supplies the energy needed for the endothermic steam reforming process for converting natural gas fuel to H_2.

Case study: We show example results based on realistic input assumptions.

- The competing H_2 generator is assumed to be a stand-alone steam methane reformer (SMR) with a fixed CO_2 to H_2 production ratio of 7.49 kg CO_2/kg H_2.
- The fuel cell systems can sell back electricity to the grid at the same price as the competing electricity generator charges (similar to net-metering but without a constraint on the total quantity of electricity sold back to the grid in one year).
- Each 1 kWt of fuel cell system waste heat can produce 1 kW of H_2 energy, up to a maximum. Heat is transferred with 100% efficiency between the fuel cell waste heat and endothermic steam reforming to produce additional H_2.
- The H_2 production rate is limited to 5% of the total fuel energy entering the system resulting in maximum H_2 production of about 17% of total recoverable heat produced.
- The total increase in fixed costs for the H_2 production, compression, and dispensing equipment and installation is estimated at 25% of the total capital and installation cost of the standard fuel cell system (not including warranty or shipping costs).
- H_2 is produced on demand just-in-time, with no H_2 storage.
- No tax on carbon dioxide (CO_2) emissions exists, but all California state and U.S. federal incentives are available.
- Case study results are shown for optimizing for both cost & CO_2 emission reductions. Sensitivity study results are shown for three different commercial H_2 prices.

Case study: We realistically describe the engineering performance characteristics of novel H_2-FCS.

Fuel Cell System Operating Data	Quantity	Units
Maximum Electrical Output	1000	kilowatts (kw)
Minimum Electrical Output	880	kilowatts (kw)
Maximum Heat-to-Electric Power Ratio	1.35	
Minimum Heat-to-Electric Power Ratio	0.7	
Baseline Heat-to-Electric Power Ratio for Fixed Heat-to-Power Ratio Operation	0.7	
Natural Gas Fuel Consumption (in Units of Energy) Per Unit of Electric Power Output	6,824	British Thermal Units (BTU) of natural gas /kwh of recovered heat
Marginal Increase in Natural Gas Fuel Consumption (in Units of Energy) Per Unit of Additional Heat Demanded (Variable Heat to Power Ratio Scenarios Only)	3,791	British Thermal Units (BTU) of natural gas /kwh of recovered heat
Baseline System Electrical Efficiency	50%	
Baseline System Heat Recovery Efficiency	30 to 35%	
Baseline Hydrogen Recovery Efficiency	5% to 0%	
Baseline System Heat Losses (Percent)	15%	
Baseline System Combined Electrical, Heat and Hydrogen Recovery Efficiency	85%	
Heat Recovery Efficiency of Burner-Heater for Marginal Heating (Variable Heat to Power Ratio Scenarios Only)	90%	
Fuel Cell System Lifetime	5	years

1 MWe MCFC system performance is based on system currently in production at Fuel Cell Energy, Inc. Baseline heat recovery efficiency is 30% up to 35%. Baseline H_2 recovery efficiency is 5% down to 0%.

Approach; Objectives 1.3 & 2.1

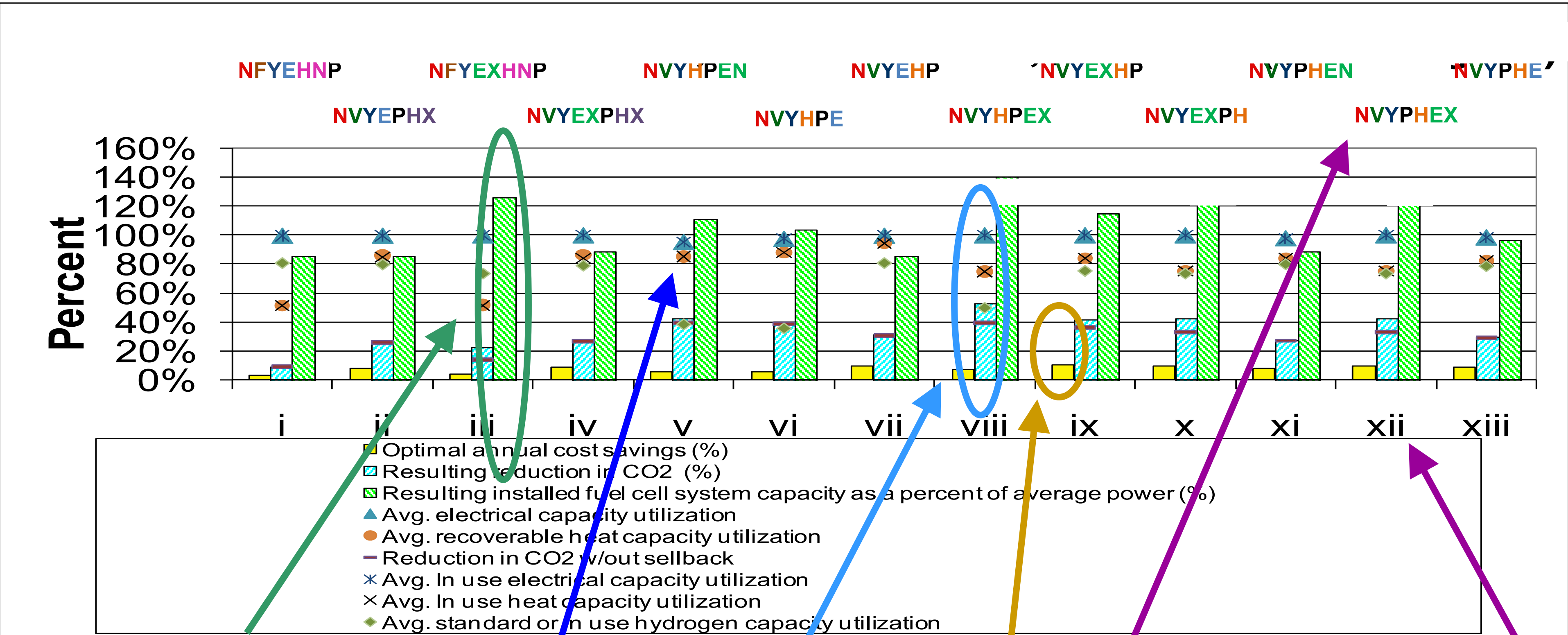
Case study: We realistically describe financial operating data for H_2-FCS and competing generators.

Fuel Cell System and H2 Co-Production Cost -- Fixed Cost per year	Amount Borrowed (or Credited) at Time t = zero [P] ($)	Annuity [A] ($)
Capital Costs of 1000 kW Fuel Cell System and H2 Generator	$ 4,000,000	$ 986,446
Installation Costs Including H2 Generator	$ 1,250,000	$ 308,264
Commissioning Costs (Start-up, Testing, Tutorials for Operators)		$ -
Shipping	$ 100,000	$ 24,661
Premium Service Contract (Maintenance and Replacement) -- Annuity Payments		$ 400,000
Fuel Cell System Incentives -- Federal and State		
California Self-Generation Incentive Program (CA SGIP) at $2500/kWe	$ 2,500,000	$ 616,529
Federal Investment Tax Credit (FITC) at $3,000/kWe or 30% of Capitol Costs	$ 1,605,000	$ 395,811
Fuel Cell System Fixed Costs -- Total Yearly Fixed Costs		707,031

Competing Generator: Natural Gas Combined Cycle Gas Turbine Plant	Quantity	Units
Price of steam for heating including carbon tax impact	0.056	$/kWh steam
Price of electricity including carbon tax impact	0.085	$/kWh electricity
Baseline System Heat Recovery Efficiency	0.22	
Baseline System Electrical Efficiency	0.40	
Baseline System Heat Losses	0.38	
Competing Generator: Distributed Steam Methane Reforming Hydrogen Generator	**Quantity**	**Units**
H2 Price	2.00 or 4.00 or 23.64	$/kg H2
CO2 Emission	7.49	kg CO2/kg H2 produced

1 MWe MCFC system costs are based on Fuel Cell Energy's system. The MCFC is tested against a CHP combined cycle gas turbine (CCGT) and a SMR H_2 generator.

Case study: We show benefits to electricity, heat & H_2 consumers; FCS manufactures; and the environment.



Highest Green = $$$ money, highest fuel cell manufacturer revenues

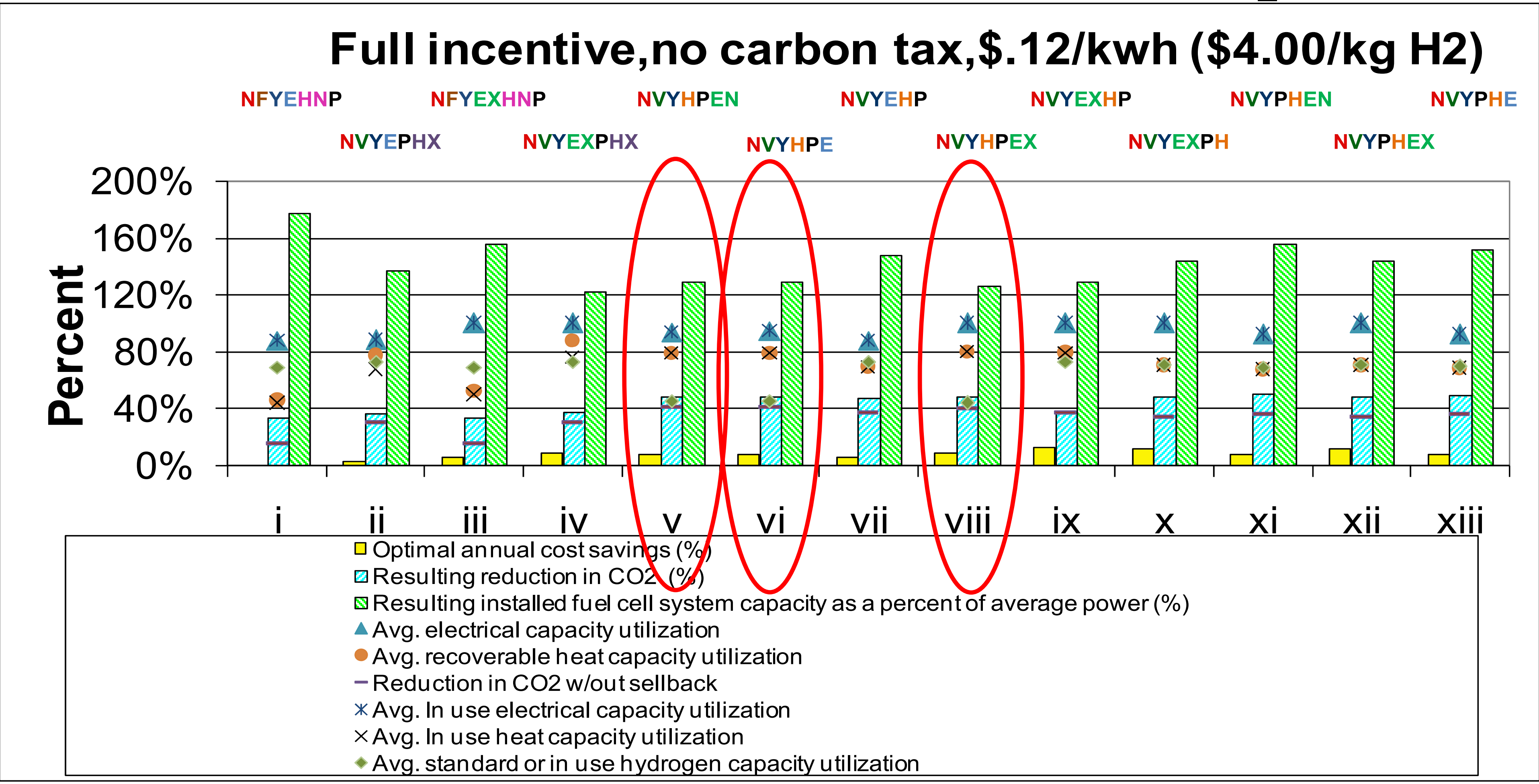
- ▲ Electrical capacity utilization
- ● Heat capacity utilization
- ✳ In use electrical capacity utilization
- X In use heat capacity utilization
- ◆ Hydrogen capacity utilization

Highest Blue = “blue skies”, lowest CO_2

Highest yellow = highest combined energy cost savings for building owners and H_2 consumers

Strategy name and number

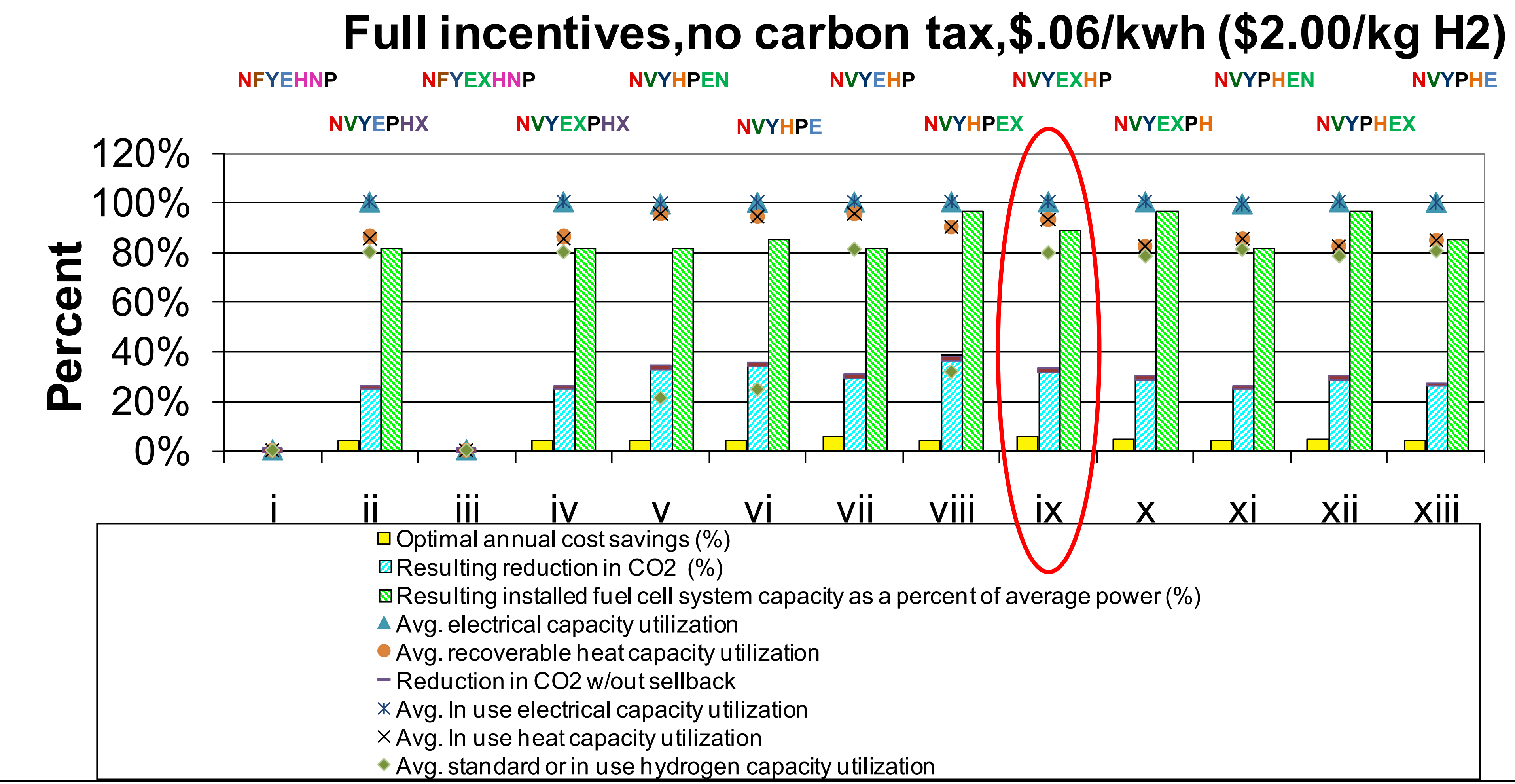
CO_2 emissions are lowest with our approach of networking, variable heat-to-power & H_2-to-heat ratios, first load following heat & then load following H_2.



Strategies with the lowest CO_2 emissions are v [NVYHPEN], vi [NVYHPE], and viii [NVYHPEX]. These strategies first follow heat demand [H] as the primary control, and then load follow H_2 demand [P] as the secondary control. Less fuel is wasted.

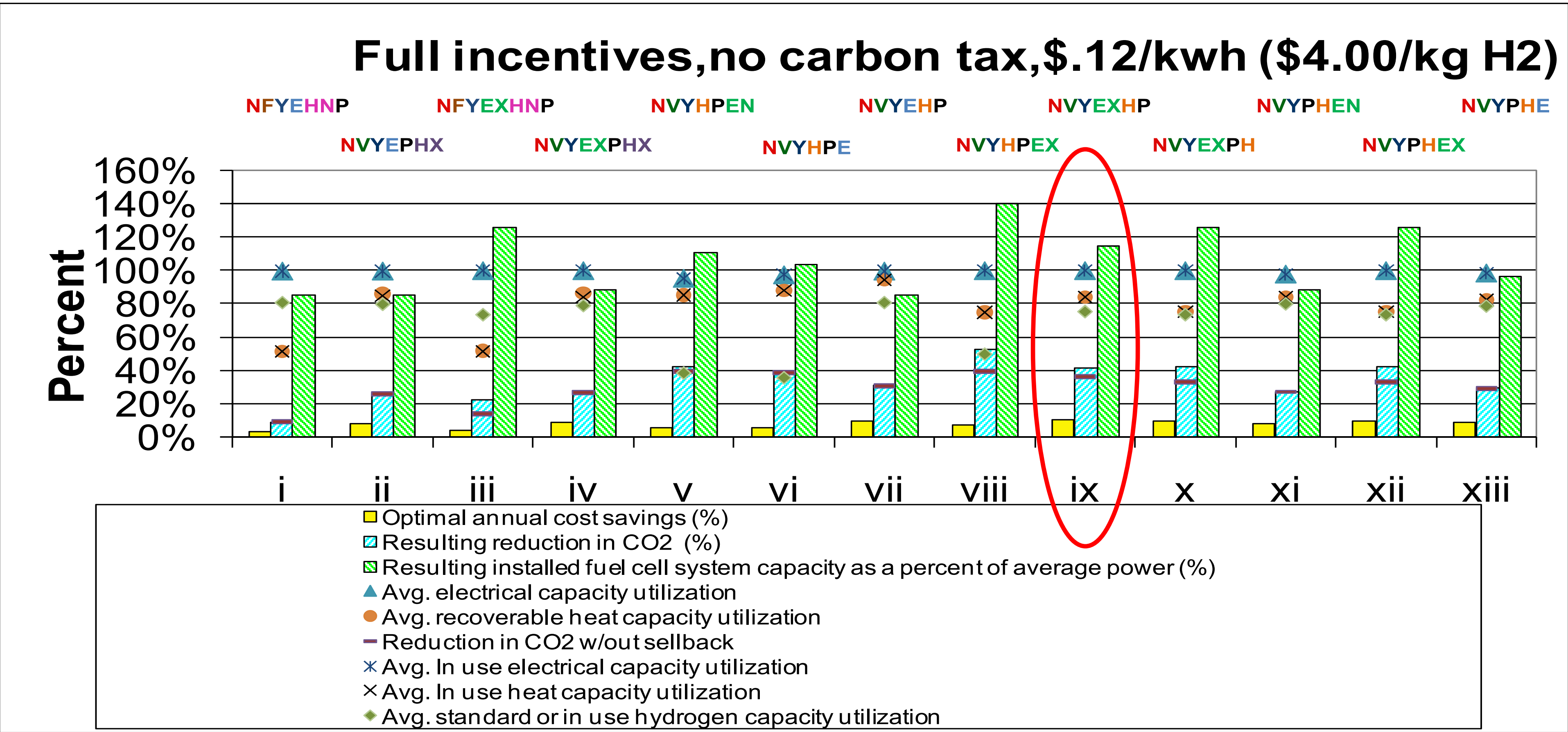
Technical Accomplishments and Progress; Objective 2.1

Energy costs are lowest with our approach of maximum FCS electrical output, with heat & then H_2 load following.



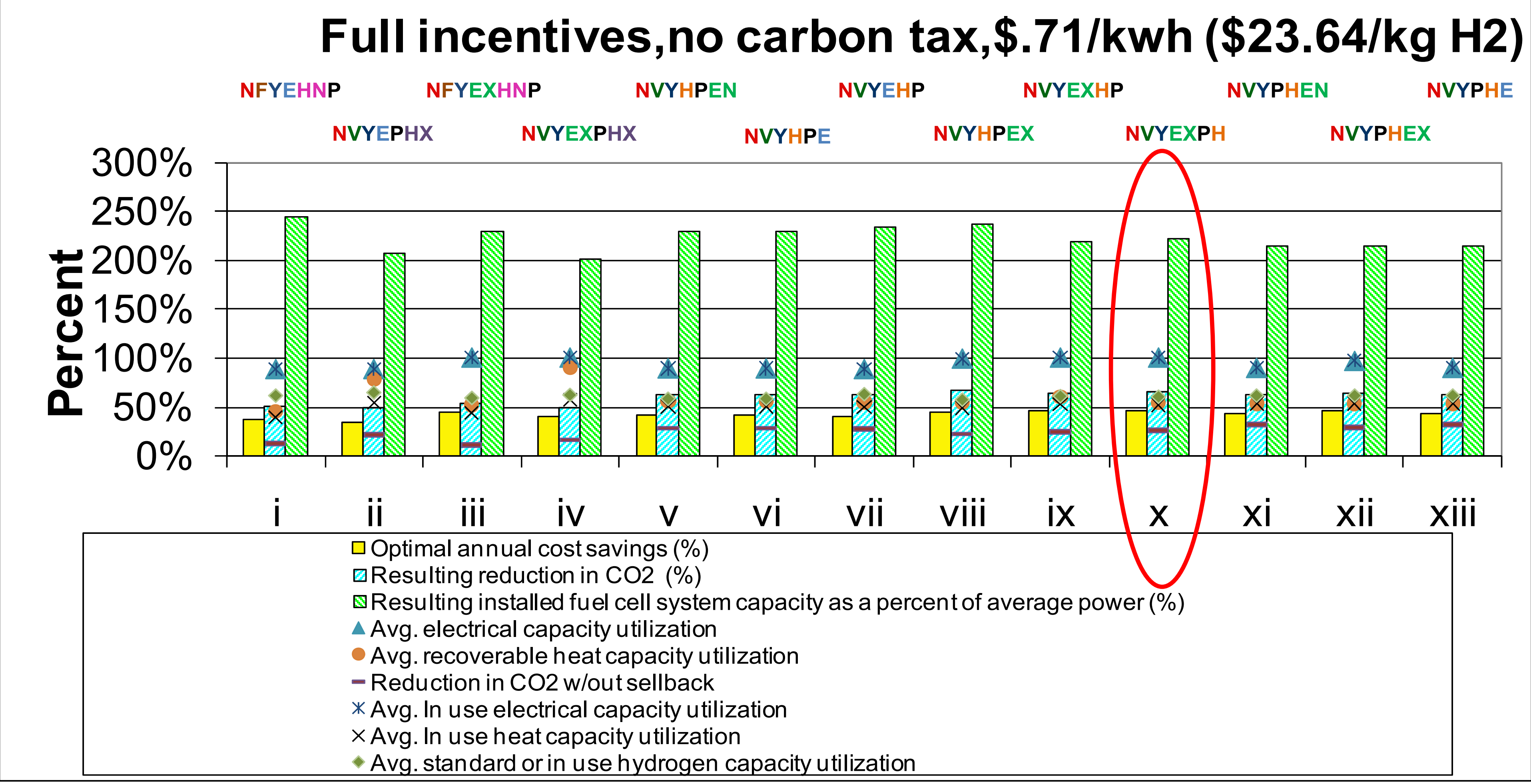
When the competing H_2 generator's price is $2/kg H_2, the most economical strategy is ix [NVYEXHP]. The second best strategy is vii [NVYEHP]. In this scenario, the electrical load following (E) is close to the maximum and therefore mimics EX.

Energy costs are lowest with our approach: H_2-FCS make the most electricity, sell any excess back to the grid, and locally make heat and H_2 with load following.



When the competing H_2 generator's price is $2 or $4/kg H_2, the most economical strategies are ix [NVYEXHP] (1st) & vii [NVYEHP] (2nd). Grid-connected systems can sell excess electricity to the grid. By contrast, heat and H_2 demand are locally constrained; less fuel is wasted when they are made via load following, yielding higher cost savings.

Energy costs are lowest with our approach of maximum electricity, heat & H_2 load following, but in a different control order depending on the competitive H_2 price.



For a competing generator H_2 price of $23.64/kg H2, the most economical strategy changes to x [NVYEXPH]. The second best strategy is again xii [NVYPHEX].

Cost optimization favors maximum electrical output, and heat & H_2 load following.

The most economical strategies investigated tended to combine a) electrical and thermal networking (N), b) a variable heat-to-electric power ratio (V), and c) a variable heat-to-H_2 ratio (Y) with these three characteristics 1) maximum electrical output (EX), 2) heat load following (H), and 3) H_2 load following (P).

- As long as systems are grid-connected with a competitive electricity sell-back price, they can sell excess electricity not used in the local area for revenue.
- By contrast, both heat and H_2 demand are locally constrained, without storage in these models. Less fuel is wasted when they are produced in load following mode, yielding higher energy cost savings.

As the competing generator H_2 price changes, the strategies with the highest cost savings change.

- As the competing generator H_2 price changes, the optimal order changes for primary, secondary, and tertiary control of 1) maximum electrical output, 2) heat load following, and 3) H_2 load following.
- For example, as the H_2 price increases from $4/kg to $23.64/kg, the most economical strategy changes from [NVYEXHP] with H_2 load following as the tertiary control to [NVYEXPH] with H_2 load following as the secondary control.
- In other words, as the competing generator H_2 price increases, it becomes more important to operate fuel cells with H_2 load following.

Future Work; Objective 1

We intensify thermodynamic models to analyze the maximum H_2 available with no added CO_2 emissions.

- Develop more intricate AspenPlus™ models to analyze co-produced H_2 available under different operating conditions with no added fuel use or CO_2 emissions.
- Enhance AspenPlus™ model fidelity to better analyze available H_2 in the context of
  - higher heat exchanger efficiency for preheating anode and cathode inlet gases,
  - different anodic fuel and cathode oxidant utilization rates,
  - the synergistic benefits of a lower fuel utilization increasing overall efficiency (i.e., via a higher Nernst Voltage, lower mass transport losses, lower cooling needs for the fuel cell stack & lower associated air compressor parasitic load.)
  - Both theoretical and practical ancillary loads (pumps, compressors, etc.),
  - more optimal heat exchanger loop designs through Pinch Point Analysis,
  - recycling more streams (such as steam) to lower reactant demand & heat loss,
  - trade-offs between external and internal reforming,
  - more complex thermodynamic cycle designs,
  - more cycle design configurations for thermally integrating the hydrogen separation unit (HSU) and fuel cell system,
  - additional hydrogen separation technologies, including not only PSA, but also electrochemical hydrogen separation pumps,
  - a greater variety of operating conditions (steam-to-carbon ratio, operating pressure, H_2 recovery methods, etc.), and
  - a greater variety of low or zero carbon, and renewable fuels (biofuels, etc.).
- Publish analytical models and equations describing the quantities of co-produced H_2 available under different conditions.

We strengthen techno-economic-environmental models to optimize more H_2 co-production cases.

- Evaluate the "low hanging fruit" markets, such as the current industrial market for H_2 demand in petroleum and chemical processing plants, and test H_2-FCS against these plants' time-dependent H_2 demand curves.
- Study the transition from low H_2 vehicle fleet penetration levels to high.
- Investigate more innovative H_2-FCS design, operating, and control strategies.
- Re-work the model to determine optimal operating strategies at each time-step.
- Analyze a larger range of viable efficiencies for H_2-FCS electricity, heat, and H_2.
- Model advanced H_2 & energy storage, compression, and dispensing concepts.
- Delineate the engineering, economic, and environmental benefits of
  - avoided long-distance H_2 transport associated with centralized H_2 production,
  - avoided transmission losses association with centralized electricity production

  including reduced capital costs for infrastructure.
- Quantify the benefits of relying on a secure fuel supply by using local feedstock.
- Examine a greater variety of low carbon, renewable fuels (biofuels, etc.).
- Standardize key model input parameters across DOE H_2 program models (in collaboration with fellow DOE Lab researchers and industry experts)

We collaborate with academia, industry, & federal entities to greatly advance R&D and technology transfer.

#	Collaborator	Relation-ship	Entity Type	In DOE H_2 program?	Extent of Collaboration
1	University of California at Irvine, Mechanical & Aerospace Engineering Dept.	sub-contractor	academia	yes	Actively collaborating on a daily basis to develop chemical engineering models of hydrogen separation units thermally integrated with fuel cell systems. Conducting related energy system analyses.
2	Fuel Cell Energy, Inc.	partner with data disclosure sensitivity	industry	yes	Actively partnering on a bi-weekly or monthly basis to validate model inputs, assumptions, and operating data. Verifying molten carbonate fuel cell (MCFC) performance, system integration approaches with fuel cells, design cycle configurations, and current and expected costs.
3	Technology Management Inc.	partner with data disclosure sensitivity	industry	no	Actively partnering on a monthly basis to validate model inputs, assumptions, and operating data. Verifying solid oxide fuel cell (SOFC) performance, system integration approaches, operation on low-carbon fuels.
4	Transportation and Stationary Power Integration (TSPI) team: SNL, NREL, LANL, ORNL, BNL, ANL	research team partners	federal	yes	Sandia National Laboratories (SNL), National Renewable Energy Laboratory (NREL), Los Alamos National Laboratories (LANL), Oak Ridge National Laboratories (ORNL), Brookhaven National Laboratories (BNL), and Argonne National Laboratories (ANL) are meeting on a monthly basis to enhance their engineering, economic, & environmental models to include H_2-FCS scenarios. Sandia has provided advice on relevant H_2-FCS literature, analyses, model results, & model feedback to team members.

We actively collaborate with many entities to speed the evaluation and development of H_2-FCS.

#	Collaborator	Relation-ship	Entity Type	In DOE H_2 program?	Extent of Collaboration
5	National Renewable Energy Laboratory (NREL)	partner	federal	yes	SNL has provided three separate rounds of detailed technical feedback on nascent versions of NREL's H2A model. SNL and NREL collaborated to develop TSPI invited workshops.
6	Fuels Pathways Integration Technology Team (FPITT)	technology transfer	federal and industry	yes	Federal laboratories -- including SNL, NREL, ANL, and Lawrence Livermore National Laboratories (LLNL) -- develops models related to alternative transportation supply chains, and industry -- including Exxon Mobil, Shell, ConocoPhillips, and Chevron critically evaluate model results. Sandia presented model results to FPITT working group and included feedback in subsequent model development.
7	International Energy Agency (IEA) Advanced Fuel Cells Annex: Stationary applications Annex XIX and Annex 25	knowledge transfer	federal, industry, and academia	no	Sandia presented model results to IEA stationary fuel cell systems working group experts and included their feedback in subsequent model development and proposed future work.

Leading international research organizations also advise us on our model development: École Polytechnique Fédérale de Lausanne (EPFL), Laboratoire d’énergétique industrielle (Swiss academia); E4Tech (European industry); and the Fraunhofer Institute for Solar Energy (ISE) Systems (German federal & industry).

Summary – Key take-away points

Our novel H_2-FCS designs have the lowest CO_2 emissions & costs of any H_2 production method to-date.

A 1 MWe fuel cell can make enough H_2 to fuel ~220 to 660 H_2 fuel cell cars/day, with no added CO_2 emissions. (Objective 1.1)

Daily H_2 output can increase by > 132% with no added CO_2 emissions, if the fuel cell reuses waste heat internally. (Objective 1.2)

Global CO_2 emissions from H_2, electricity, and heat are lowest when H_2-FCS are electrically and thermally networked, use variable heat-to-power & H_2-to-heat ratios, and load follow heat and H_2 demands. (Objective 1.3)

Global energy costs from H_2, electricity, and heat are lowest when H_2-FCS are networked, use variable heat-to-power & H_2-to-heat ratios, produce at their maximum electrical output continuously, and load follow heat and H_2 demands. (Objective 2.1)