Energy & Environmental Science

Electronic Supplementary Information

Life-cycle net energy assessment of large-scale hydrogen production via photoelectrochemical water splitting

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Tables

Table S1. Low, base-case, and high values of system model parameters. Low values result in reduced system performance relative to the base-case, while high values result in improved system performance.

Parameter description	Units	Low	Base-case	High
System				
Capacity factor of facility	percent	80%	90%	95%
Primary energy-to-electricity conversion	percent	40%	50%	60%
Life span of balance of system	years	20	40	60
Decommissioning energy	percent	20%	10%	5%
PEC cell				
Solar-to-hydrogen efficiency	percent	5%	10%	20%
Life span of PEC cell	years	5	10	20
Cell degradation threshold	percent	70%	80%	90%
Transmittance loss (dust, glass, electrolyte)	percent	20%	10%	5%
Photo-active cell materials energy use	$MJ\ m^{-2}$	23	14	5
Other cell materials energy use	$MJ\ m^{-2}$	1227	692	469
Photo-active cell fabrication energy use	$MJ\ m^{-2}$	1668	1001	715
Other cell fabrication energy use	$MJ\ m^{-2}$	517	407	359
Electrolyte energy intensity	multiplier	1.5	1.0	0.8
Panel				
Panel inactive area	percent	10%	5%	2%
Panel material use	multiplier	1.2	1.0	0.8
Panel material energy intensity	multiplier	1.2	1.0	0.8
Panel internal frame spacing	meter	0.5	1.0	1.5
Panel transport (truck and train)	kilometer	1300	300	0
Containment vessel thickness	meter	0.008	0.004	0.002
Containment vessel material energy	multiplier	1.5	1.0	0.8
Piping				
Maximum velocity, uncompressed H2	$m\ sec^{-1}$	0.5	1.0	2.0
Maximum velocity, compressed H2	$m\ sec^{-1}$	20	40	60
Maximum velocity, H2O	$m\ sec^{-1}$	1.0	3.0	5.0
Material energy intensity	multiplier	1.2	1.0	0.8
Allowance for valves and fittings	percent	50%	25%	10%
Pipe transport (train)	kilometer	3000	1000	300
Gas handling				
Panels per blower	units	50	100	150

Gas blower power	kW	3.0	1.5	0.7
Gas blower average use	percent of capacity	100%	75%	50%
Gas dryer power	kW	5.0	2.4	1.4
Gas dryer average use	percent of capacity	100%	75%	50%
Compressor specific energy use	W h m^{-3}	82	70	57
Compressor interstage loss	psi	10	5	0
Gas intake temperature	degree C	80	60	40
Compressor fan load	percent	10%	7.5%	5%
Gas handling hardware embodied energy	multiplier	2.0	1.0	0.5
Storage				
Gas storage capacity	day	2.0	1.0	0.5
Allowable stress in tank wall	multiplier	0.8	1.0	1.2
Corrosion allowance	mm	12	9	6
Allowance for valves and fittings	percent	20%	10%	5%
Water				
Water treatment electricity	MJ ton^{-1} of treated water	43.1	21.5	16.1
Water treatment brine waste	liter ton^{-1} of treated water	774	387	71
Water use for panel cleaning	liter m^{-2} $year^{-1}$	100	25	10
Water transport electricity	kWh m^{-3} km^{-1}	0.0073	0.0047	0.0018
Roads				
Road width	meter	8	6	4
Asphalt thickness	meter	0.10	0.05	0.03
Subbase thickness	meter	0.30	0.15	0.08
Percent bitumen in asphalt	percent	6%	5%	4%
Material energy intensity	multiplier	1.2	1.0	0.8
Operations				
Number of trucks and cranes	units	12	6	3
Horsepower of engines	brake hp	600	400	200
Daily operating time	hours	24	12	8
Equipment load factor	ratio	0.70	0.54	0.38
Panel heat requirement	kWh m^{-2} $year^{-1}$	11.1	5.4	0.5

Table S2. Mass (kg) of panel components

Component	Mass (kg)	Notes
Structure	340	Perimeter frame of steel channel section (ASTM C4x5.4), with internal elements of steel angle section (ASTM L2½x2x3/16) spaced at 1 m.
P5 piping	7	
PVC cell chamber	163	Based on Zhai *et al*. [28]
Glass cover	207	Based on Zhai *et* al. [28]
PEC cell elements	4	Based on Zhai *et al*. [28]
Electrolyte	569	1M H_2SO_4, assume density of 1.045 kg m^{-3}
Total	1290	
Total without electrolyte	721	

Table S3. Characteristics of modeled PEC cells (Source: Zhai *et al.* [28])

Category	Component	Lower case	Medium case	Higher case
Material choices	Photocathode	Silicon (Si)	Silicon (Si)	Silicon (Si)
	Photoanode	Tungsten trioxide (WO_3)	Tungsten trioxide (WO_3)	Gallium arsenide (GaAs)
	Catalysts for photocathode	Cobalt (Co)	Platinum (Pt)	Platinum (Pt)
	Catalysts for photoanode	No catalyst	No catalyst	Platinum (Pt)
	Encapsulation	Polyvinyl chloride (PVC)	Polyvinyl chloride (PVC)	Polycarbonate
	Thickness of chamber	3 mm	5 mm	7 mm
	Thickness of membrane	30 µm	50 µm	70 µm
Fabrication	Thermodynamic efficiency of processes used to fabricate photocathode/anode and membrane	70%	50%	30%

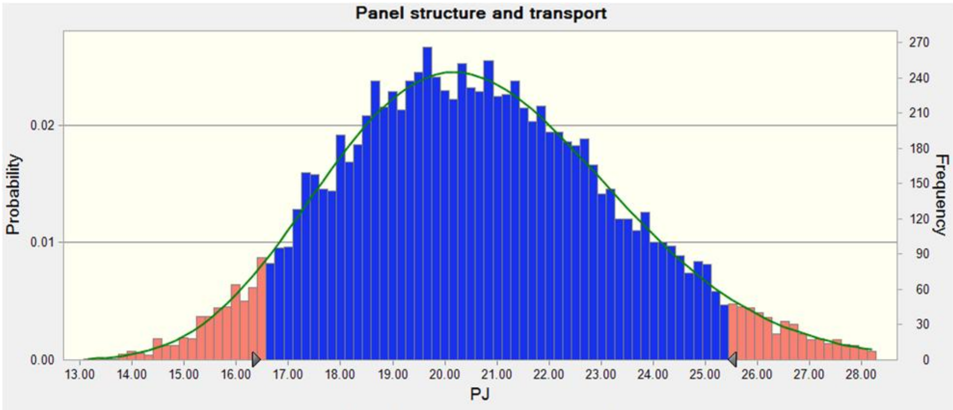
Table S4. Characteristics of base-case pipe levels P0 through P5 for H_2, O_2 and H_2O. Shaded pipe sizes are determined by minimum size (nominal ½ inch), not flow properties.

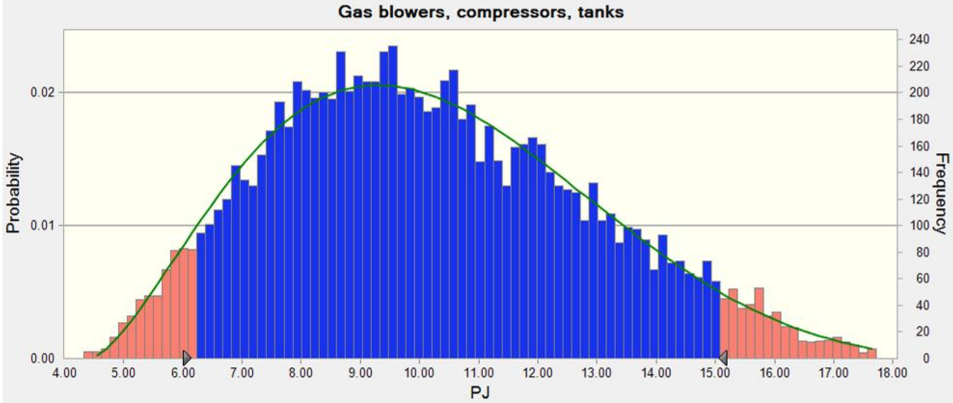
		P0	P1	P2	P3	P4	P5
Length	km	300	15	144	1891	14385	21752
Maximum velocity	m sec^{-1}						
H2		40	40	40	1	1	<<1
O2		40	40	40	1	1	<<1
H2O		3	3	3	3	3	<<3
Flow rate	kg sec^{-1}						
H2		8.0	2.0	0.33	0.0045	0.00004	<<
O2		63	16	2.6	0.035	0.00035	<<
H2O		142	18	3.0	0.040	0.00040	<<
Pipe interior diameter	inch						
H2		14	7.2	2.9	10	1.0	0.62
O2		10	5.1	2.1	7.3	0.73	0.62
H2O		9.7	3.4	1.4	0.62	0.62	0.62
Pipe material							
H2		PVC S80	PVC S80	PVC S80	PVC S40	PVC S40	PVC S40
O2		PVC S80	PVC S80	PVC S80	PVC S40	PVC S40	PVC S40
H2O		PVC S40	PVC S40	PVC S40	PVC S40	PVC S40	PVC S40

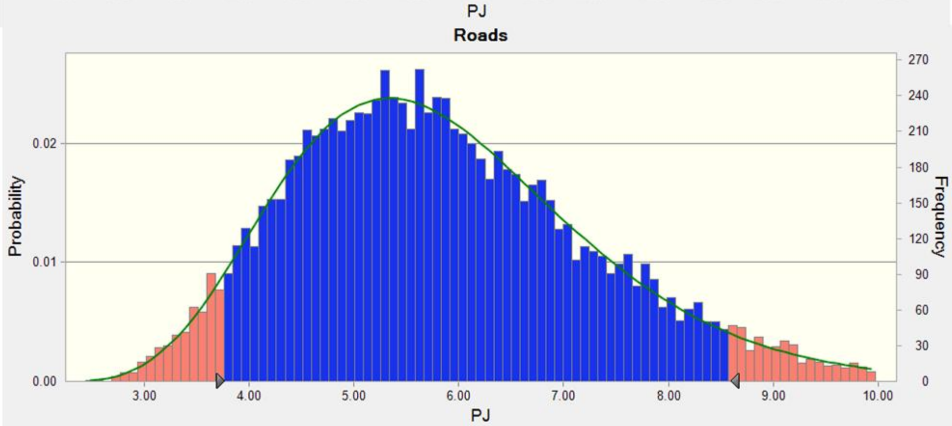
Table S5. Annual electricity requirement for panel heating to prevent freezing. The separate and combined effects of several possible design and operation conditions were assessed to estimate a likely range for the annual heating energy input. These were 1) to vary the minimum allowable temperature of the electrolyte from 0 °C to -2.5 °C; 2) to reduce the thermal radiation energy losses by reducing the emissivity of the window material from 0.94 to 0.8 using an optical coating; and 3) to add an additional 2 cm layer of R12 polystyrene insulation to the back of the device. Results indicate that variation of local climate has greater effect on panel heating energy than does variation of these conditions. The base-case conditions (shown in bold font in the table) assume a -2.5 °C temperature threshold, no insulation, and no low-emissivity coating.

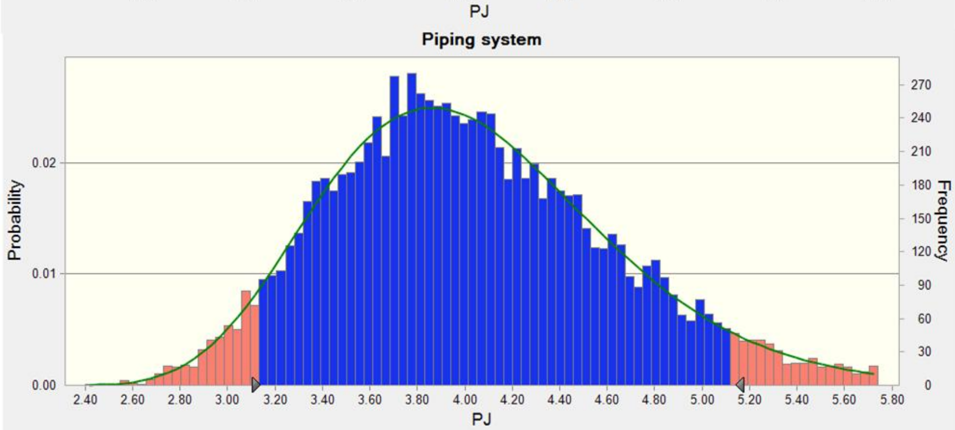
Conditions			**Heating energy (kWh m^{-2} $year^{-1}$)**			
Temperature threshold	Insulation	Low-emissivity coating	Barstow	Phoenix	Las Vegas	Tucson
-2.5 °C	**none**	**none**	**11.0**	**0.6**	**6.1**	**4.2**
0 °C	none	none	23.9	3.1	16.1	14.0
0 °C	2 cm R12	none	19.1	3.8	13.6	12.5
0 °C	none	top emissivity = 0.8	18.9	1.4	12.7	10.9
-2.5 °C	none	top emissivity = 0.8	7.4	0.4	3.8	3.1

Figures


Panel structure and transport
Probability
Frequency
PJ


Gas blowers, compressors, tanks
Probability
Frequency
PJ


Roads
Probability
Frequency
PJ


Piping system
Probability
Frequency
PJ

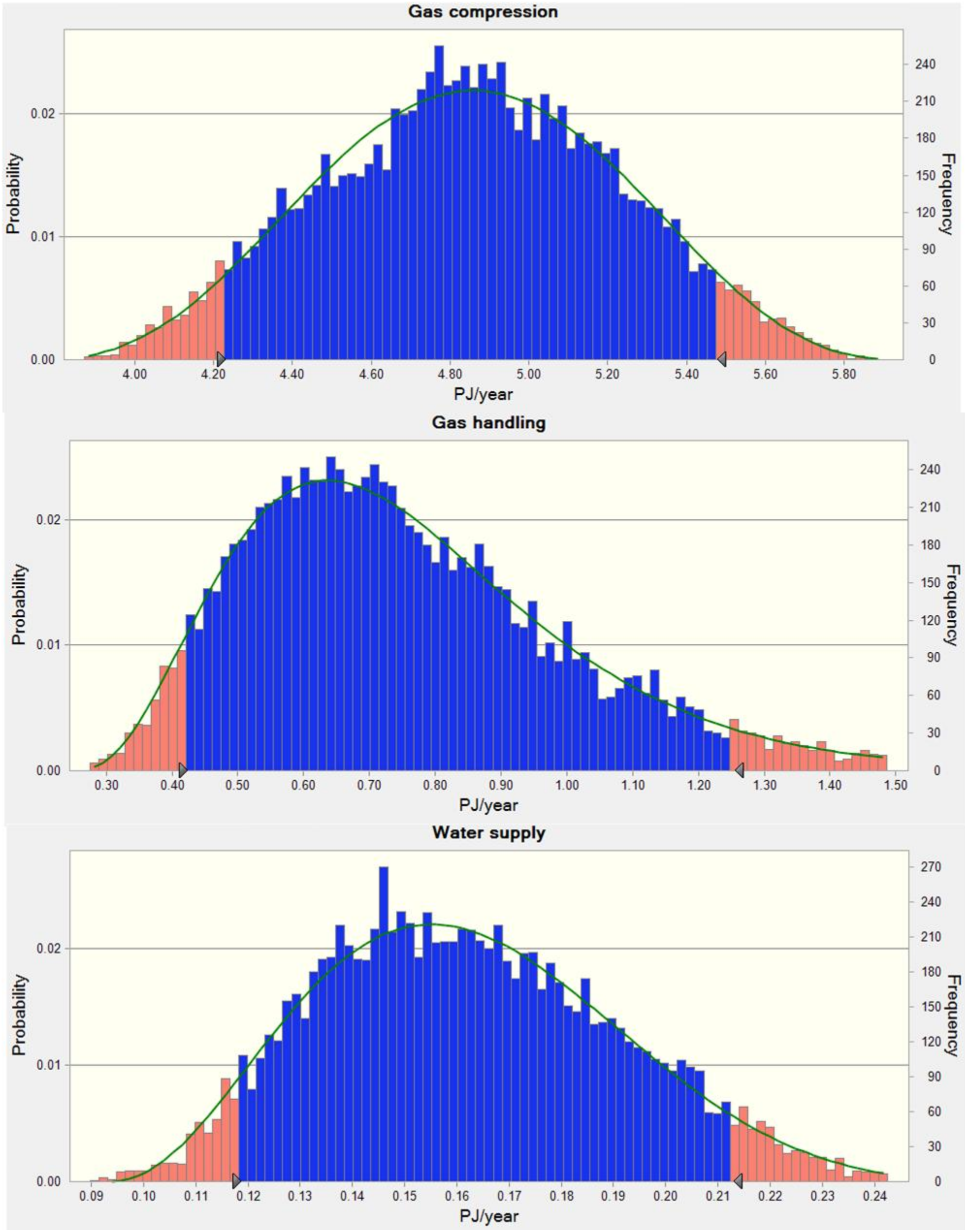


Figure S1. Outcomes of Monte Carlo simulations of parameter categories. Facility production energy use (top) is in units of PJ, and facility operation energy use (bottom) is in units of PJ year^{-1}.

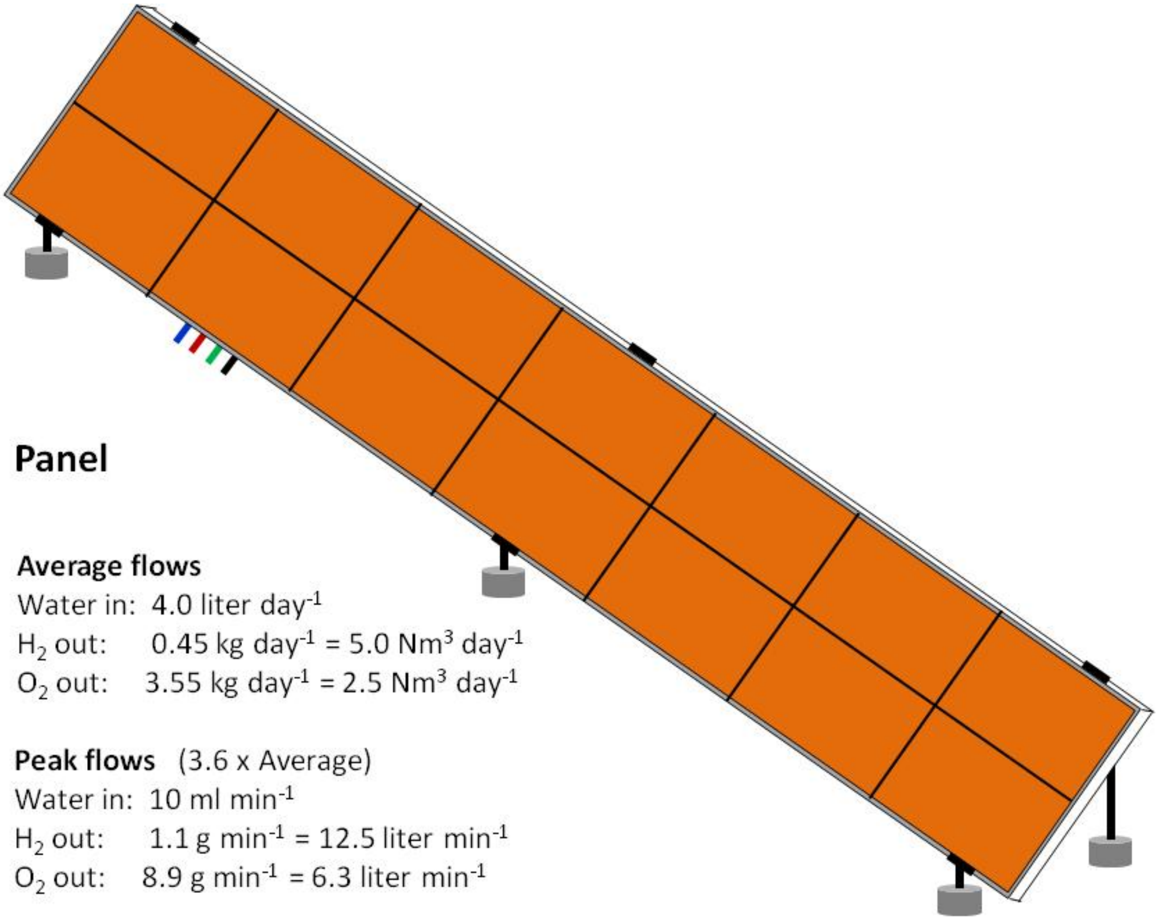


Figure S2. PEC panel with dimensions of 12.0 m long and 2.4 m wide. Flow rates are based on base-case conditions, and do not include water vapor lost with vented O_2.

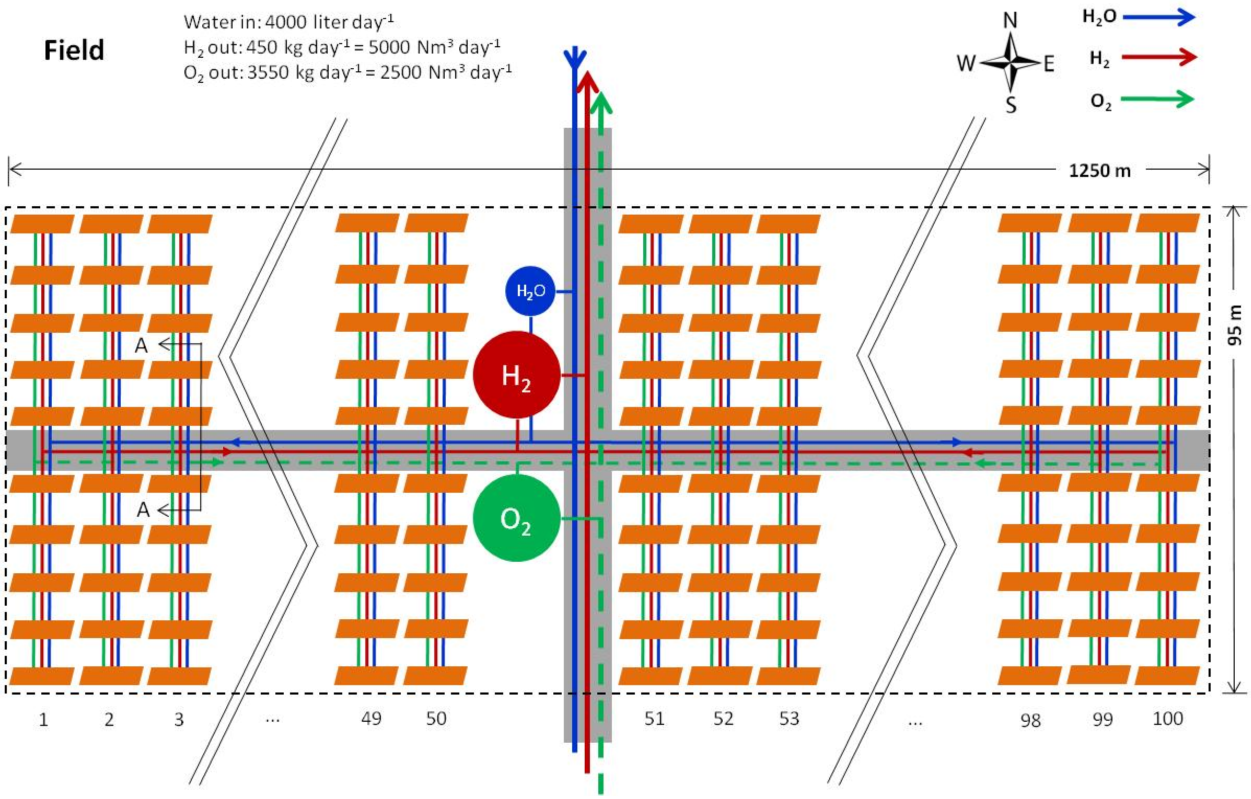


Figure S3. Diagram of a PEC field, comprising 1000 panels (100 rows of ten panels) plus compression and storage equipment for one day's production of H_2 (and O_2, if collected). Water flow rates do not include water vapor lost with vented O_2.

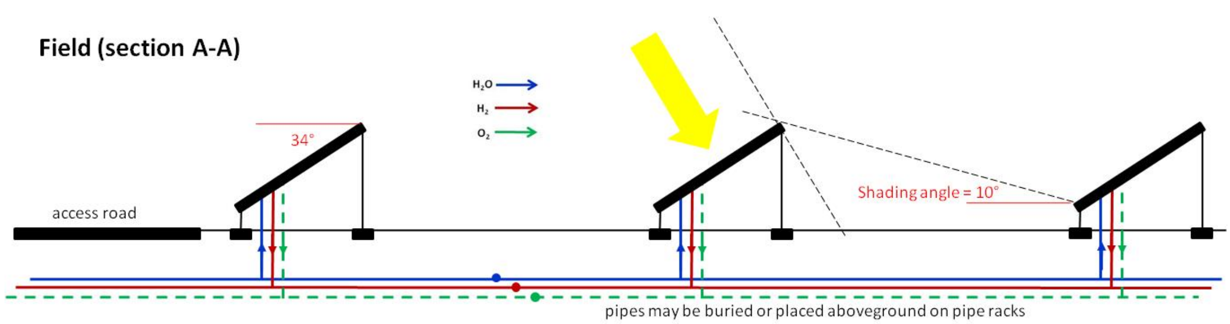


Figure S4. Cross sectional diagram of a PEC field, showing geometry of panel layout. Section A-A corresponds to indicator on Figure S3.

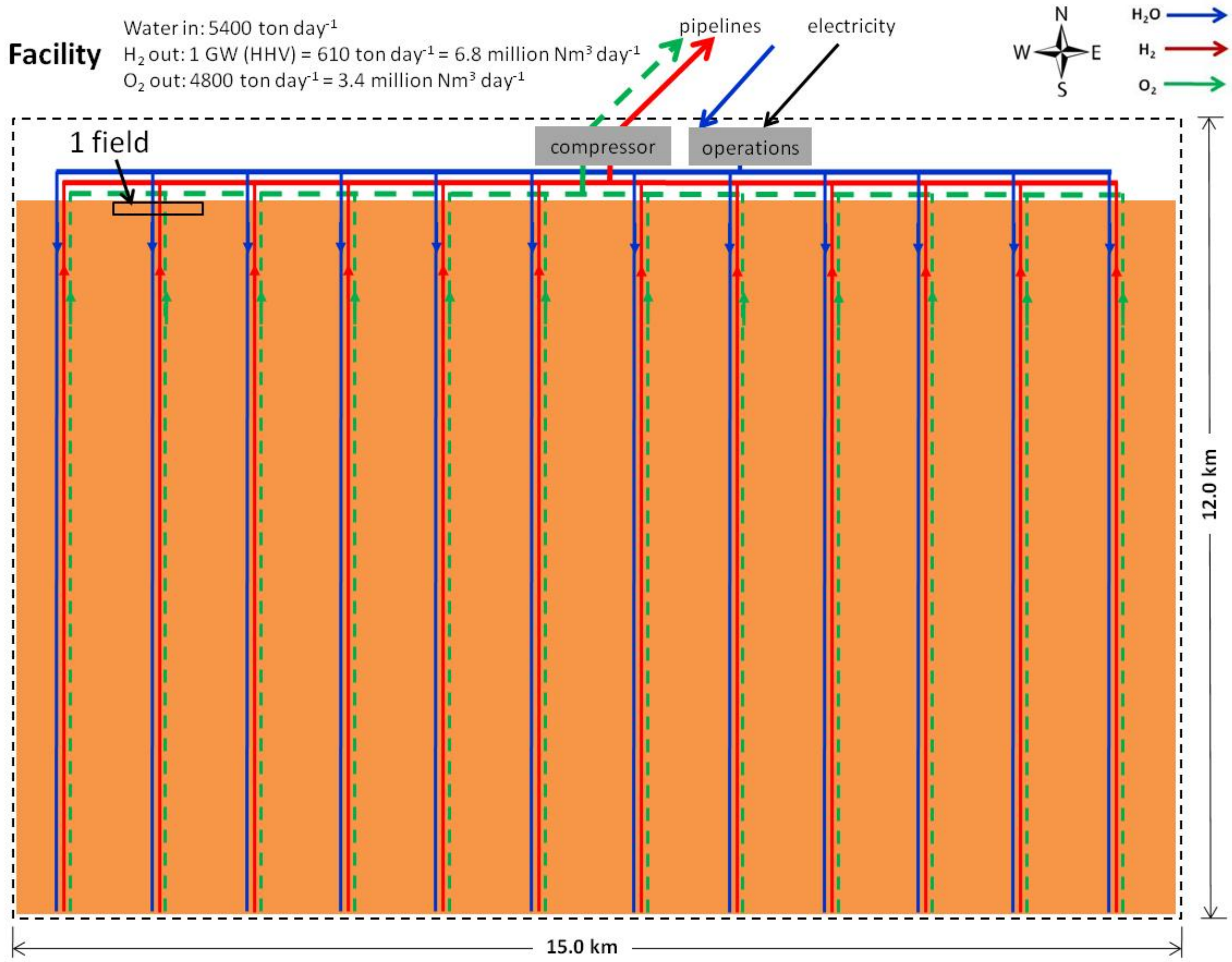


Figure S5. Diagram of PEC facility producing 1 GW (annual average) H_2. Water flow rates do not include water vapor lost with vented O_2.

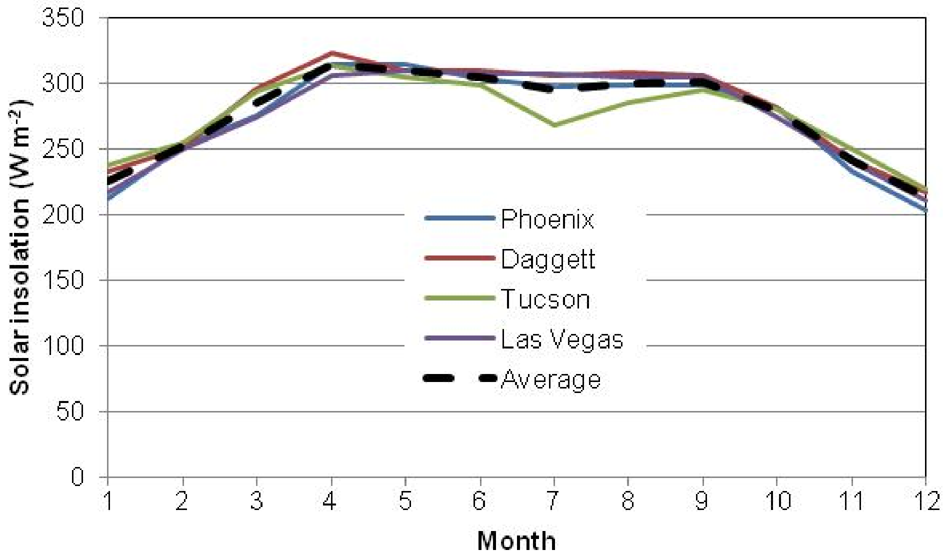


Figure S6. Monthly solar insolation (W m^{-2}) at four sites across the U.S. southwest. The assumed insolation on the facility is the average of the four sites, shown as a dashed line.

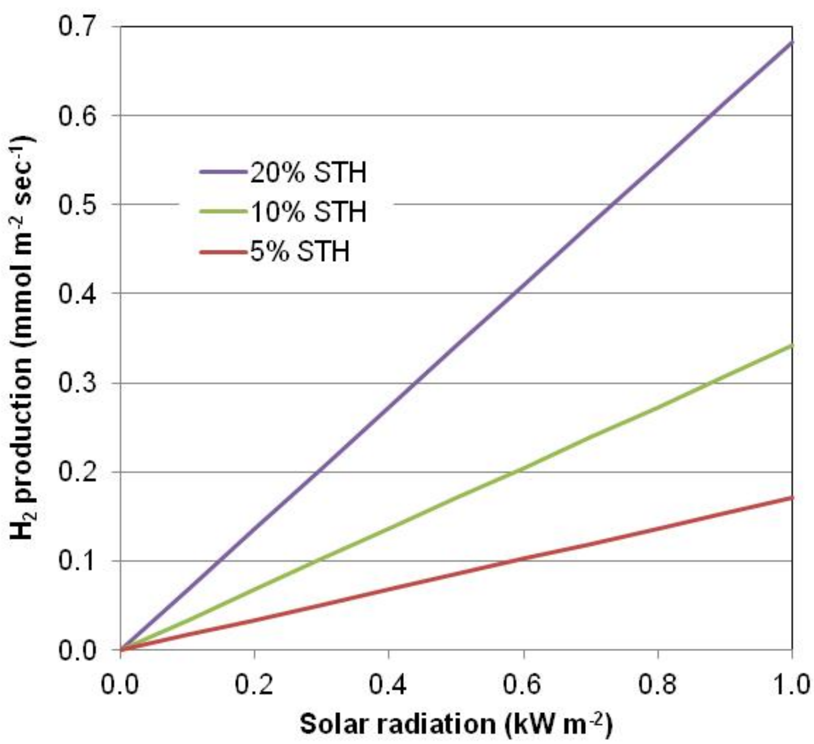


Figure S7. Assumed relation between instantaneous solar radiation and H_2 production.

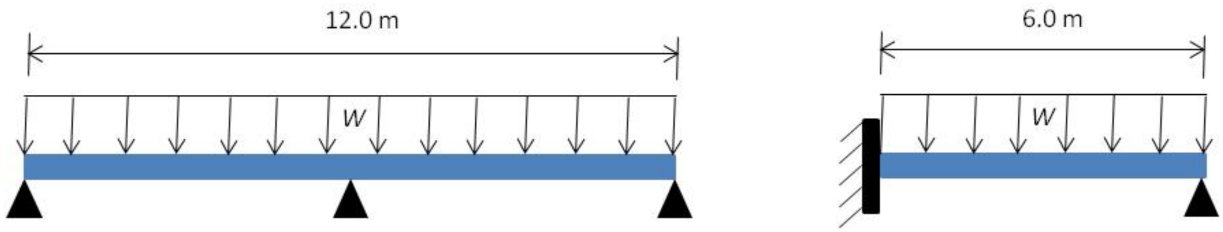


Figure S8. Estimation of panel deflection under load. Considering the panel as a uniformly-loaded beam that is simply supported at three points (left), symmetry implies that deflection will be equal to a beam fixed on one end and simply supported on the other (right). Based on Pope,[44] maximum deflection (inches) for such a beam will be:

$$y_{max} = \frac{-0.0054\, W\, L^4}{E\, I}$$

where W is the uniform load (pounds inch^{-1}), L is the length of the beam (inch), E is the modulus of elasticity of the material (psi), and I is the moment of inertia of the beam (inch^4). In this deflection analysis we assume the panel is laying flat; the uniform load is composed of the dead load of the steel structure (1.6 pounds inch^{-1}) plus the load of the PEC components and electrolyte (4.4 pounds inch^{-1}), to which is applied a safety factor multiplier of 3. The length of the (half) panel is 6.0 m or 237 inches. The modulus of elasticity of steel is about 3.1×10^7 psi. The moment of inertia of each of the two perimeter steel channel sections (ASTM C4x5.4) is 3.85 inch^4. These properties yield a maximum calculated deflection of 1.2 inches. The calculated length-to-deflection ratio is about 190, which is marginally acceptable for typical structural solutions. There appears to be significant scope for increasing material use efficiency through creative design that integrates PEC cell materials into a structural solution.

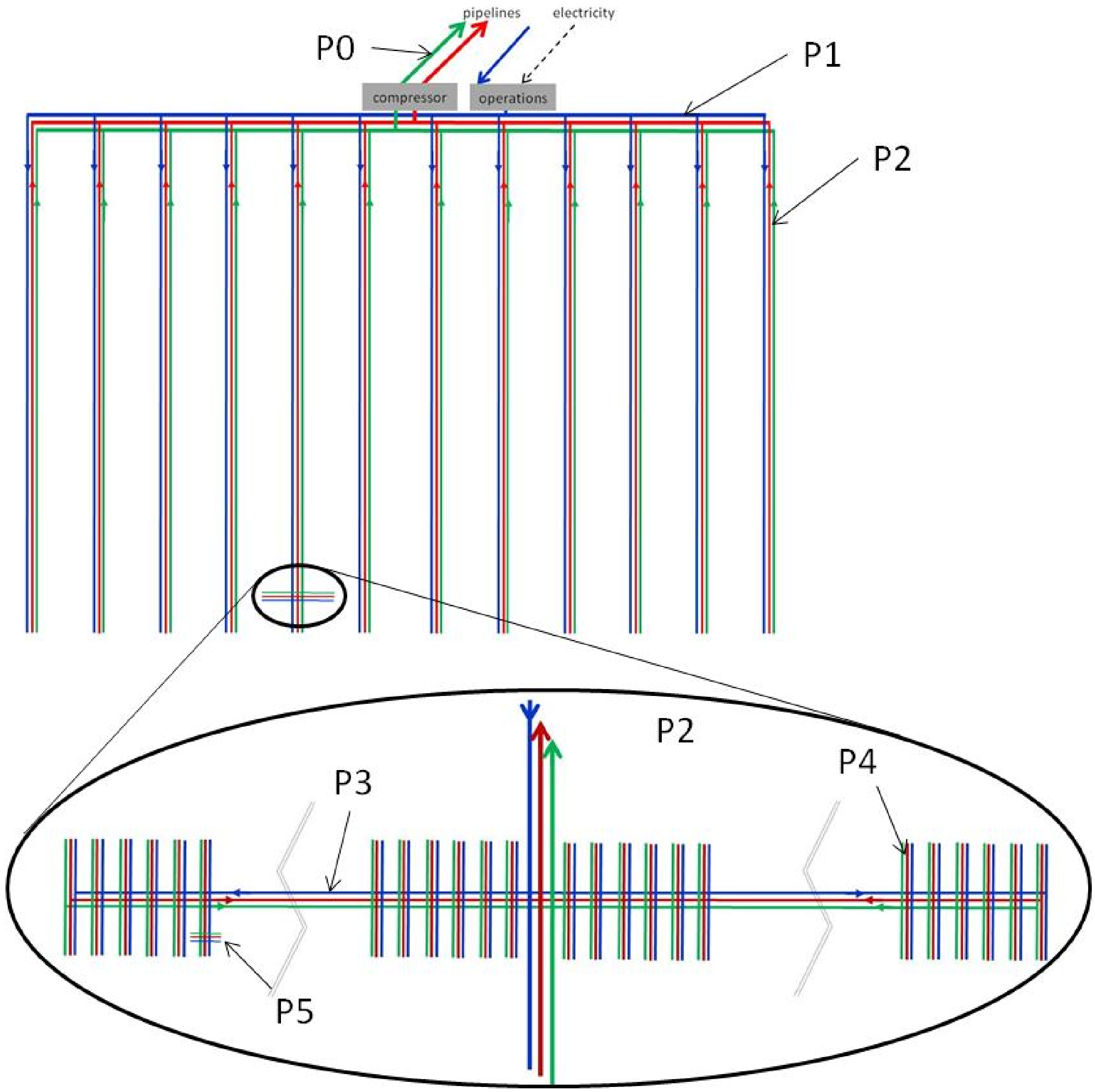


Figure S9. Hierarchical piping networks to transport fluids. Water, hydrogen and oxygen conduits are represented by blue, red and green lines, respectively.

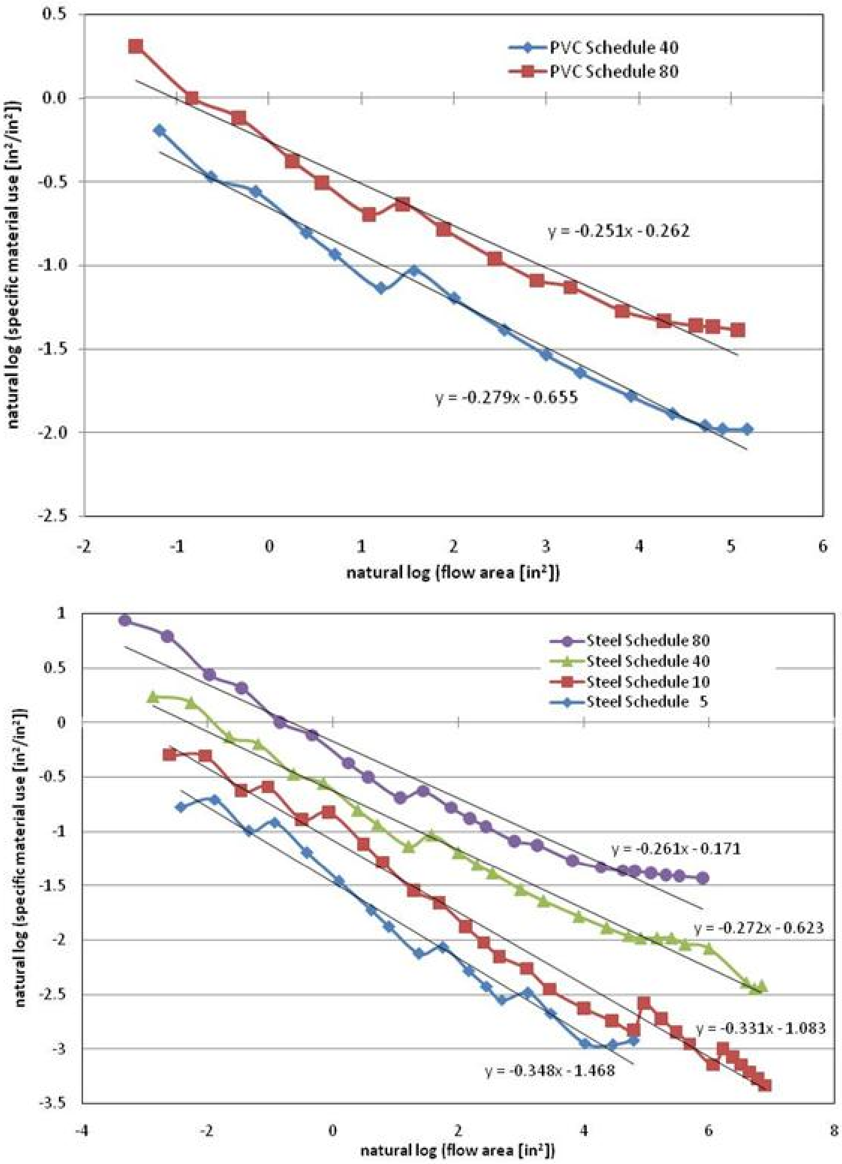


Figure S10. Relation between the flow area and specific material use of standard sizes of pipes made of PVC (top) and steel (bottom). Pipe dimensions are based on open-source data reporting agreed standards, namely ASTM D1785 (Poly Vinyl Chloride Plastic Pipe) and ASME B36.10 (Welded and Seamless Wrought Steel Pipe). Pipe sizing in this analysis is based on the fit lines.

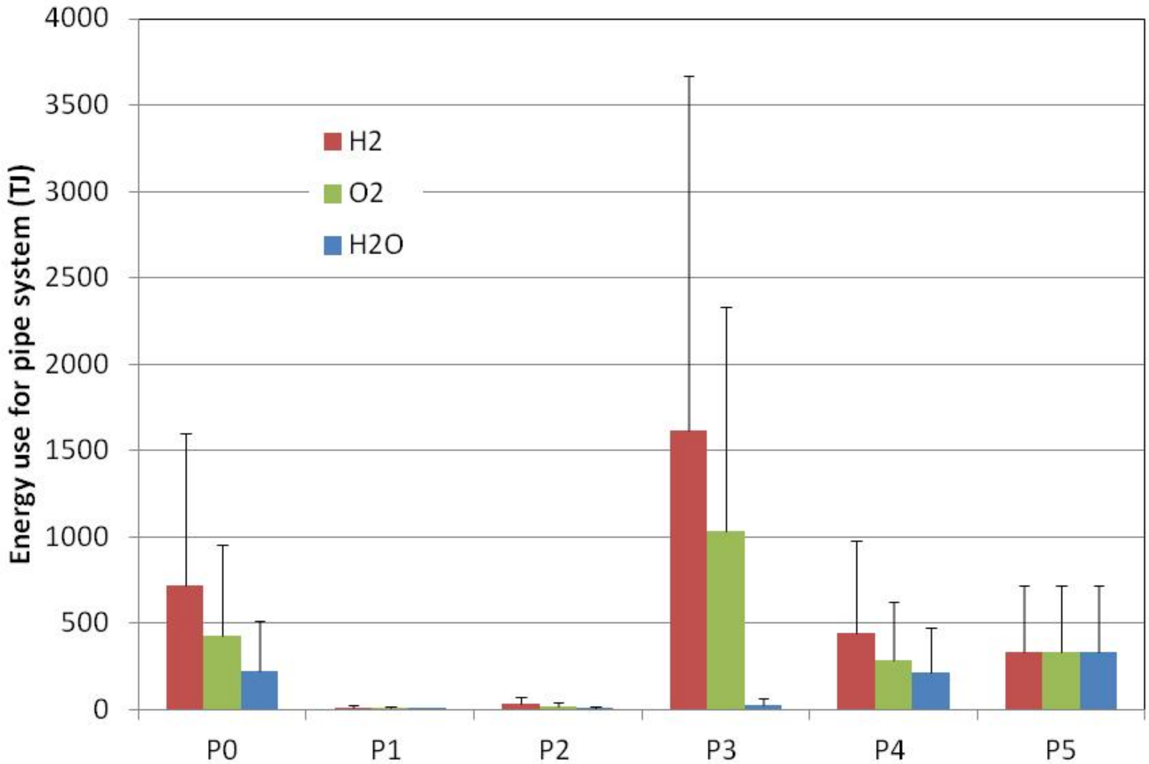


Figure S11. Energy use for production of piping system for the gas and liquid flows in the facility (H_2O, H_2, O_2). Colored bars show energy use for base case PVC pipes, error bars show additional energy use for steel pipes.

Details of H_2 demand scenarios

Light-duty vehicle travel demand in 2014 is approximately 2.70 trillion miles (EIA 2014). Based on NRC (2013), we assume that average light-duty vehicle hydrogen fuel cell efficiency is 13.5 kg H_2 per 1000 miles (based on the average of passenger car and light truck efficiencies), roughly 3.5 times more efficient than conventional gasoline engines. This results in an annual demand of 35.4 billion kg H_2. Assuming each 1 GW facility produces 222 million kg H_2 per year, 160 such facilities would be required. By 2050, NRC (2013) projects average fuel cell efficiency will decrease fuel consumption to 7.5 kg H_2 per 1000 miles, while we project travel demand will increase to 3.76 trillion miles (based on extrapolation of EIA projections through 2040). These combined changes result in a 2050 demand of 28.2 billion kg H_2, requiring 127 1 GW facilities to produce it.

EIA (US Energy Information Agency), *Annual Energy Outlook 2014 Early Release*, 2014. Web-accessed at http://www.eia.gov/forecasts/aeo/er/index.cfm

National Research Council, *Transitions to Alternative Vehicles and Fuels*, Washington, DC: The National Academies Press, 2013. Web-accessed at http://www.nap.edu/catalog.php?record_id=18264