Supporting Information for

How much technological progress is needed to make solar hydrogen cost-competitive?

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Other supplementary materials for this manuscript:

pyH2A along with original data and analysis for this publication are publicly available at: https://github.com/jschneidewind/pyH2A

Documentation for pyH2A is available at: https://pyh2a.readthedocs.io/en/latest/

1 Table of Contents

1.1 Table of Figures

1.2 Table of Tables

2 General Methodology

All calculations and visualizations were performed using pyH2A (https://github.com/jschneidewind/pyH2A). pyH2A calculates the levelized cost of hydrogen ($LCOH_2$) by modelling a hydrogen production plant using a specified technology across its entire lifetime. The general methodology can be divided into four parts: input parameters, workflow, discounted cash flow (DCF) calculation and analysis.

2.1 Input Parameters

The input parameters are the collection of all input information that is used in the techno-economic model. They contain financial input parameters (see Section 6.2), information about the workflow (see Section 2.2 and Section 6.2) and model specific information. Input parameters for each model are shown in Section 6.

2.1.1 Shared parameters

A number of input parameters are shared across the three different technologies (PV+E, PEC and photocatalysis) to facilitate comparison. All plant designs are scaled to produce roughly 1 ton of H_2 per day (365 t H_2 per year). To calculate labor cost, it is assumed that ten identical plants (ten "plant modules") are operated together and can share their labor force. This is done because the labor force calculation assumes that each staffer can oversee a certain amount of solar collection area, which is typically larger than the area of single plant. Operation of multiple plants therefore allows for calculation of the optimal labor cost.

Regarding location and irradiation, Daggett (California, USA) was chosen as the location for all plants due to its high solar irradiation and to facilitate comparison with previous studies.[1] Hourly irradiation data for a typical meteorological year in Daggett was obtained from the Photovoltaic Geographical Information system (https://re.jrc.ec.europa.eu/pvg_tools/en/#TMY). Based on this hourly data, incident power for a dual axis solar tracking (PEC), single axis solar tracking (PV+E) and no tracking (photocatalytic) configuration was calculated using a methodology reported by Chang and co-workers.[2] In the techno-economic models, either the mean daily incident power (PEC and photocatalytic) or the hourly incident power (PV+E) was used.

Financial input parameters are shared by all models (see Section 6.2).

2.2 Workflow

Each computation in pyH2A is structured by the workflow that is specified in the input parameters (see Section 6). The workflow determines which functions and plugins are executed during the DCF calculation as well as their order of execution. Functions are part of the core DCF calculation and are always executed. Plugins are modular pieces of code that are responsible for handling a specific part of the calculation. There are general purpose plugins shared by all models (see Section 6.2) as well plugins which are specific to a given technology. The actions of technology-specific plugins are described in the respective model description sections. By invoking plugins, specific pieces of input information are processed (e.g. by using the Photocatalytic_Plugin, information in the "Catalyst" input table is processed).

In general, all plugins ultimately feed information (such as total capital and operating costs) into the core functions, where this information is used to perform the DCF calculation.

2.3 Discounted Cash Flow (DCF) Calculation

In the DCF calculation, the inflation adjusted cash flow over the entire lifetime of the hydrogen production plant is modelled. For this modelling, capital and operating cost (CAPEX and OPEX), income from H_2 sales as well as financial parameters (taxes, working capital, loan payments, depreciation, salvage and decommissioning) are considered. Based on the cashflow and specified internal rate of return, the $LCOH_2$ is calculated. The DCF calculation is based on the H2A model by the U.S. Department of Energy and National Renewable Energy Laboratory.[3] The detailed DCF procedure can be found in the "Discounted_Cash_Flow" module of pyH2A.

2.4 Analysis

Four different methods are used to analyze the results of the DCF calculation as well as the response of the techno-economic models to perturbations of the input parameters: cost contribution, sensitivity and waterfall analysis as well as Monte Carlo analysis with the associated concept of development distance.

2.4.1 Cost Contribution Analysis

Cost contribution analysis is concerned with determining how much each underlying aspect of the model contributes to the observed cost.
For the overall cost breakdown, the contribution of each component in the DCF calculation to the $LCOH_2$ is determined. The DCF calculation's components are shown in Table 2.4-1.

Table 2.4-1 DCF calculation components that constitute $LCOH_2$ breakdown

Name	Description
Initial equity depreciable capital	Depreciable capital costs at the beginning of plant construction, including direct capital costs such as equipment purchases and installation costs as well as indirect capital costs such as permitting and contingency costs.
Non depreciable capital	Non-depreciable capital costs, e.g. cost for land on which the plant is built.
Fixed operating costs	Operating costs which do not vary in the short-term, e.g. staffing cost.
Variable operating costs	Variable operating costs, e.g. cost of utilities such as water or electricity.
Replacement costs	Cost for replacement of plant components. These might either be planned replacement costs (e.g. replacing electrolyzer stacks after they have reached their maximum operational lifetime) or unplanned replacement costs, e.g. for repairs.
Interest	Interest payments for purchases which were financed using a loan.
Principal payment	Principal payment for purchases which were financed using a loan.
Working capital reserve	Cost arising from maintaining a working capital reserve, depends on total operating costs.
Taxes	Applicable local and/or federal taxes paid on taxable income derived from H_2 sales.
Decommissioning	Cost of decommissioning H_2 production plant at the end of life.
Salvage	Income from selling salvaged components of decommissioned plant.

Furthermore, cost contribution analysis was also applied to the direct capital cost of each technology, showing how much each component of the plant contributed to the total direct capital cost.

2.4.2 Sensitivity Analysis

Sensitivity analysis investigates how the $LCOH_2$ changes when a single input parameter value is varied. To obtain the new $LCOH_2$, a DCF calculation is performed where all parameters values are the same as in the reference calculation except for the parameter value of interest. Typically, two separate calculations are performed, for which the parameter value of interest is both decreased and increased. For the sensitivity analyses herein, input parameter values were typically doubled and halved, except in cases where this would not be physically reasonable (e.g. in case of electrolyzer efficiency, which cannot be higher than 0.0253 kg(H_2)/kWh on thermodynamic grounds).
In the sensitivity analysis plots, the parameter name is shown in bold and below it three values are listed: the center value is the reference one, on the left is the value which led to a decrease and on the right is the value which led to an increase of the $LCOH_2$. The bar chart illustrates the reference $LCOH_2$ (black dotted line), the decreased $LCOH_2$ (green bar on the left) and increased $LCOH_2$ (red

bar on the right). For a given sensitivity plot, parameters are sorted by the $LCOH_2$ increase in descending order.

2.4.3 Waterfall Analysis

Waterfall analysis investigates how the combined variation of multiple input parameter values changes the $LCOH_2$. To determine how much each parameter contributes to the $LCOH_2$ change, parameter values are varied sequentially: first, only one parameter value is adjusted and the $LCOH_2$ is calculated. Subsequently, the next parameter value is adjusted (maintaining the previous parameter value change) and the resulting $LCOH_2$ is calculated again. This procedure is repeated until all desired adjustments were made. Based on the intermediate $LCOH_2$ results, it can be determined how much each parameter variation contributed to the total $LCOH_2$ change.

The waterfall analysis plot shows this sequential progression from left to right: on the very left, the base case $LCOH_2$ is shown. To its right, the varied input parameter values and their contribution to the $LCOH_2$ change are displayed in the order they were applied. The x-axis label for each parameter shows the adjusted parameter value, the parameter name as well as original parameter value in the base case. Finally, the adjusted $LCOH_2$ is shown on the right, which is obtained when all parameter values have been varied.

A key limitation for this type of waterfall analysis is that the contribution of each parameter depends on the order in which the parameter values are changed. In case of the waterfall analysis for Photovoltaic + Electrolysis (PV+E) for example (see Figure 5.2-4), the contribution of the electrolyzer efficiency change is $-0.28 when it is applied third (as is the case for Figure 5.2-4) but it is $-0.93 when applied first. This can be explained by the fact that an improvement of electrolyzer efficiency is more impactful when the electrolyzer is expensive (applying efficiency change before CAPEX change) compared to a situation where the electrolyzer is cheap (applying efficiency change after CAPEX change).

Due to this limitation waterfall analysis has to be used with care when trying to determine which parameters are actually most impactful for reducing the $LCOH_2$.

2.4.4 Monte Carlo Analysis and Development Distance

Monte Carlo analysis aims to determine how simultaneous progress for multiple input parameters changes the $LCOH_2$. Hence, it maps a trajectory for the impact of future technological improvements. The analysis proceeds via four steps:

1. The input parameters to be varied in the analysis are chosen. In case of PV+E, for example, PV CAPEX, electrolyzer CAPEX, electrolyzer efficiency and electrolyzer stack replacement cost are varied. Sensitivity analysis was used to determine the parameters with the strongest impact on $LCOH_2$ in the base case and the top four were selected.
2. For each chosen parameter, a [base, limit] interval of the parameter value is defined. The base value is typically the value from the base case model, representing the state-of-the-art for the parameter (e.g. 0.0185 kg(H_2)/kWh for electrolyzer efficiency). The limit value describes the limiting value which can reasonably be obtained for this parameter through future improvements (e.g. 0.025 kg(H_2)/kWh for electrolyzer efficiency, which is close to 99% of the maximum theoretical efficiency of 0.0253 kg(H_2)/kWh[2]). In Section 6, the "Parameters – Monte_Carlo_Analysis" tables for each model describe how each limit value was chosen.
3. 50,000 sets of the chosen input parameters are generated. Each set contains a random value (uniform distribution) for each parameter within its [base, limit] interval. Each set is therefore a random point within the *n*-dimensional box spanned by *n* chosen parameter intervals.

4. For every set of input parameter values, the values are substituted into the reference (base case) model and the $LCOH_2$ is calculated. Therefore, each set of random parameter values can be mapped to its corresponding $LCOH_2$ value.

2.4.4.1 Development distance

To analyze the results from the Monte Carlo analysis, the concept of "development distance" was developed. It aims to reduce the simultaneous variation of multiple input parameters into a single variable that describes technological progress. This is done by assigning each set of input parameter values a single number between 0 and 1, which describes how far this set is between base and limit case. Base case refers to the model where all chosen input parameters are at their base value, limit case refers to the model where all chosen input parameters are at their limit value. A development distance of 0 means that the set of input parameters is identical to the base values while a distance of 1 means that it is identical to the limit values.

The development distance of a given set of input parameter values is calculated in three steps:

1. Coordinate normalization: every value in the set is normalized to be between 0 and 1 based on its [base, limit] interval. This is done using either a linear or logarithmic normalization function (for details see 2.4.4.2). Unless mentioned otherwise, the linear normalization function is used for analysis. For example, using the linear normalization function in case of electrolyzer efficiency, an efficiency of 0.02175 kg(H_2)/kWh would have a normalized value of 0.5, since it is halfway between the base value of 0.0185 kg(H_2)/kWh and the limit value of 0.025 kg(H_2)/kWh. This normalization transforms each set from being a random point within a *n*-dimensional box to being a random point within a *n*-dimensional unit cube.
2. Distance calculation: for the *n*-dimensional unit cube, one vertex corresponds to the base case while the opposite vertex (vertex with maximum distance to base case vertex) corresponds to the limit case. In a four-dimensional case, for example, point (0, 0, 0, 0) might correspond to the base case while (1, 1, 1, 1) corresponds to the limit case. For the set of normalized values, its distance from the base case vertex is calculated using the city block metric (L_1 distance).
3. Distance normalization: the maximum city block distance (distance between base case and limit case vertex) depends on the number of dimensions of the *n*-dimensional unit cube (e.g. 3 for a three-dimensional unit cube, 4 for a four-dimensional one). The obtained distance value is therefore divided by the number of chosen parameters (which corresponds to the number of dimensions *n*). Hence, the normalized distance is obtained, which will be referred to as "development distance".

Using this methodology, a development distance can be calculated for each set of input parameter values. One should note that the mapping of input parameter values to development distance is not unique: two different sets of values can have the same development distance.
Each set of parameter values has an associated $LCOH_2$. As the mapping of sets to development distance is not unique, sets can have the same development distances but different $LCOH_2$. However, it is observed that development distance shows a good correlation with $LCOH_2$, allowing it to be used as simple metric that correlates technological progress with future $LCOH_2$.
Coupling Monte Carlo analysis with the described development distance calculation leads to a dataset with the following information: sets of input parameter values, their associated development distance and $LCOH_2$.

2.4.4.2 *Normalization function*

To ensure that every parameter contributes equally to the calculated development distance, parameter values are normalized to be between 0 and 1, based on their [base, limit] interval. To accomplish this, either a linear (Equation (1)) or logarithmic normalization function (Equation (2)) is used:

$$f(x) = \frac{x - x_{base}}{x_{limit} - x_{base}} \qquad \text{Equation (1)}$$

$$f(x) = \frac{\log_{10}(\frac{x}{x_{base}})}{\log_{10}(\frac{x_{limit}}{x_{base}})} \qquad \text{Equation (2)}$$

Where x is the parameter value to be normalized and x_{base} and x_{limit} are the base and limit values for the given parameter. Figure 2.4-1 shows a visual comparison of the two normalization functions for two selected parameters: PV CAPEX ($/kW(PV)) and electrolyzer efficiency (kg(H_2)/kWh(Electricity)).

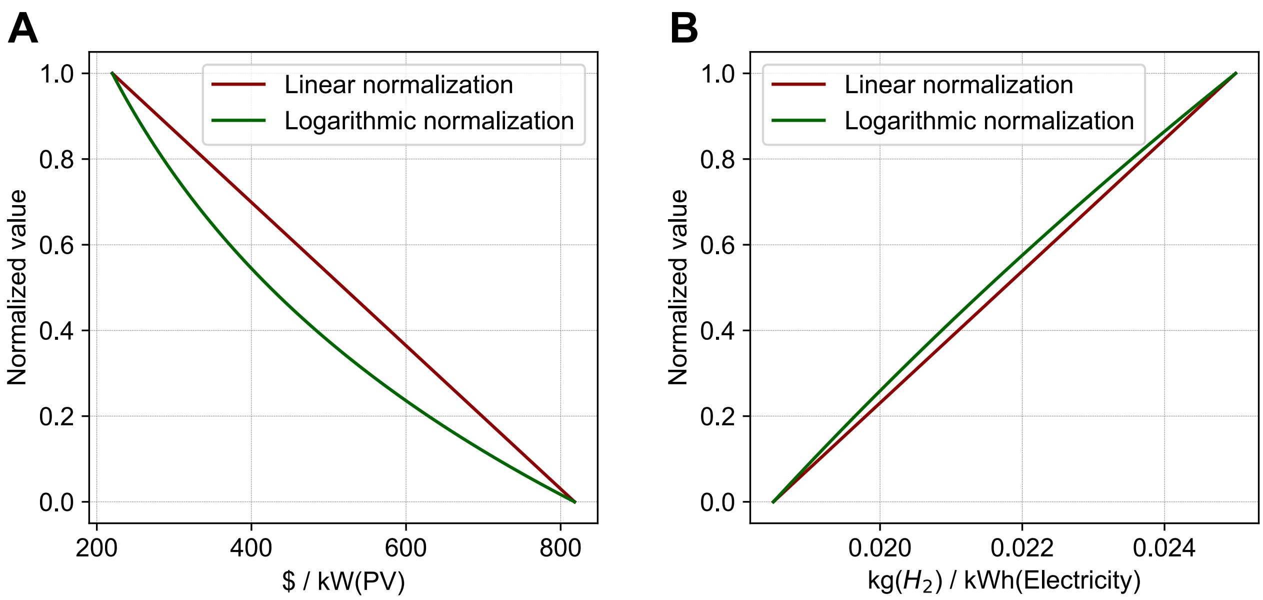


Figure 2.4-1 Comparison of linear and logarithmic normalization functions for PV CAPEX ($/kW(PV)) and electrolyzer efficiency (kg(H_2)/kWh(Electricity)

The two functions yield comparable results, with the deviation being smaller when the parameter range covers a smaller range. In case of PV CAPEX, base and limit values are separated by a factor of about four, while they are only separated by a factor of ca. 1.35 for electrolyzer efficiency. Hence, the deviation between linear and logarithmic normalization is smaller for electrolyzer efficiency.

The difference between linear and logarithmic normalization becomes most significant when normalizing values which lie outside of the [base, limit] interval, as in the case of development distance/time analysis (see Section 2.4.4.6): for example, a historical PV CAPEX of 3200 $/kW(PV) has a normalized value of ca. -4 when using linear normalization while the value is ca. -1 when logarithmic normalization is used. This is because 3200 $/kW(PV) is four times the [base, limit] interval ([818, 220], range of 598 $/kW(PV)), minus the base value of 818 $/kW(PV). Linear normalization assumes that each 598 $/kW(PV) step corresponds to one normalized unit, hence the normalized value is -4. Logarithmic normalization, on the other hand, assumes that a fourfold reduction from 3200 \$/kW(PV) to 818 \$/kW(PV) corresponds to the same unit as a fourfold reduction from 818 \$/kW(PV) to 220 \$/kW(PV), with the normalized value therefore being -1.

Historically, logarithmic instead of linear improvements often occur (see Section 5.4): going from 3200 \$/kW(PV) to 818 \$/kW(PV) is about as challenging/time-consuming as going from 818 \$/kW(PV) to 220 \$/kW(PV). Hence, logarithmic normalization, where both of the steps correspond to one normalized unit is sensible. In contrast, linear normalization would imply that going from 3200 \$/kW(PV) to 2600 \$/kW(PV) would be as challenging as going from 818 \$/kW(PV) to 220 \$/kW(PV), which is usually not the case since progress becomes more challenging when approaching a limit. Therefore, logarithmic normalization is used when analyzing historical data and when comparing historical development distances to Monte Carlo development distances (which are then also calculated using logarithmic normalization to facilitate comparison).

However, as shown in in Figure 2.4-1, within the [base, limit] interval the differences between the two normalization functions are small. Linear normalization has the advantages of being fully symmetrical and being independent of the range covered by the [base, limit] interval. Therefore, linear normalization is used for regular Monte Carlo development distance analysis, where all parameter values are within the [base, limit] intervals.

2.4.4.3 Development distance/LCOH$_2$ relationship

Using the Monte Carlo dataset, one can plot the development distance of each datapoint against the associated LCOH$_2$. The resulting plot shows the relationship between development distance and LCOH$_2$, describing how technological progress among the chosen input parameters affects LCOH$_2$. The plots are typically shown including a Savitzky-Golay filtered trendline and an indication of the target cost region (grey horizontal bar, for further information on target cost region see below).

2.4.4.4 Development distance histogram

The Monto Carlo results can be used to quantify how much technological progress is required to reach a defined target cost range. In this case the target cost range is set to 1.5 – 1.6 \$/kg(H$_2$). The development distance histogram shows the distribution of development distances for input parameter sets that have an associated LCOH$_2$ within the target cost range. It therefore provides information on which range of development distances are needed to achieve the defined target cost. Plots typically include a fitted and scaled normal distribution, from which the mean development distance and standard deviation are derived.

2.4.4.5 Colored scatter plot

Colored scatter plots visualize the input parameter sets that have an associated LCOH$_2$ within the target cost range. Each point in the scatter plots represents one such set of input parameter values. The point's x-axis coordinate is determined by the first input parameter value, the y-axis coordinate by the second input parameter value and color axis (z-axis) by the third input parameter value. In this case, the raw (unprocessed) parameter values are shown. The fourth (and any further parameter values) are not shown in this visualization.

Visualization of the data in this form illustrates which region of the parameter space gives rise to a model instance that reaches the target cost range. A light blue area further highlights this region: it corresponds to the biggest possible two-dimensional area in which the parameter sets that reach the target cost range can be located. This area is calculated by setting the third (and any further parameters) to their limit value and then determining the edge values of the first (x-axis) and second (y-axis) parameter, which just reach the target cost range.

For reference, the base case datapoint is also shown (labelled "Base"), and by definition it will always be in one of the corners of the scatter plot. Comparing the base case coordinate to the region which contains the sets that reach the target cost range gives a visual idea of the required technological progress.

2.4.4.6 Development distance/time relationship

Using historical data, it is possible to establish a relationship between development distance and time. This is done by collecting historical parameter values for a given technology. For example, in case of PV+E, historical PV CAPEX, electrolyzer CAPEX and electrolyzer efficiency values are collected. Each datapoint in the historical dataset corresponds to a given year with the associated parameter values in that year.

Using the development distance methodology described in Section 2.4.4.1, the development distance of each historical datapoint is obtained. As laid out in Section 2.4.4.2, logarithmic normalization instead of linear normalization is used when analyzing this historical data. Since development distance typically increases with time, historical development distance values are negative in most cases (indicating that historical datapoints are associated with parameter values which are less advanced than the base parameter values). A new dataset is thus obtained, describing how development distance has historically changed over time.

Using the historical development distance trend, different models can be fitted to the data to extrapolate into the future. Using this extrapolation, one can estimate when certain positive development distances (between 0, base case, and 1, limit case) may be achieved. In the 'Development_Distance_Time_Analysis" module implemented in pyH2A, two models are used for fitting: a linear and an asymptotic model. The linear model assumes that the historical rate of development distance increase remains unchanged. Hence, it is the optimistic scenario for relating development distance to time. The asymptotic model assumes that the limit case (development distance of 1) is approached asymptotically, meaning that the rate of development distance increase goes down as the development distance approaches 1. It is therefore the conservative scenario for relating establishing the development distance/time relationship.

Based on the extrapolated models, development distance values between 0 and 1 can be mapped to the respective years in which they may be achieved. This information can then be added to development distance/LCOH$_2$ relationship or development distance histogram plots. To ensure that the development distance/time relationship is comparable to the development distances shown in these plots, the Monte Carlo development distances are recalculated using logarithmic normalization. Since logarithmic and linear normalization yield comparable results within the [base, limit] interval (see Section 2.4.4.2), the Monte Carlo development distances are typically very similar to those obtained using linear normalization.

3 Photoelectrochemical Water Splitting (PEC)

3.1 Model Description

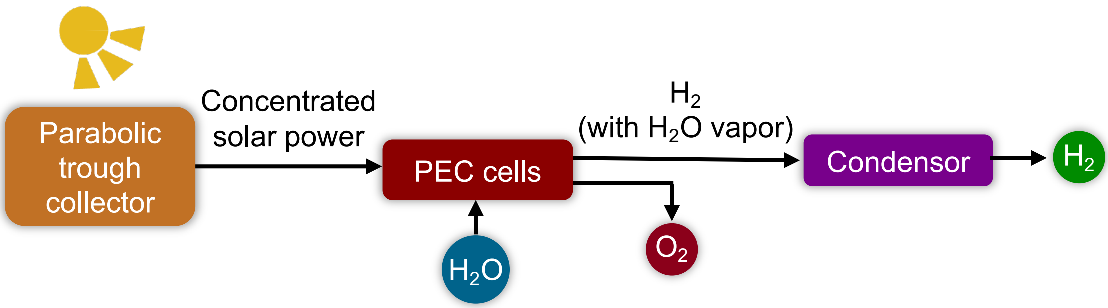


Figure 3.1-1 Simplified process model for photoelectrochemical water splitting (PEC)

3.1.1 General description

For the photoelectrochemical water splitting plant, dual-axis tracking parabolic trough collectors are used for solar concentration (providing a specified solar concentration factor). The concentrated solar power irradiates PEC cells, which split water into H_2 and O_2. Those gases are formed on opposite sides of the cell, providing intrinsic separation (akin to an electrolyzer).[4,5] Generated H_2 is then transported to a gas processing unit, where residual water vapor is removed using a condenser, obtaining pure H_2. Overall plant layout and operating is based on Pinaud *et al.* (type 4: tracking concentrator array).[1]

3.1.2 Specific plugins and methodology

Hydrogen production by PEC cells is modelled using the "PEC_Plugin". Based on the specified dimensions of a single cell, the STH efficiency and incident irradiation (mean daily solar irradiation multiplied by solar concentration factor), daily H_2 production per cell is calculated. Given the plant's design capacity, the total number of required PEC cells is obtained, which in turn determines the total PEC cell area and cost. The "Solar_Concentrator_Plugin" uses the total PEC cell area and solar concentration factor to determine the required solar collector/concentrator area and resulting cost. Just like the photocatalyst in photocatalytic water splitting, PEC cells are assumed to undergo degradation, requiring replacement after a specified lifetime. It is assumed that the entire PEC cell is replaced, since they are, by definition, highly integrated devices. This means that cell replacement cost is equal to the full PEC cell cost.

3.1.3 Estimation of PEC cell cost

Just like photocatalysts for water splitting, PEC cells are not currently in use on an industrial scale. To estimate cell cost, we therefore turned to cost information for solar cells, which are similar to the light-absorbing component of PEC devices. Regular silicon solar cells do not generate a potential that is sufficient for water splitting. Therefore, state-of-the-art PEC cells[4,5] typically utilize (multi-junction) III-V semiconductors, similar to III-V solar cells. Such solar cells are used commercially and we can use their cost as a proxy.

Horowitz *et al.*[6] estimate a lower cost bound of 70 $\$/W_{DC}$ for III-V solar cells, equivalent to 21,000 $\$/m^2$ (assuming 30% efficiency). This was used as the base value for PEC cell cost per m^2. It should be noted that this is likely a quite optimistic estimate for the current cost of PEC cells: aside from the light-absorbing component, these cells also incorporate electrocatalysts, membranes and other balance of system components not required for a solar cell. The cost of these components is neglected in this estimate (however, the cost of solar cell-specific parts such as conductive interconnections, is included instead). Furthermore, PEC cells are less commercially mature compared to III-V solar cells, which would likely also increase their relative current cost.

3.1.4 Base and limit parameter values

Four parameters were varied between the base and limit case models: STH efficiency, PEC cell cost, PEC cell lifetime and the solar concentration factor (Table 3.1-1). Using sensitivity analysis, these were found to have the strongest impact on $LCOH_2$ in the base case model (see Figure 3.2-3).

Table 3.1-1 Parameters varied between base and limit case for photoelectrochemical water splitting (PEC)

Parameter	Base value	Limit value
STH efficiency	14%	30%
PEC cell cost ($/m^2(PEC cell))	21000	700
PEC cell lifetime (years)	0.33	3
Solar concentration factor	50	100

Table 3.1-2 Source/rationale for PEC base case parameter values

Parameter	Base value	Source/rationale
STH efficiency	14%	Value is based on 14% STH efficiency for a vapor-fed PEC device reported in Kistler 2020[4]. This system has one of the most favorable combinations of STH efficiency and lifetime as was therefore chosen as a reference. However, in this case no solar concentration was used. In Idriss 2020[5] STH efficiencies of 18% (15 suns solar concentration) and 13% (200 suns solar concentration) are reported, corroborating a value of ca. 14% for 50 suns solar concentration.
PEC cell cost ($/m^2(PEC cell))	21000	Based on current cost of III-V solar cells, see 3.1.3
PEC cell lifetime (years)	0.33	Based on 1000 h lifetime reported in Kistler 2020.[4] Assuming eight hours of daily irradiation this would correspond to an operation time of ca. 125 days.
Solar concentration factor	50	Solar concentration factor which can typically be achieved with a parabolic trough design, as reported in Gharbi 2011.[7]

Table 3.1-3 Source/rationale for PEC limit case parameter values

Parameter	Base value	Source/rationale
STH efficiency	30%	The achievable STH efficiency is the product of solar concentrator efficiency (ca. 76% for state-of-the-art parabolic trough concentrators, see Filas 2018[8]) and PEC STH efficiency (maximum possible STH efficiency is ca. 40% for multi junction devices based on Hellgardt 2018[9]), leading to a value of ca. 30%. Solar concentrator efficiency might improve in the future, but the 40% PEC STH efficiency limit reported in Hellgardt 2018[9] neglects energy loss channels which are likely unavoidable and would lower the obtainable STH efficiency limit. Hence, an overall value of 30% for the STH efficiency limit was assumed.
PEC cell cost ($/m^2(PEC cell))	700	30-fold cost reduction for PEC cells relative to base case value analogous to the 30-fold cost reduction assumed for the photocatalyst in photocatalytic water splitting
PEC cell lifetime (years)	3	Assumption of a 9-fold lifetime improvement relative to the base case value. The lifetime of PEC cells (even in the limit case) is likely substantially lower compared to solar cells since various components are exposed to a reactive chemical environment.
Solar concentration factor	100	Doubling of solar concentration factor relative to the base case value, with a factor of 100 being in the upper range of what is typically achievable with parabolic trough concentrators (see Gharbi 2011[7]).

3.2 Base Case

3.2.1 Cost Breakdown

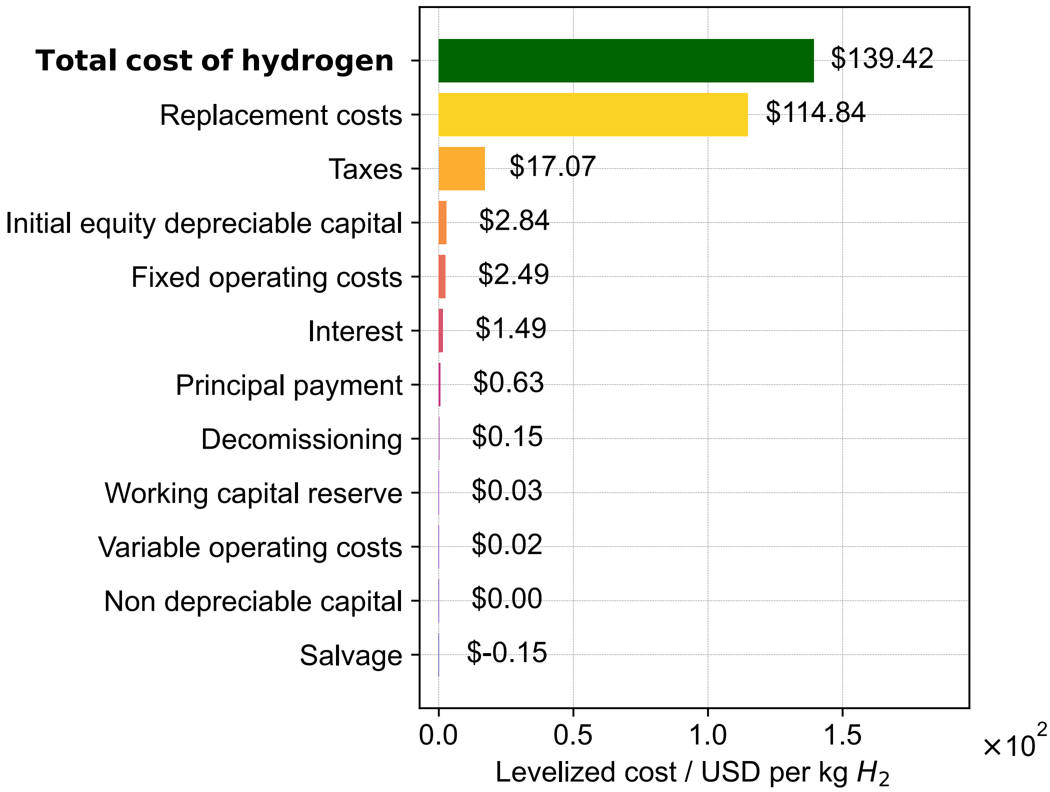


Figure 3.2-1 Overall cost breakdown plot for PEC base case

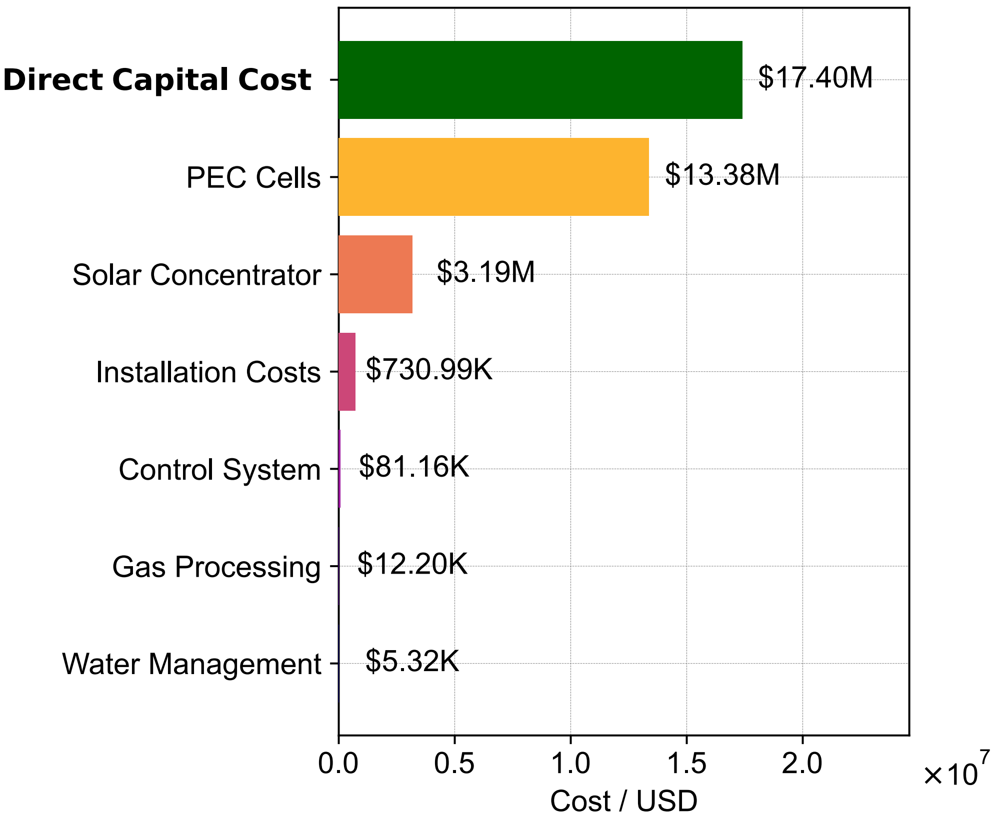


Figure 3.2-2 Capital cost breakdown plot for PEC base case

3.2.2 Sensitivity Analysis

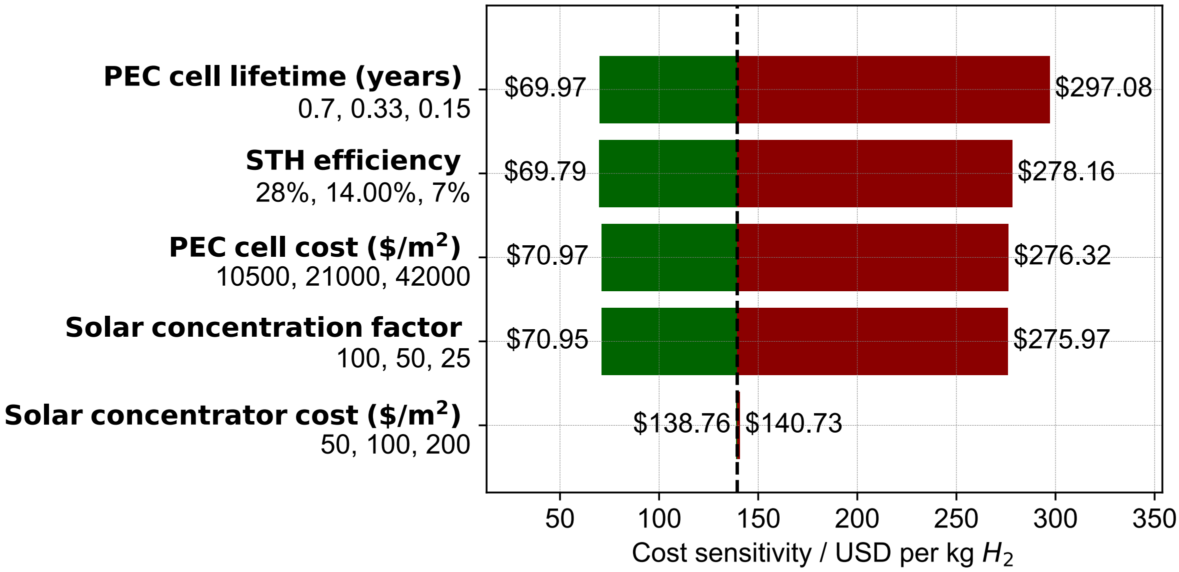


Figure 3.2-3 Sensitivity analysis plot for PEC base case

3.3 Limit Case

3.3.1 Cost Breakdown

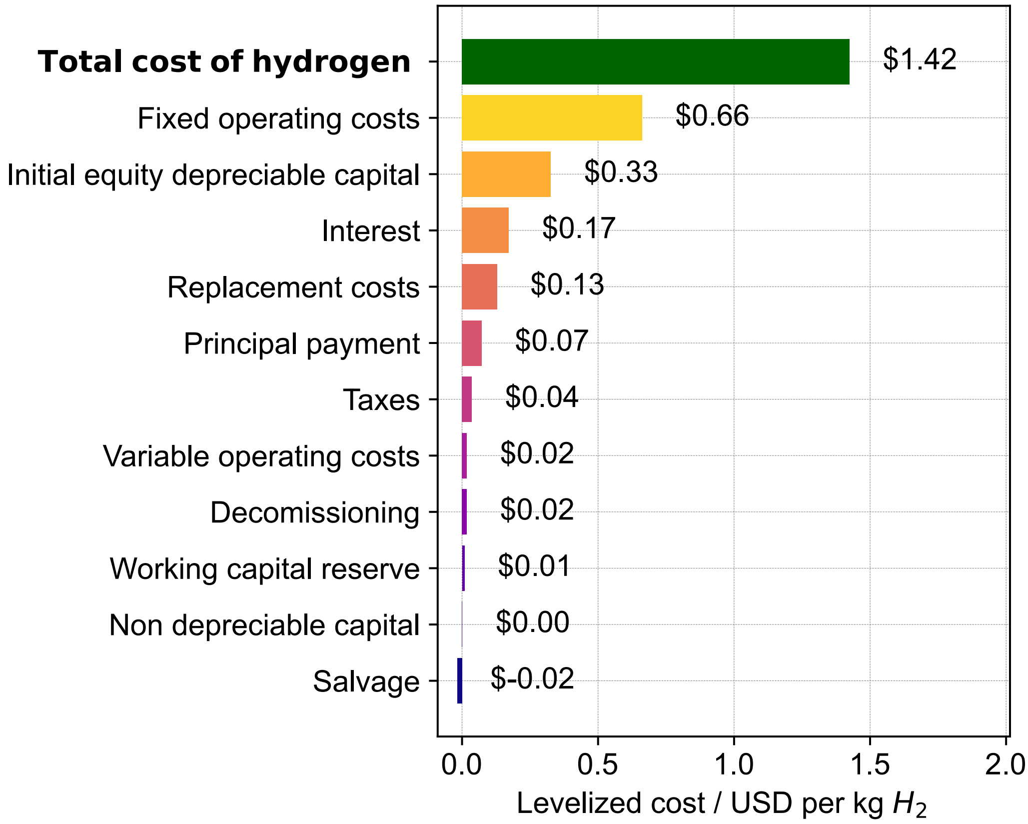


Figure 3.3-1 Overall cost breakdown plot for PEC limit case

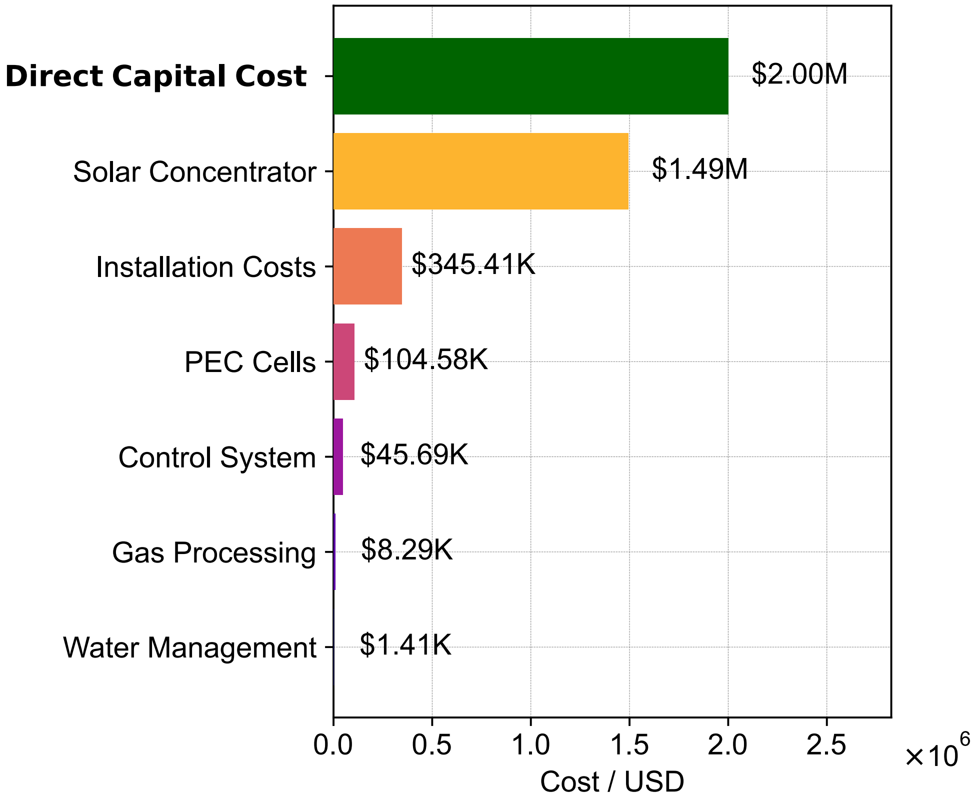


Figure 3.3-2 Capital cost breakdown plot for PEC limit case

3.3.2 Sensitivity Analysis

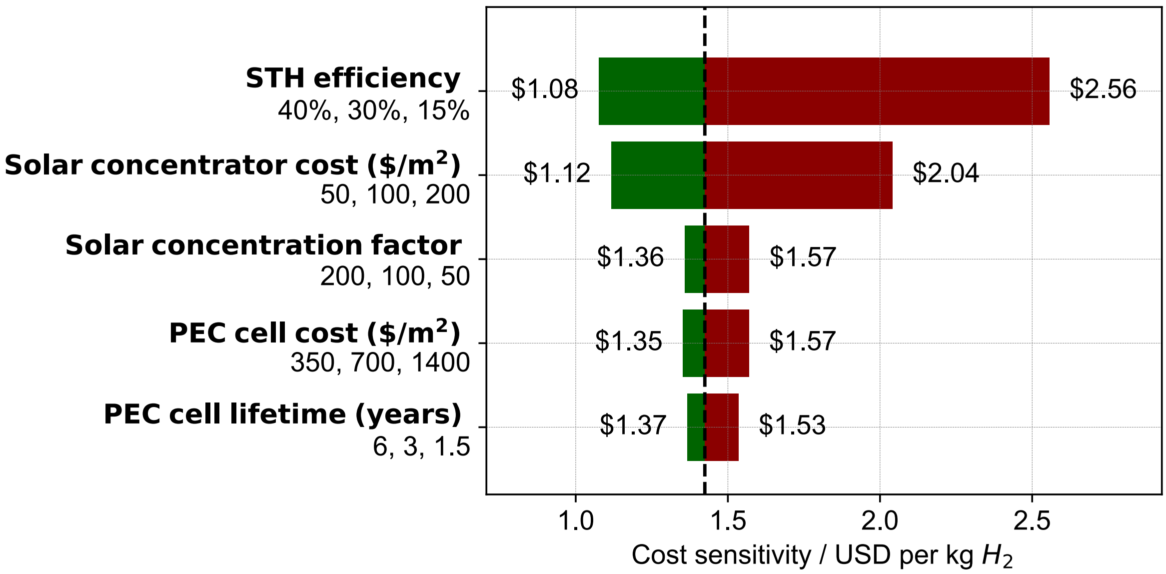


Figure 3.3-3 Sensitivity analysis plot for PEC limit case

3.4 PEC Limit Case without Solar Concentration (PEC Type 3)

The PEC limit case without solar concentration is identical to the regular PEC limit case, except that no solar concentration is used. All sunlight is therefore directly collected by PEC cells, leading to a significantly larger PEC cell area. This configuration is similar to the “type 3: fixed panel array” described by Pinaud *et al.*[1]

3.4.1 Cost Breakdown

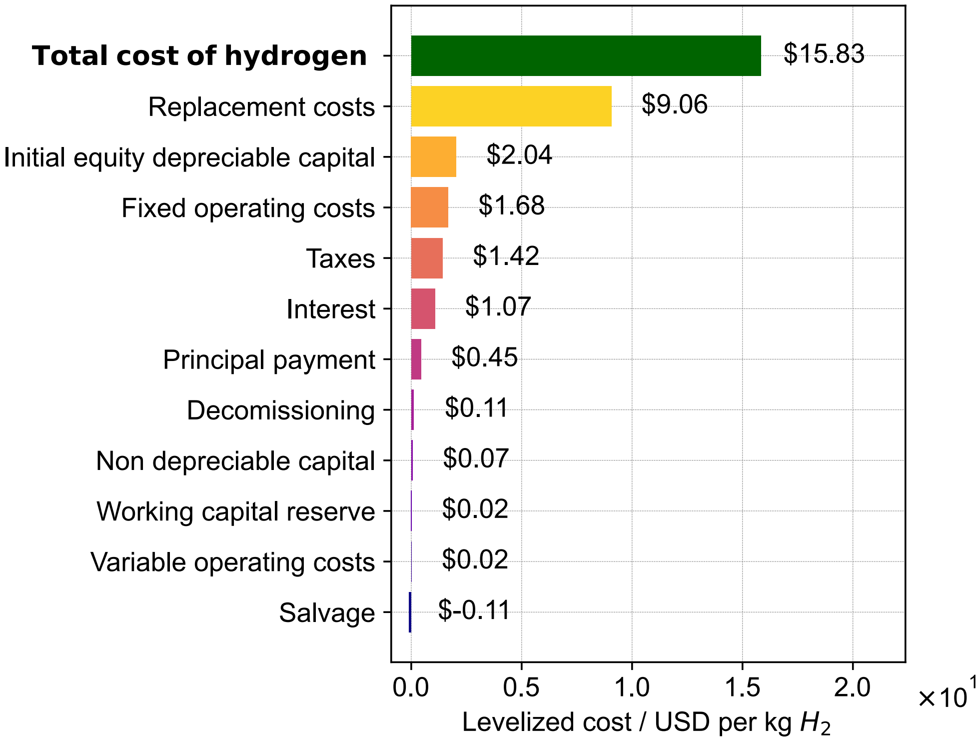


Figure 3.4-1 Overall cost breakdown plot for PEC type 3 limit case

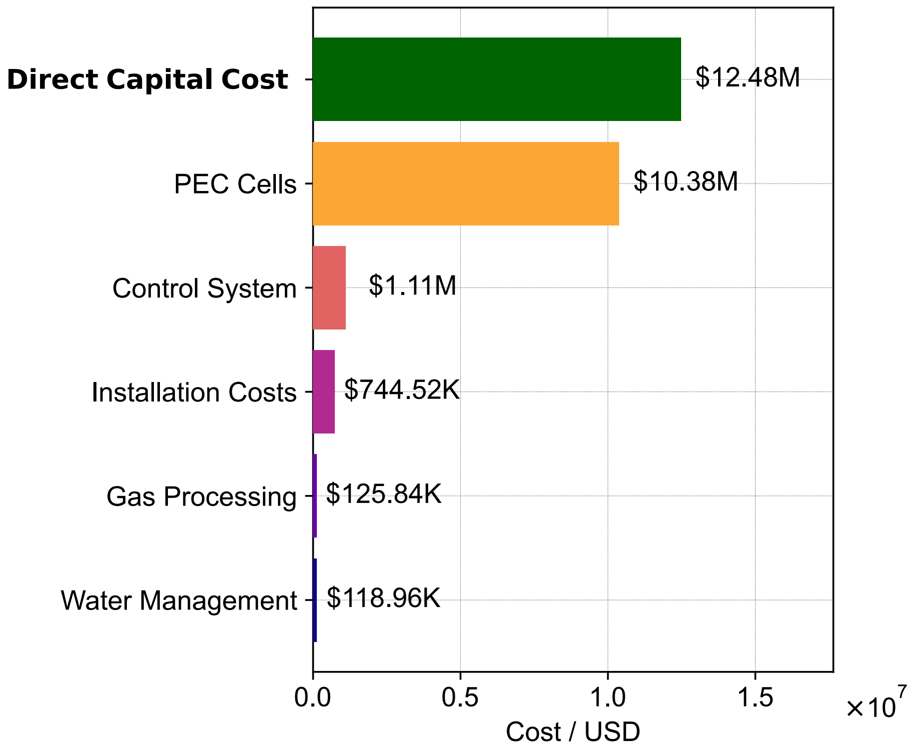


Figure 3.4-2 Capital cost breakdown plot for PEC type 3 limit case

3.4.2 Sensitivity Analysis

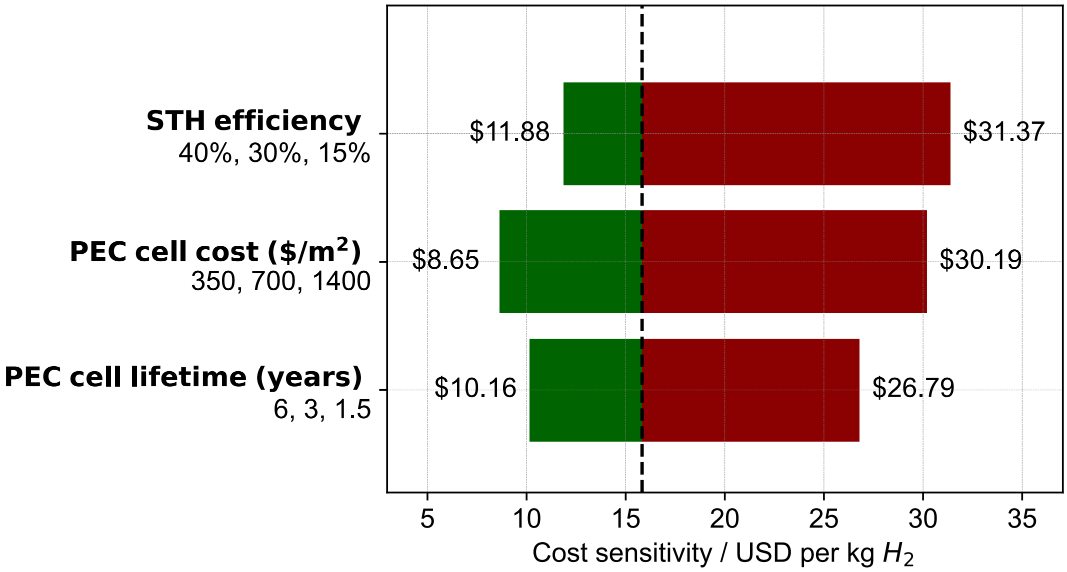


Figure 3.4-3 Sensitivity analysis plot for PEC type 3 limit case

4 Photocatalytic Water Splitting (Photocatalytic/PC)

4.1 Model Description

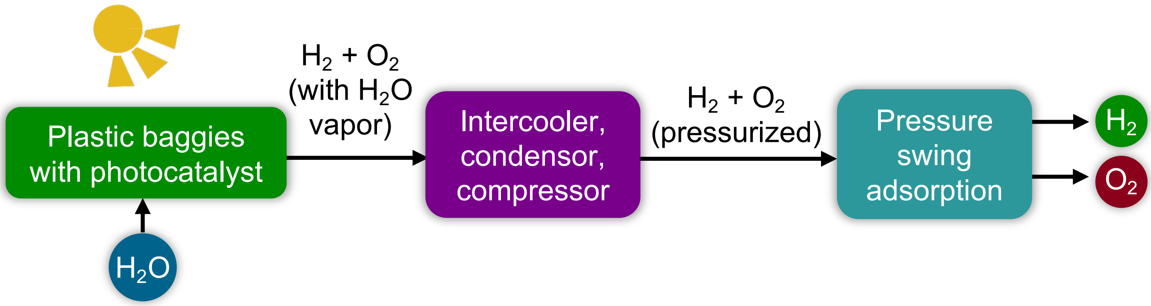


Figure 4.1-1 Simplified process model for photocatalytic water splitting (photocatalytic/PC)

4.1.1 General description

In the photocatalytic water splitting plant, hydrogen production takes place in multiple large plastic baggie reactors. These reactors are placed on flat ground and filled with a mixture of photocatalyst and water. Solar irradiation leads to the production of a H_2/O_2 mixture in the baggies, which is transported to a central gas processing site via suitable connecting pipes. At the gas processing site, water vapor in the H_2/O_2 mixture is removed using intercoolers and condensers and the mixture is compressed. Separation of the compressed H_2/O_2 stream is achieved using pressure swing adsorption, obtaining pure hydrogen. It is assumed that the separation step leads to a 10% loss of H_2.[1] The plant's design capacity is therefore scaled up by ca. 10% to compensate for this loss. Overall plant layout and operation is based on Pinaud *et al.* (type 1: single bed particle suspensions).[1]

4.1.2 Specific plugins and methodology

Hydrogen production in plastic baggie reactors is modelled using the "Photocatalytic_Plugin". In this model, mean daily solar irradiation, solar-to-hydrogen (STH) efficiency and baggie size are used to calculate the daily H_2 production per baggie. Based on the plant's design capacity, the necessary number of baggie reactors is calculated. The dimensions of a single baggie, number of required baggies and catalyst concentration determine the amount of photocatalyst which is needed for plant operation. Due to catalyst degradation, the photocatalyst is assumed to have a limited lifetime, after which it has to be replaced with new catalyst. This incurs replacement costs and creates the need for removal of deactivated catalyst. The "Catalyst_Separation_Plugin" models the removal process by calculating the amount of water/catalyst mixture that has to be separated every year based on the catalyst lifetime. To approximate the cost of this separation it is assumed to be similar to a nanofiltration step. Deactivated catalyst is not recycled in the modelled plant.

4.1.3 Estimation of catalyst cost

Estimating the photocatalyst cost is challenging since no comparable catalysts are currently being used in a large-scale industrial context. Therefore, the CatCost catalyst cost estimation tool by the National Renewable Energy Laboratory (NREL)[10] was used to obtain appropriate estimates. A catalyst costing model was created based on the carbon dots (CDot)/C_3N_4 (0.48 wt% CDots) photocatalyst reported by Kang and co-workers,[11] prepared on a conservative 5 ton/year scale (the base case hydrogen production plant would actually use around 17 tons of catalyst per year). Since this is a carbon nitride material, urea and melamine were selected as starting materials and a mass yield of 5% was assumed (comparable to the one reported by Kang and co-workers[11]). The impact of CDots on the catalyst cost was taken into account by replacing them with 0.5 wt% ruthenium as an approximate cost placeholder. Furthermore, the electricity consumption was set to

60 kWh/kg(Catalyst) since Kang and co-workers employed an electrochemical route for CDot preparation.[11] Equipment and operating costs were modelled using the CatCost process template "Metal on Metal Oxide - Strong Electrostatic Adsorption". Using this catalyst costing methodology, a final cost of 890 \$/kg was obtained. Given that particulate photocatalysts are not a well-established technology in industry, the base case catalyst cost was increased to 3000 \$/kg.
For the limit case catalyst cost, the production scale was increased to 100 t/year, which led to a cost reduction to 140 \$/kg. The limit case catalyst cost was therefore set to 100 \$/kg.
CatCost JSON files containing all information for the CatCost models are available in the GitHub repository.

4.1.4 Base and limit parameter values

Four parameters were varied between the base and limit case models: STH efficiency, catalyst concentration, catalyst cost and catalyst lifetime (see Table 4.1-1). Using sensitivity analysis, these were found to have the strongest impact on $LCOH_2$ in the base case model (see Figure 4.2-3).

Table 4.1-1 Parameters varied between base and limit case for photocatalytic water splitting

Parameter	Base value	Limit value
STH efficiency	2%	20%
Catalyst concentration (g(Catalyst)/L)	0.533	0.01
Catalyst cost (\$/kg(Catalyst))	3000	100
Catalyst lifetime (years)	0.5	1

Table 4.1-2 Source/rationale for photocatalytic water splitting base case parameter values

Parameter	Base value	Source/rationale
STH efficiency	2%	Based on STH efficiency of CDot/C_3N_4 catalyst reported in Kang 2015[11]
Catalyst concentration (g(Catalyst)/L)	0.533	Based on catalyst concentration reported in Kang 2015 (80 mg catalyst in 150 ml of water)[11]
Catalyst cost (\$/kg(Catalyst))	3000	Cost estimation using CatCost tool,[10] see Section 4.1.3
Catalyst lifetime (years)	0.5	Based on catalyst lifetime reported in Kang 2015: catalyst was reported to be stable for 45 days of continuous irradiation (assuming eight hours of daily solar irradiation this would be equal to 135 days in operation) and it could also be used for 200 days with daily drying of the catalyst at 60 °C. Hence, a lifetime of ca. six months was assumed.

Table 4.1-3 Source/rationale for photocatalytic water splitting limit case parameter values

Parameter	Limit value	Source/rationale
STH efficiency	20%	The maximum theoretical STH efficiency of dual absorber water splitting photocatalyst is ca. 28%.[12] Since it likely very challenging to fully exhaust this potential a limit value of 20% was assumed.
Catalyst concentration (g(Catalyst)/L)	0.01	The limit catalyst concentration has to be high enough so that most sunlight is still absorbed. To estimate this concentration a model calculation for a homogeneous photocatalyst (which allows for easier calculation of the absorption behavior based on the Beer-Lambert law) was used: assuming a molar mass of 500 g/mol as well as a molar attenuation coefficient of 10,000 $M^{-1}cm^{-1}$ ($[Ru(bpy)_3]^{2+}$ has a maximum molar attenuation coefficient of 14,600 $M^{-1}cm^{-1}$[13]) and given the water height in the reactor of 5 cm in our model, a concentration of 0.01 g/L leads to an absorbance of 1 (meaning that 90% of light is absorbed and 10% is transmitted).
Catalyst cost (\$/kg(Catalyst))	100	Cost estimation using CatCost tool[10] for large catalyst production scale, see Section 4.1.3
Catalyst lifetime (years)	1	Doubling of the base case lifetime to 1 year. Due to the challenging reaction conditions (irradiation, presence of oxygen and water) a relatively short catalyst is assumed even in the limit case.

4.2 Base Case

4.2.1 Cost Breakdown

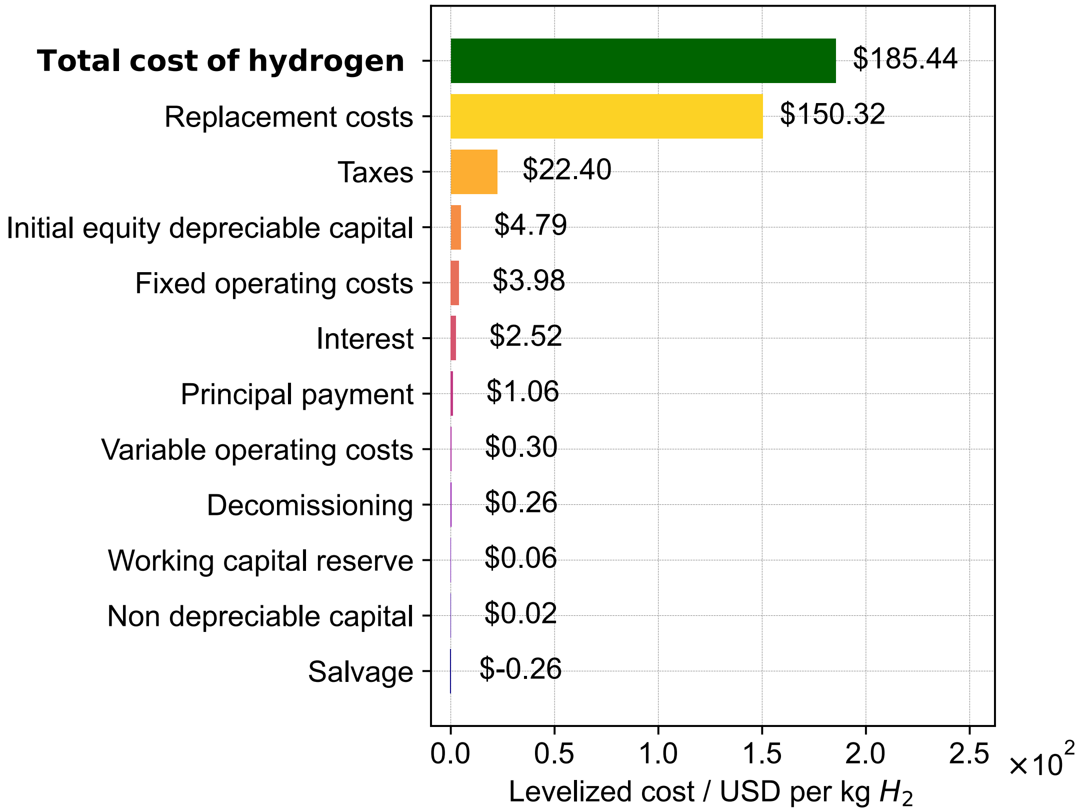


Figure 4.2-1 Overall cost breakdown plot for PC base case

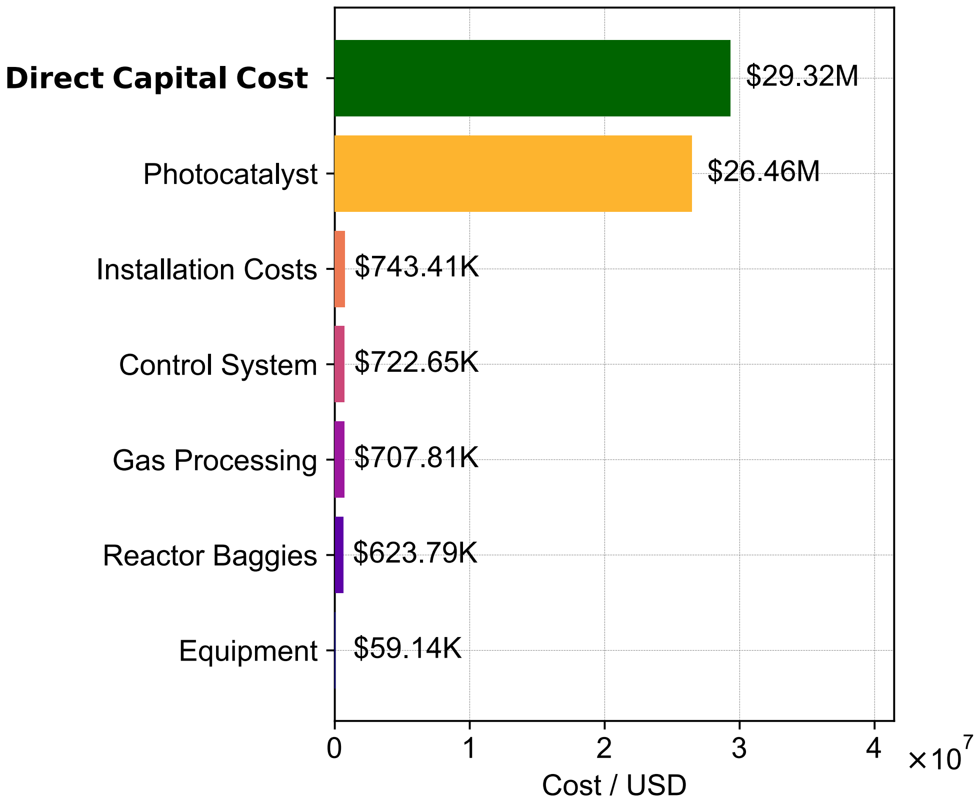


Figure 4.2-2 Capital cost breakdown plot for PC base case

4.2.2 Sensitivity Analysis

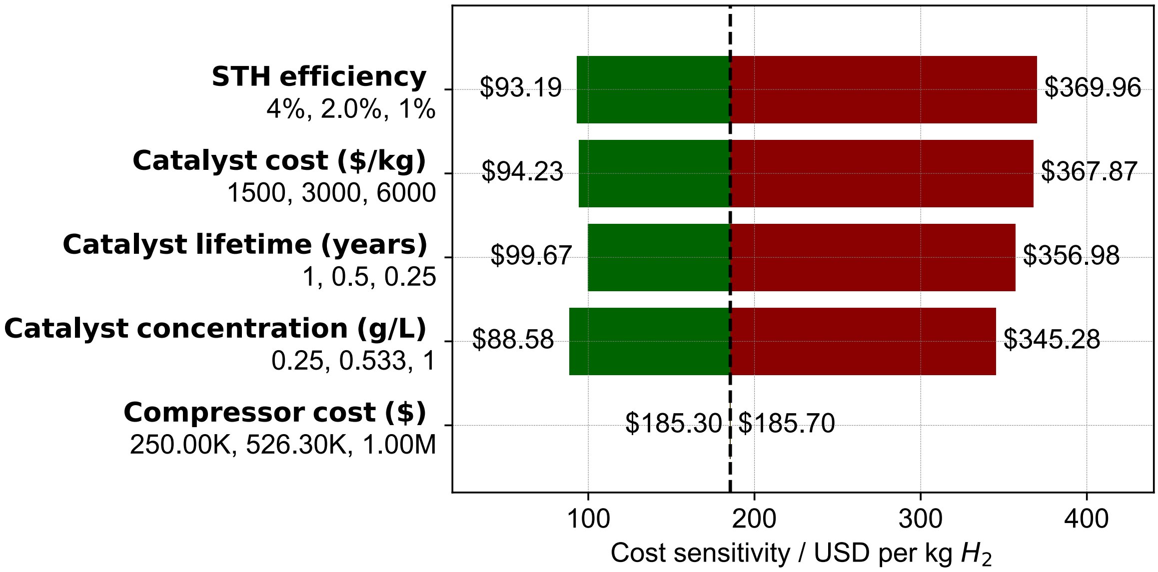


Figure 4.2-3 Sensitivity analysis plot for PC base case

4.3 Limit Case

4.3.1 Cost Breakdown

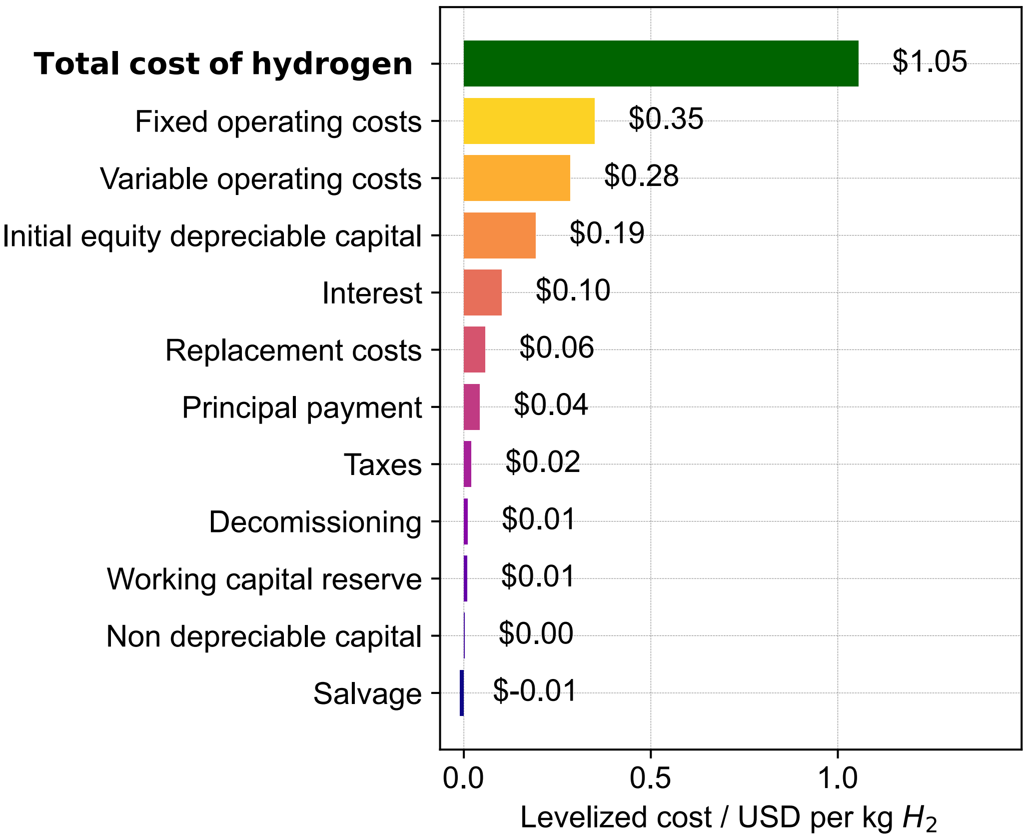


Figure 4.3-1 Overall cost breakdown plot for PC limit case

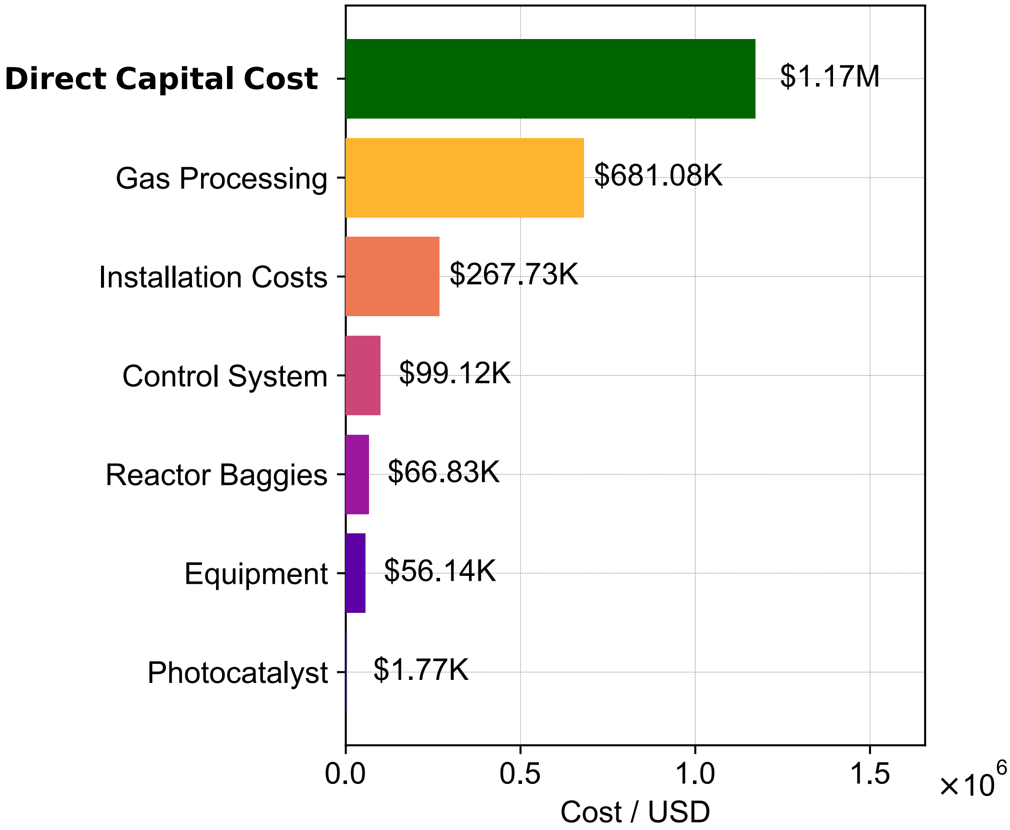


Figure 4.3-2 Capital cost breakdown plot for PC limit case

4.3.2 Sensitivity Analysis

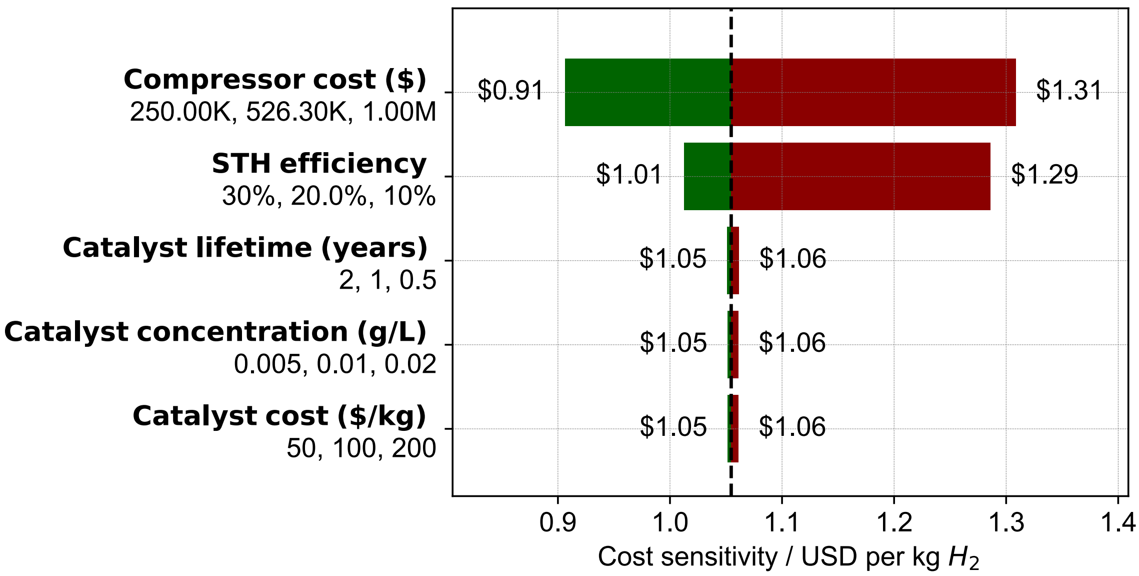


Figure 4.3-3 Sensitivity analysis plot for PC limit case

5 Photovoltaic + Electrolysis (PV+E)

5.1 Model Description

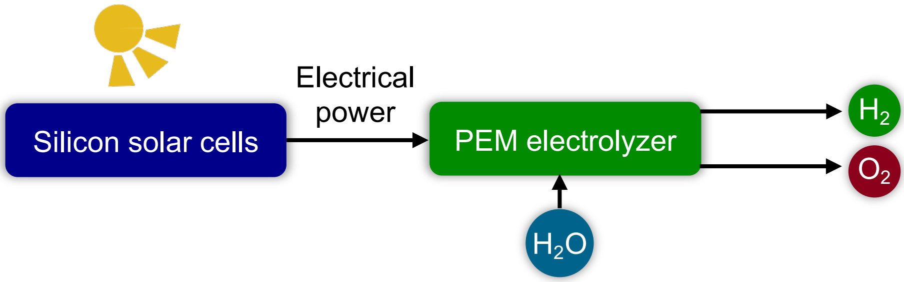


Figure 5.1-1 Simplified process model for photovoltaic + electrolysis (PV+E)

5.1.1 General description

The photovoltaic + electrolysis (PV+E) solar hydrogen production plant assumes the use of bifacial silicon solar cells in a single-axis tracking configuration for power generation. This represents the state-of-the-art for low cost solar electricity production.[14] The solar cells are coupled with a proton-exchange membrane electrolyzer for hydrogen production and the whole plant is operated off-grid (meaning that the solar cells are the only source of power).

5.1.2 Specific plugins and methodology

Combined operation of the solar cells and the electrolyzer is modelled by the "Photovoltaic_Plugin", which uses a methodology based on the one reported by Chang and co-workers.[2] In this model, power produced by the solar cells is used directly by the electrolyzer. Power production is calculated using hourly incident irradiation data. Power produced by the solar cells has to exceed the minimum capacity of the electrolyzer for H_2 production to occur. Furthermore, power exceeding the nominal power of the electrolyzer is wasted and does not contribute to H_2 production. Using this methodology, H_2 production for every hour of the year is calculated. Furthermore, solar cell and electrolyzer degradation over time are taken into account and the resulting decline in H_2 production is modelled over the entire lifetime of the plant. The electrolyzer stacks have a specified lifetime, after which they require replacement. Since only the stacks are replaced, replacement cost is a specified fraction of the total electrolyzer CAPEX.

5.1.3 Base and limit parameter values

Four parameters were varied between the base and limit case models: PV CAPEX, electrolyzer CAPEX, electrolyzer conversion efficiency and electrolyzer stack replacement cost (see Table 5.1-1). Using sensitivity analysis, these were found to have the strongest impact on $LCOH_2$ in the base case model (see Figure 5.2-3).

Table 5.1-1 Parameters varied between base and limit case for PV+E

Parameter	Base value	Limit value
PV CAPEX ($/kW(PV))	818	220
Electrolyzer CAPEX ($/kW(Electrolyzer))	784	200
Electrolyzer conversion efficiency (kg(H_2)/kWh(Electricity))	0.0185	0.025
Electrolyzer Stack replacement cost (% of Electrolyzer CAPEX)	40%	20%

Table 5.1-2 Source/rationale for PV+E base case parameter values

Parameter	Base value	Source/rationale
PV CAPEX ($/kW(PV))	818	Value based on Chang 2020,[2] also in the range of values reported by Chiesa

		2021[14] and Shah 2021[15]
Electrolyzer CAPEX ($/kW(Electrolyzer))	784	Value based on Chang 2020,[2] also in the range reported by IRENA 2020[16] and Shah 2021[15]
Electrolyzer conversion efficiency (kg(H_2)/kWh(Electricity))	0.0185	Value based on Chang 2020[2]
Electrolyzer Stack replacement cost (% of Electrolyzer CAPEX)	40%	Value based on Chang 2020[2]

Table 5.1-3 Source/rationale for PV+E limit case parameter values

Parameter	Limit value	Source/rationale
PV CAPEX ($/kW(PV))	220	Based on Waldau 2021[17] PV CAPEX projection for 2050 (PV module learning rate of 25%, balance of system learning rate of 7.5%, base PV growth scenario)
Electrolyzer CAPEX ($/kW(Electrolyzer))	200	CAPEX reduction to 200 $/kW in 2050 based on IRENA 2020[16] and learning curve model in Waldau 2021[17] (using their cost reduction factor of ca. 4-5 until 2050 due to learning)
Electrolyzer conversion efficiency (kg(H_2)/kWh(Electricity))	0.025	Maximum possible efficiency: 0.02538 kg(H_2)/kWh(Electricity) (see Chang 2020,[2] based on reaction enthalpy), chosen value represents 98.5% of maximum possible efficiency.
Electrolyzer Stack replacement cost (% of Electrolyzer CAPEX)	20%	Halving stack replacement cost from 40% of electrolyzer CAPEX to 20%

5.2 Base Case

5.2.1 Cost Breakdown

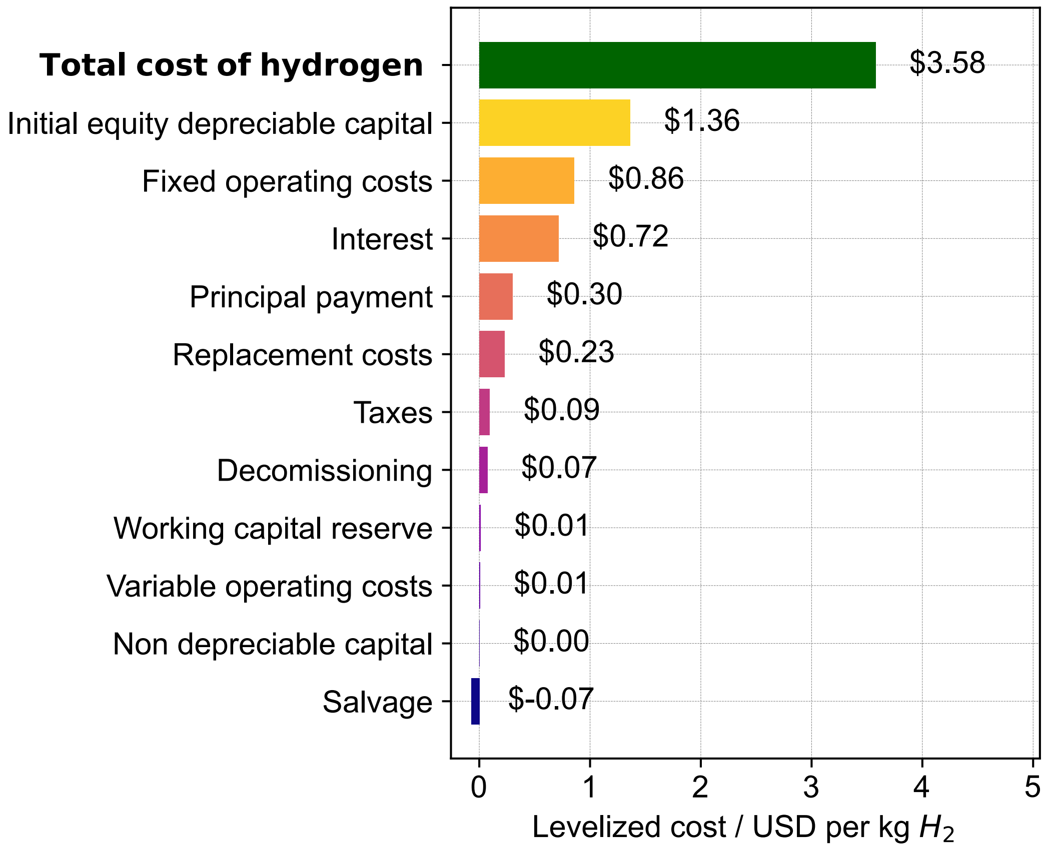


Figure 5.2-1 Overall cost breakdown plot for PV+E base case

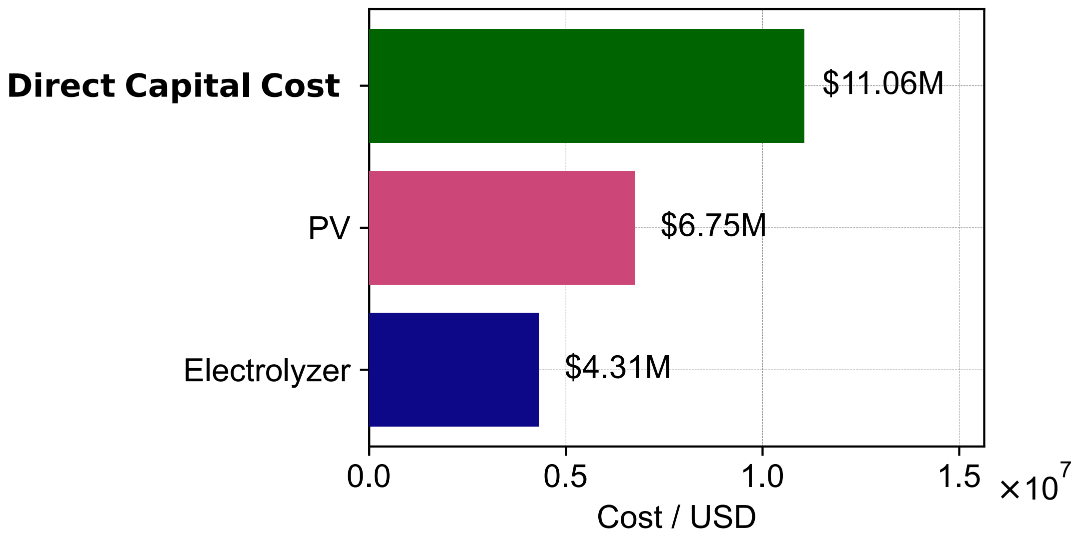


Figure 5.2-2 Capital cost breakdown plot for PV+E base case

5.2.2 Sensitivity Analysis

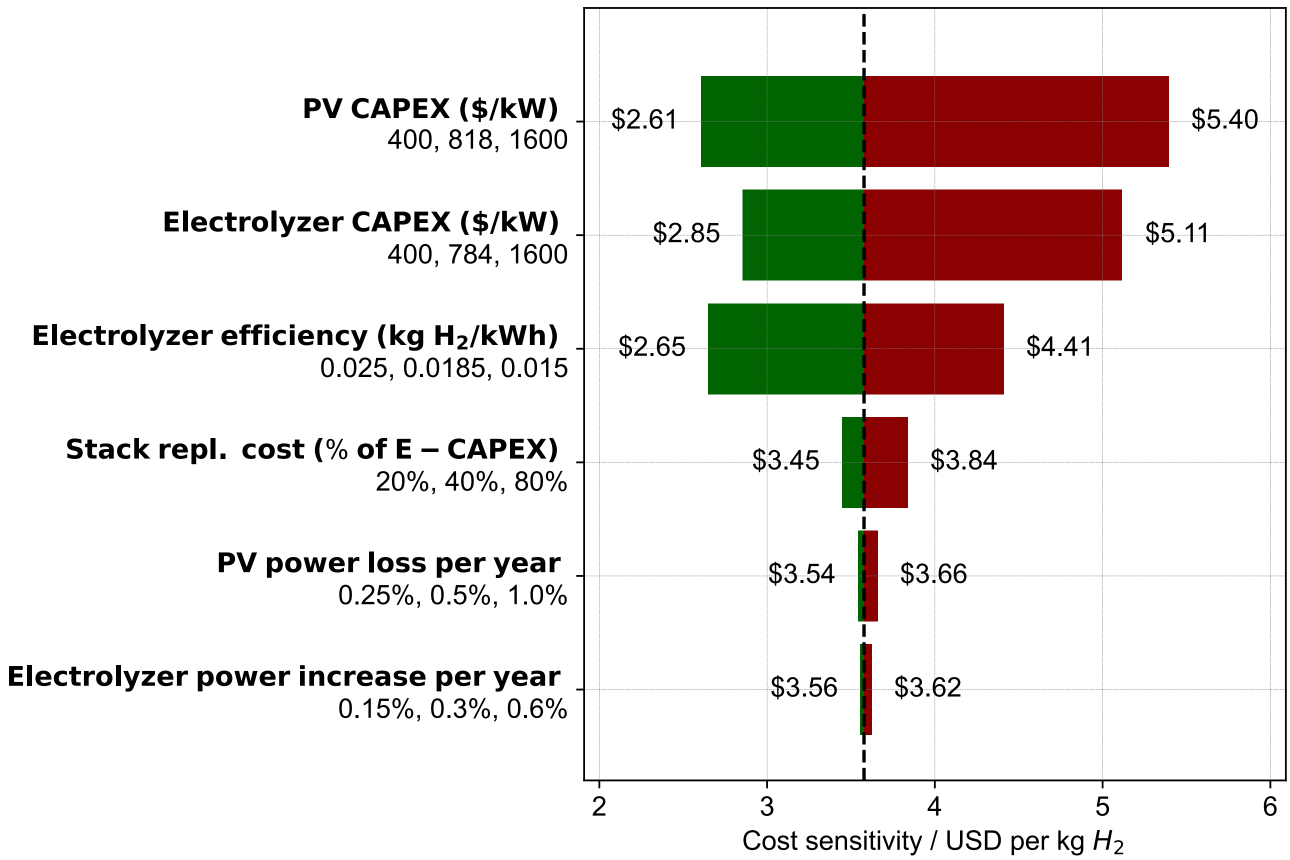


Figure 5.2-3 Sensitivity analysis plot for PV+E base case

5.2.3 Waterfall Analysis

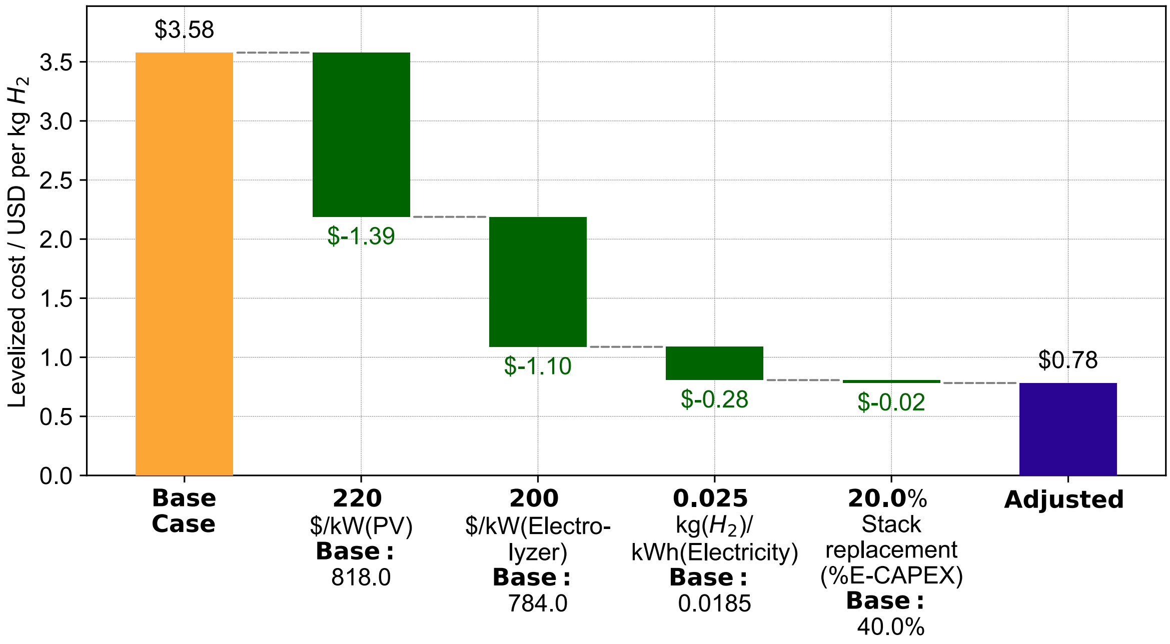


Figure 5.2-4 Waterfall analysis plot for PV+E base case transitioning to limit case

5.3 Limit Case

5.3.1 Cost Breakdown

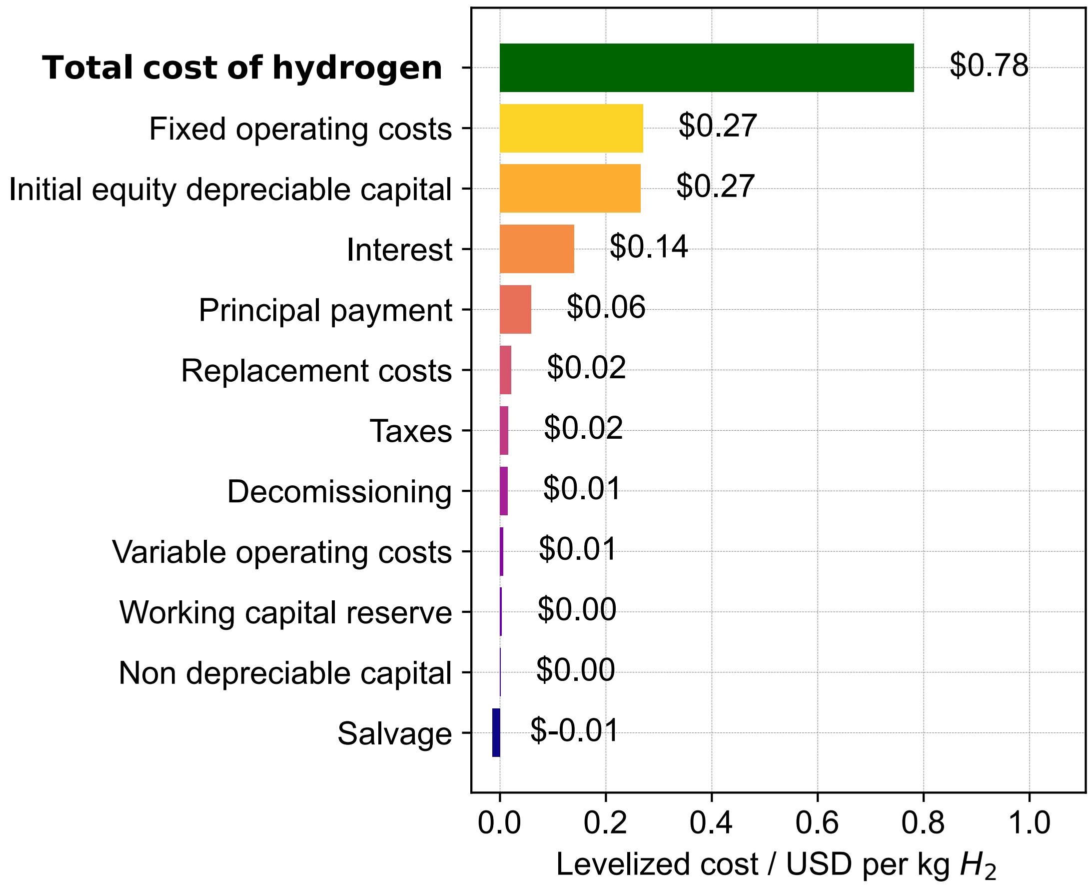


Figure 5.3-1 Overall cost breakdown plot for PV+E limit case

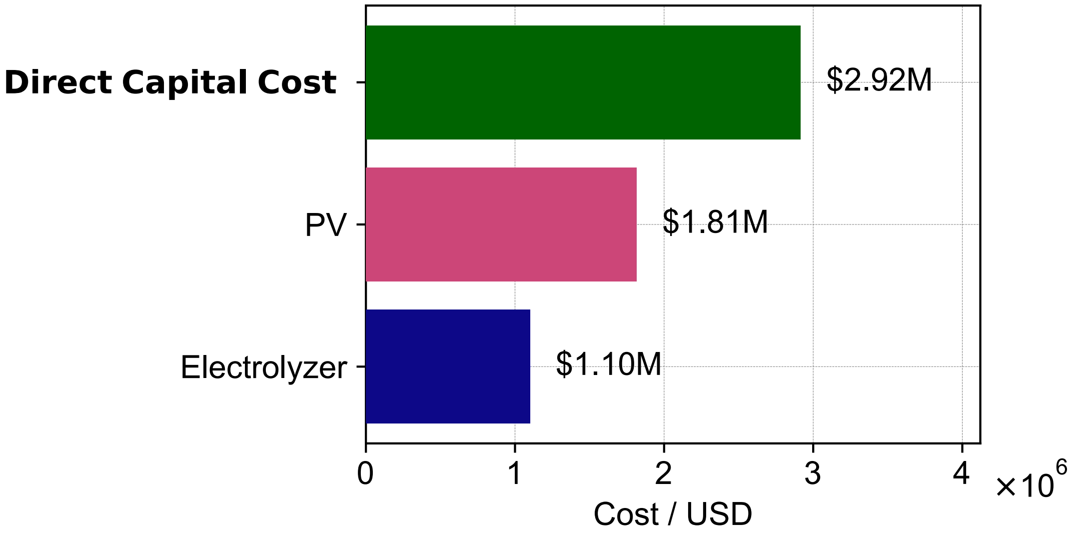


Figure 5.3-2 Capital cost breakdown plot for PV+E limit case

5.3.2 Sensitivity Analysis

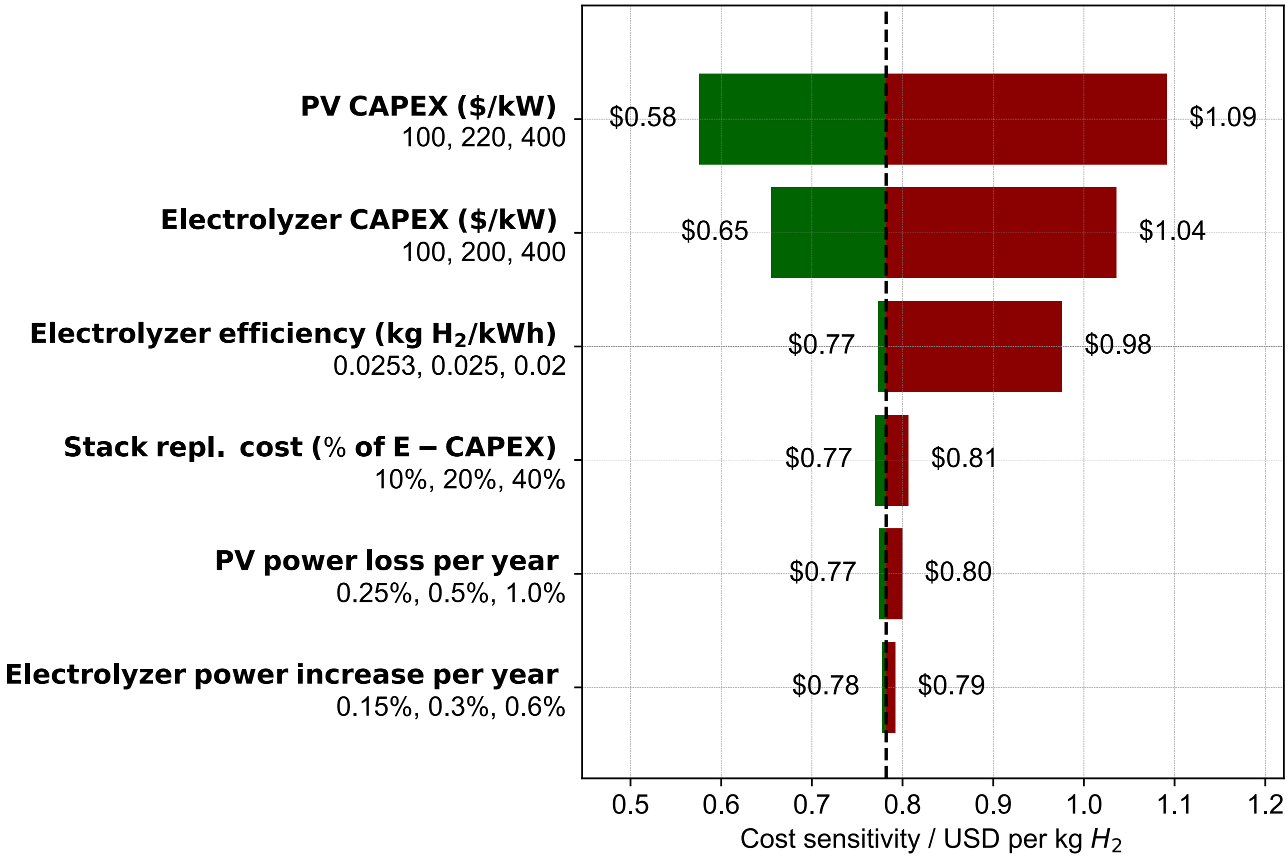


Figure 5.3-3 Sensitivity analysis plot for PV+E limit case

5.4 Historical Data and Development Distance/Time Relationship

5.4.1 Historical data for PV+E

The four parameters used for Monte Carlo analysis and development distance calculations are PV CAPEX (\$/kW(PV)), electrolyzer CAPEX (\$/kW(Electrolyzer)), conversion efficiency (kg(H_2)/kWh(Electricity)) and stack replacement cost (as a fraction of electrolyzer CAPEX). Hence, historical data for each parameter was sourced to calculate the historical development distances.

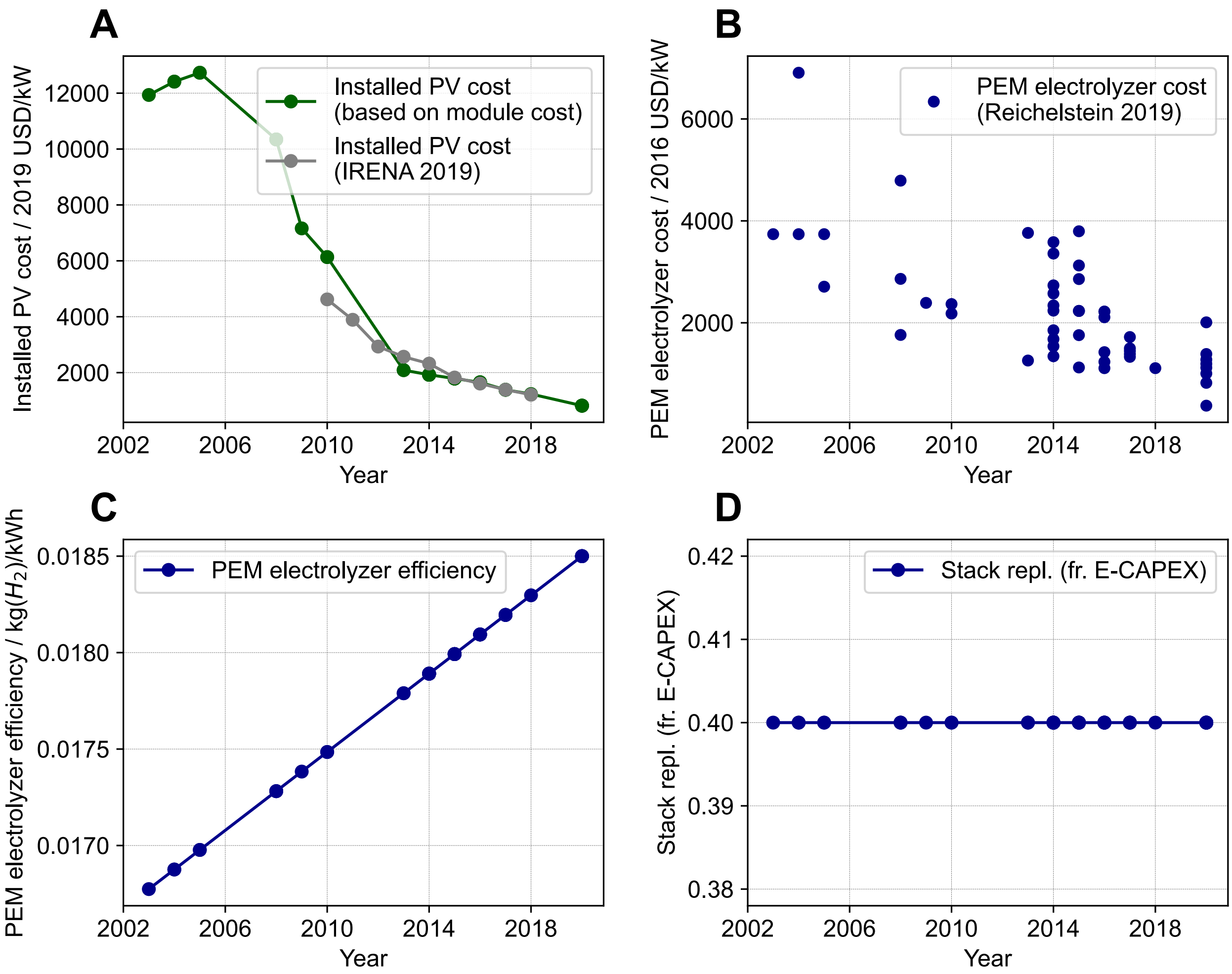


Figure 5.4-1 Historical parameter values for PV+E used for development distance/time analysis
PV cost data is sourced from Lafond *et al.*[18] and IRENA.[19] PEM cost data is from Glenk and Reichelstein.[20] Stack repl. (fr. E-CAPEX) stands for stack replacement cost as a fraction of electrolyzer CAPEX.

PV CAPEX data was calculated using solar module cost data from Lafond *et al.*[18] as well as the 2019 IRENA report on renewable power generation costs.[19] Solar module cost is only one component of the total installed PV CAPEX (which also includes balance of systems components, installation costs etc.). While these other costs differ between countries, solar module cost constitutes on average around 30 – 35% of total PV CAPEX.[19] Hence, PV CAPEX was calculated by multiplying solar module cost by a factor of 3. The thus obtained data is in good agreement with the global average of installed PV cost reported by IRENA (see Figure 5.4-1A),[19] but with the advantage of extending back to 2003.

Historical PEM electrolyzer CAPEX data was obtained from Glenk and Reichelstein.[20] In their study, the authors collected historical PEM cost values from various previous studies, hence there are multiple cost estimates for a given year (see Figure 5.4-1B). All datapoints were used for the subsequent analysis.

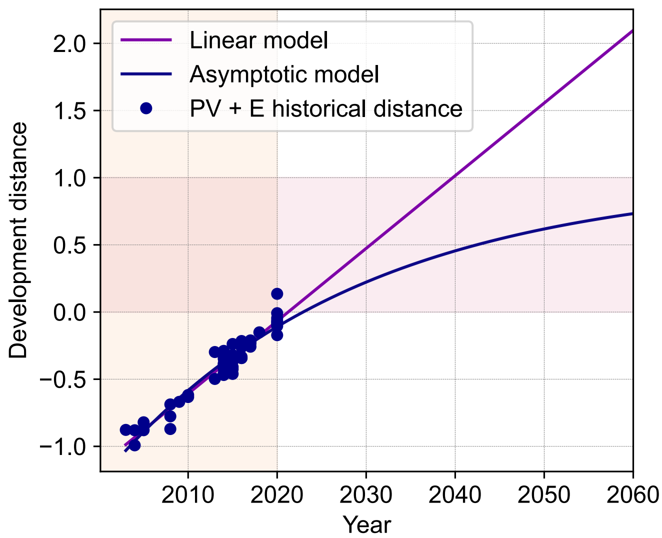
PEM cell efficiency has not significantly improved over time based on performance metrics reported in the academic literature.[21] However, the performance history of research devices may not reflect the trends for industrial electrolyzers. Vartiainen *et al.*[17] assumed an annual efficiency increase of 0.3% points for alkaline electrolyzers. For the present analysis, it was assumed that PEM cell efficiency has historically improved by 0.4% points per year (since PEM electrolyzers usually outperform alkaline electrolyzers in terms of efficiency). The reference for estimating PEM cell efficiency is an efficiency of 0.0185 kg(H_2)/kWh(Electricity) (base value) in 2020.

For stack replacement cost, it was assumed that it has remained unchanged for the studied time period, being the same as the base value (40% of electrolyzer CAPEX).

All of the data which has been used for the present analysis is shown in Figure 5.4-1. It covers a timespan from 2003 to 2020.

5.4.2 Historical development distance and model fitting

Using the historical parameter values, the historical development distance was calculated as described in Section 2.4.4.6. Furthermore, a linear as well as an asymptotic model were fitted to the data and extrapolated into the future. These results are shown in Figure 5.4-2.

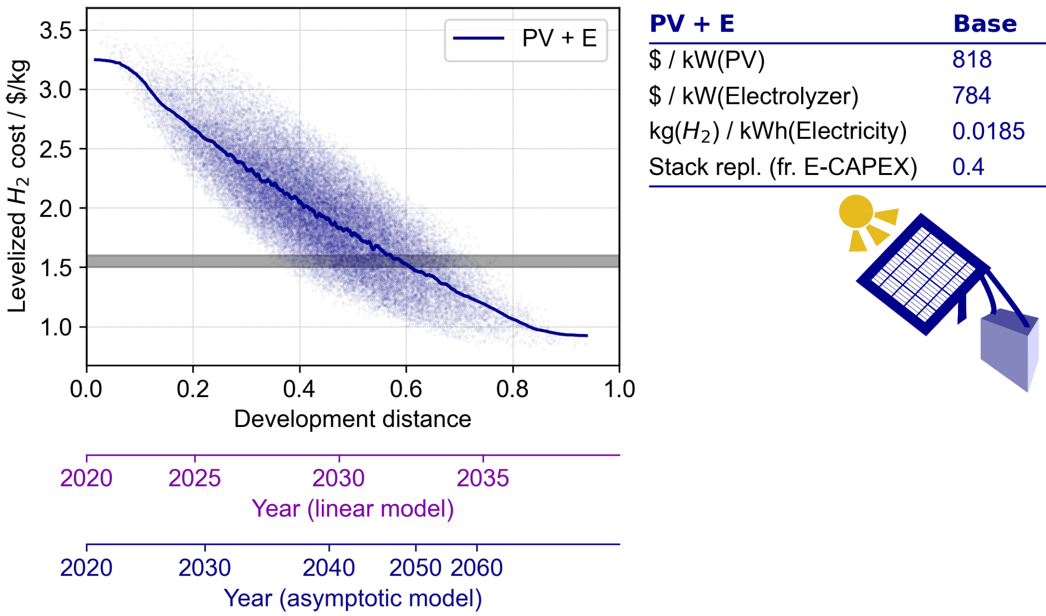


PV + E	Base	Limit
$ / kW(PV)	818	⟶ 220
$ / kW(Electrolyzer)	784	⟶ 200
kg(H_2) / kWh(Electricity)	0.0185	⟶ 0.025
Stack repl. (fr. E-CAPEX)	0.4	⟶ 0.2

Figure 5.4-2 Historical development distance and fit of linear and asymptotic models
The development distance region from 0 to 1 is highlighted, as well as the future region, into which the models are extrapolated. The parameters which constitute the development distance and their base as well as limit values are shown in the table on the right.

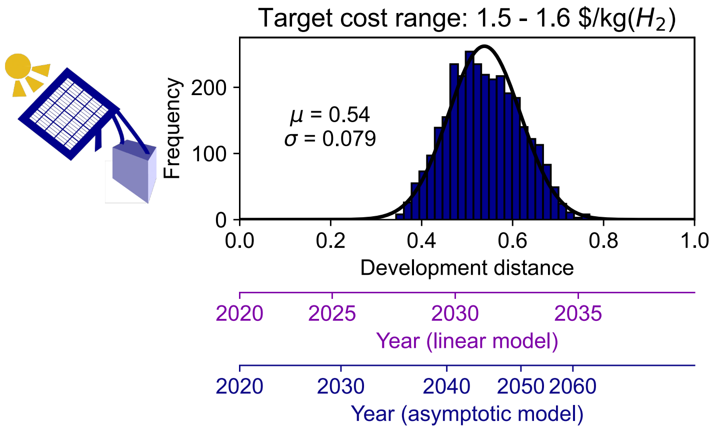
5.4.3 Mapping of development distance to time for Monte Carlo plots

Using the linear and asymptotic models, development distances between 0 and 1 were mapped to future years. This mapping is shown for the PV+E development distance/time plot (Figure 5.4-3) and development distance histogram (Figure 5.4-4).



PV + E	Base	Limit
$ / kW(PV)	818	⟶ 220
$ / kW(Electrolyzer)	784	⟶ 200
kg(H_2) / kWh(Electricity)	0.0185	⟶ 0.025
Stack repl. (fr. E-CAPEX)	0.4	⟶ 0.2

Figure 5.4-3 Development distance/time plot for PV+E with mapping of distances to years
Logarithmic instead of linear normalization was used to calculate the Monte Carlo distances. The parameters which constitute the development distance and their base as well as limit values are shown in the table on the right.



PV + E	Base	Limit
$ / kW(PV)	818	⟶ 220
$ / kW(Electrolyzer)	784	⟶ 200
kg(H_2) / kWh(Electricity)	0.0185	⟶ 0.025
Stack repl. (fr. E-CAPEX)	0.4	⟶ 0.2

Figure 5.4-4 Development distance histogram for PV+E with mapping of distances to years
Logarithmic instead of linear normalization was used to calculate the Monte Carlo distances, leading to slightly different μ and σ values. The parameters which constitute the development distance and their base as well as limit values are shown in the table on the right.

6 Input Parameters

In the following, the detailed input parameters for each techno-economic model are shown. pyH2A uses Markdown formatted input files which were converted to formatted tables for presentation herein. The original Markdown input files are available at https://github.com/jschneidewind/pyH2A.

Shown are the input parameters for the base case models (except for PEC without solar concentration, PEC type 3, for which the limit case model is shown). The limit case models are identical to the base case models except that the limit values for the varied parameters are used. These parameters and their respective limit values are shown in the “Parameters - Monte_Carlo_Analysis” table for each model.

A note on notation used in the input tables: in most cases, the “Value” column contains the specific input parameter value. Instead of an actual parameter value, it may also contain a path to reference another parameter value. Paths use the format “table name > row > column”. If an input table contains a separate “Path” column, the referenced value in “Path” is multiplied by the value in “Value”.

6.1 References used in Input Tables

The input tables contain additional comments/descriptions which also contain references to the literature. The following table maps these references (which are in *author*, *year* format) to the references used in this document.

Table 6.1-1 Mapping of input file references

Input file reference	Numbered reference in document
Chang 2020	[2]
Chiesa 2021	[14]
Costa 2006	[22]
Driess 2021	[23]
Filas 2018	[8]
Gharbi 2011	[7]
Hellgardt 2018	[9]
Horowitz 2018	[6]
Idriss 2020	[5]
IRENA 2020	[16]
Kang 2015	[11]
Kibria 2021	[24]
Kistler 2020	[4]
Pinaud 2013	[1]
Schneidewind 2021	[12]
Shah 2021	[15]
Stolten 2020	[25]
Tremblay 2020	[26]
Waldau 2021	[17]
Zhao 2021	[27]

6.2 Workflow and Financial Input Parameters

Workflow and financial input parameters are shared by all techno-economic models. Models add specific plugins to the workflow, but the core workflow shown below is shared by all models.

Workflow

Name	Type	Position	Description
Production_Scaling_Plugin	plugin	1	Computes plant output and scaling factors (if scaling is requested)
production_scaling	function	2	core function to process yearly plant output
Capital_Cost_Plugin	plugin	3	Calculation of direct, indirect and non-depreciable capital costs
initial_equity_depreciable_capital	function	4	core function to process depreciable capital costs
non_depreciable_capital_costs	function	5	core function to process non-depreciable capital costs
Replacement_Plugin	plugin	6	Calculation of replacement costs
replacement_costs	function	7	core function to process replacement costs
Fixed_Operating_Cost_Plugin	plugin	8	Calculation of fixed operating costs
fixed_operating_costs	function	9	core function to process fixed operating costs
Variable_Operating_Cost_Plugin	plugin	10	Calculation of variable operating costs, including utilities
variable_operating_costs	function	11	core function to process variable operating costs

Financial Input Values

Name	Full Name	Value
ref year	Reference year	2016
startup year	Assumed start-up year	2020
basis year	Basis year	2016
current year capital costs	Current year for capital costs	2016
startup time	Start-up Time (years)	1
plant life	Plant life (years)	20
depreciation length	Depreciation Schedule Length (years)	20
depreciation type	Depreciation Type	MACRS
equity	% Equity Financing	40%
interest	Interest rate on debt (%)	3.7%
debt	Debt period	Constant
startup cost fixed	% of Fixed Operating Costs During Start-up	100%
startup revenues	% of Revenues During Start-up	75%
startup cost variable	% of Variable Operating Costs During Start-up	75%
decommissioning	Decommissioning costs (% of depreciable capital investment)	10%
salvage	Salvage value (% of total capital investment)	10%
inflation	Inflation rate (%)	1.9%
irr	After-tax Real IRR (%)	8.0%
state tax	State Taxes (%)	6.0%
federal tax	Federal Taxes (%)	21.0%
working capital	Working Capital (% of yearly change in operating costs)	15.0%

6.3 Photoelectrochemical Water Splitting (PEC)

Workflow

Name	Type	Description	Position
Hourly_Irradiation_Plugin	plugin	Plugin to calculate solar irradiation from typical meteorological year data	0
PEC_Plugin	plugin	Plugin to model photoelectrochemical water splitting	2
Solar_Concentrator_Plugin	plugin	Plugin to model solar concentration	2
Multiple_Modules_Plugin	plugin	Modelling of module plant modules, adjustment of labor requirement	3

Display Parameters

Name	Value
Name	PEC Type 4
Color	darkred

Technical Operating Parameters and Specifications

Name	Value	Path	Full Name
Operating Capacity Factor (%)	90.0%		
Plant Design Capacity (kg of H2/day)	1,000		
Plant Modules	10	None	10 identical modules, only affects labor requirement calculation.

Construction

Name	Full Name	Value
capital perc 1st	% of Capital Spent in 1st Year of Construction	100%

Hourly Irradiation

Name	Value	Comment
File	pyH2A.Lookup_Tables.Hourly_Irradiation_Data~tmy_34.859_-116.889_2006_2015.csv	Location: Dagget, CA, USA

Irradiance Area Parameters

Name	Value	Comment
Module Tilt (degrees)	0	Two axis tracking, module tilt and array azimuth change are not relevant.
Array Azimuth (degrees)	0	
Nominal Operating Temperature (Celcius)	45	Temperature is stabilized even under solar concentration through intrinsic water cooling.
Mismatch Derating	98%	
Dirt Derating	98%	Values taken from Chang 2020, analogues to silicon PV.
Temperature Coefficienct (per Celcius)	0.0%	No assumed efficiency loss with higher temperature.

Solar Input

Name	Value	Path	Comment
Mean solar input (kWh/m2/day)	Hourly Irradiation > Mean solar input two axis tracking	Solar Concentrator > Concentration Factor >	Two axis tracking irradiation from hourly irradiation multiplied by solar

Name	Value	Path	Comment
	(kWh/m2/day) > Value	Value	concentration factor to give solar input incident on PEC cells.

Solar-to-Hydrogen Efficiency

Name	Value	Comment
STH (%)	14.0%	Reference Kistler 2020, 14% STH (Note: vapor-fed device used in reference, techno-economic analysis assumes liquid phase design, no solar concentration); alternative reference: Idriss 2020, 18% STH at 15 suns, 13% STH at 200 suns (triple junction III-V cell based system).

PEC Cells

Name	Value	Comment
Cell Cost ($/m2)	21,000.0	Price of III-V solar cells as reference, approximate $/W to $/m2 conversion formula: Cost ($/W) * conversion_efficiency (%) * 1000 W/m2 = Cost ($/m2), Reference: Horowitz 2018 (NREL), 70 $/W, assuming 30% efficiency = 21,000 $/m2.
Lifetime (years)	0.33	Should consider operational lifetime (irradiation for only 8 h per day), baseline 1000 h operation time (reference: Kistler 2020), 3000 h total, 0.3 years.
Length (m)	6	Based on sizing in Pinaud 2013.
Width (m)	0.3	Based on sizing in Pinaud 2013.

Solar Concentrator

Name	Value	Comment
Concentration Factor	50	Concentration factor increased from 10 (Pinaud 2013) to 50 due to high PEC cell cost, within range of typical parabolic trough concentrators, see Gharbi 2011.
Cost ($/m2)	100	100 $/m2 parabolic trough concentrator cost based on Filas 2018.

Land Area Requirement

Name	Value	Comment
Cell Angle (degree)	35	Used for total land area calculation.
South Spacing (m)	6.71	
East/West Spacing (m)	17.3	

Direct Capital Costs - Water Management

Name	Value	Path	Comment
Water pump ($)	213.0	None	Based on Pinaud 2013.
Water Manifold Piping ($ per cell)	11.58	PEC Cells > Number > Value	
Water Collection Piping ($ per cell)	1.502	PEC Cells > Number > Value	
Water Column Collection Piping ($ per cell)	1.1015	PEC Cells > Number > Value	
Water Final Collection Piping ($ per cell)	0.231	PEC Cells > Number > Value	

Direct Capital Costs - Gas Processing

Name	Value	Path	Comment
Condenser ($)	7,098.0	None	Based on Pinaud 2013.
Manifold Piping ($ per cell)	11.58	PEC Cells > Number > Value	

Name	Value	Path	Comment
Collection Piping ($ per cell)	1.502	PEC Cells > Number > Value	
Column Collection Piping ($ per cell)	1.1015	PEC Cells > Number > Value	
Final Collection Piping ($ per cell)	0.231	PEC Cells > Number > Value	

Direct Capital Costs - Control System

Name	Path	Value	Comment
PLC ($)	None	3,000.0	Based on Pinaud 2013.
Control Room Building ($)	None	17,527.0	
Control Room Wiring Panel ($)	None	3,000.0	
Computer and Monitor ($)	None	1,500.0	
Labview Software ($)	None	4,299.0	
Water Level Controllers (cost per cell, $)	PEC Cells > Number > Value	50.0	
Pressure Sensors (cost per cell, $)	PEC Cells > Number > Value	3.333	
Hydrogen Area Sensors (cost per cell, $)	PEC Cells > Number > Value	73.42	
Hydrogen Flow Meter ($)	None	5,500.0	
Instrument Wiring (cost per cell, $)	PEC Cells > Number > Value	0.252	
Power Wiring (cost per cell, $)	PEC Cells > Number > Value	0.1256	
Conduit (cost per cell, $)	PEC Cells > Number > Value	3.759	

Direct Capital Costs - Installation Costs

Name	Path	Value	Comment
Piping Installation (per cell, $)	PEC Cells > Number > Value	5.65	Based on Pinaud 2013.
Reactor Installation (per m2 of solar collection area)	Non-Depreciable Capital Costs > Solar Collection Area (m2) > Value	22.0	
Pump Installation (% of pump cost)	Direct Capital Costs - Water Management > Water pump ($) > Value	30%	
Gas processing installation (% of gas processing cost)	Direct Capital Costs - Gas Processing > Summed Total > Value	30%	
Control system installation (% of control system cost)	Direct Capital Costs - Control System > Summed Total > Value	30%	

Indirect Capital Costs

Name	Path	Value	Comment
Engineering and Design (% of total direct capital costs)	Direct Capital Costs > Total > Value	7%	Based on Pinaud 2013.
Process Contingency (% of total direct capital costs)	Direct Capital Costs > Total > Value	20.0%	
Up-Front Permitting Costs (% of total direct capital costs)	Direct Capital Costs > Total > Value	0.5%	
Site Preparation (% of total direct capital costs)	Direct Capital Costs > Total > Value	1%	

Non-Depreciable Capital Costs

Name	Value	Comment
Cost of land ($ per acre)	500.0	Land cost based on Pinaud 2013.

Fixed Operating Costs

Name	Full Name	Value	Comment
area	Area per staff (m2)	60,000	Based on Pinaud et al. 2013, smaller area per staff compared to PV+E and photocatalytic model due to smaller size of individual units, more connections and sensors.
supervisor	Shift supervisor	1	Number of shift supervisors.
shifts	Shifts	3	Number of shifts per day.
hourly labor cost	Burdened labor cost, including overhead ($ per man-hr)	50.0	

Other Fixed Operating Costs

Name	Full Name	Path	Value	Comment
g&a	G&A rate (% of labor cost)	Fixed Operating Costs > Labor Cost > Value	20.0%	Based on Pinaud 2013.
property tax	Property tax and insurance rate (% of total capital investment per year)	Total Capital Costs > Inflated > Value	2.0%	
repairs	Production Maintenance and Repairs (% of direct capital costs)	Direct Capital Costs > Total > Value	0.5%	
fees	Licensing, Permits and Fees ($ per year)	None	1000.0	

Utilities

Name	Usage per kg H2	Usage Unit	Cost	Cost Unit	Price Conversion Factor	Price Conversion Factor Unit	Comment
Industrial Electricity	0.16	kWh/kg H2	pyH2A.Lookup_Tables. Utility_Cost~Industrial_ Electricity_AEO_2017_ Reference_Case.csv	GJ	0.0036	GJ/kWh	Electricity usage based on Pinaud 2013.
Process Water	2.369	gal/kg H2	0.0023749510945008	$(2016)/gal	1.	None	Seawater reverse osmosis cost ca. 0.6 $/m3 (equal to ca. 0.0023 $/gal), based on Kibria 2021 and Driess 2021.

Unplanned Replacement

Name	Full Name	Path	Value	Comment
unplanned replacement	Total Unplanned Replacement Capital Cost Factor (% of total direct depreciable costs/year)	Depreciable Capital Costs > Inflated > Value	0.5%	Based on Pinaud 2013.

Sensitivity_Analysis

Parameter	Name	Type	Values
Solar-to-Hydrogen Efficiency > STH (%) > Value	STH efficiency	value	7%; 28%
PEC Cells > Cell Cost ($/m2) > Value	PEC cell cost ($/m^{2})	value	10,500; 42,000

Parameter	Name	Type	Values
PEC Cells > Lifetime (years) > Value	PEC cell lifetime (years)	value	0.15; 0.7
Solar Concentrator > Cost ($/m2) > Value	Solar concentrator cost ($/m^{2})	value	50; 200
Solar Concentrator > Concentration Factor > Value	Solar concentration factor	value	25; 100

Monte_Carlo_Analysis

Name	Value	Comment
Samples	50000	Number of samples in Monte Carlo simulation.
Target Price Range ($)	1.5; 1.6	
Input File	./PEC/Base/Monte_Carlo_Output.csv	

Parameters - Monte_Carlo_Analysis

Parameter	Name	Type	Values	File Index	Comment
Solar-to-Hydrogen Efficiency > STH (%) > Value	STH efficiency	value	Base; 30%	0	Practical STH efficiency is the product of solar concentrator efficiency (ca. 76% for state-of-the-art parabolic trough concentrator, see Filas 2018) and PEC STH efficiency (maximum possible STH efficiency ca. 40% for multi junction device based on Hellgardt 2018). Maximum practical STH efficiency therefore estimated to be ca. 30%.
PEC Cells > Cell Cost ($/m2) > Value	$ / m^{2}(PEC Cell)	value	700.0; Base	1	30-fold price reduction for PEC cells analogous to 30-fold reduction of photocatalyst cost in photocatalytic model.
PEC Cells > Lifetime (years) > Value	Cell lifetime / years	value	Base; 3	2	9-fold lifetime improvement relative to state of the art (0.33 years).
Solar Concentrator > Concentration Factor > Value	Solar concentration factor	value	Base; 100	3	Doubling solar concentration factor, upper range of parabolic trough concentrators (see Gharbi 2021).

6.4 PEC without Solar Concentration (PEC Type 3)

Workflow

Name	Type	Description	Position
Hourly_Irradiation_Plugin	plugin	Plugin to calculate solar irradiation from typical meteorological year data	0
PEC_Plugin	plugin	Plugin to model photoelectrochemical water splitting	2
Multiple_Modules_Plugin	plugin	Modelling of module plant modules, adjustment of labor requirement	3

Display Parameters

Name	Value
Name	PEC Type 3
Color	darkred

Technical Operating Parameters and Specifications

Name	Value	Path	Full Name
Operating Capacity Factor (%)	90.0%		
Plant Design Capacity (kg of H2/day)	1,000		
Plant Modules	10	None	10 identical modules, only affects labor requirement calculation.

Construction

Name	Full Name	Value
capital perc 1st	% of Capital Spent in 1st Year of Construction	100%

Hourly Irradiation

Name	Value	Comment
File	pyH2A.Lookup_Tables.Hourly_Irradiation_Data~tmy_34.859_-116.889_2006_2015.csv	Location: Dagget, CA, USA

Irradiance Area Parameters

Name	Value	Comment
Module Tilt (degrees)	0	Two axis tracking, module tilt and array azimuth change are not relevant.
Array Azimuth (degrees)	0	
Nominal Operating Temperature (Celsius)	45	Temperature is stabilized by intrinsic water cooling.
Mismatch Derating	98%	
Dirt Derating	98%	Values taken from Chang 2020, analogues to silicon PV
Temperature Coefficient (per Celsius)	0.0%	No assumed efficiency loss with higher temperature.

Solar Input

Name	Value	Path	Comment
Mean solar input (kWh/m2/day)	Hourly Irradiation > Mean solar input two axis tracking (kWh/m2/day) > Value	None	Two axis tracking irradiation from hourly irradiation data.

Solar-to-Hydrogen Efficiency

Name	Value	Comment
STH (%)	30.0%	30% STH Limit value from PEC Type 4 model (maximum possible STH efficiency ca. 40% for multi junction device based on Hellgardt 2018).

PEC Cells

Name	Value	Comment
Cell Cost ($/m2)	700.0	Price of III-V solar cells as reference, approximate $/W to $/m2 conversion formula: Cost ($/W) * conversion_efficiency (%) * 1000 W/m2 = Cost ($/m2), Reference: Horowitz 2018 (NREL), 70 $/W, assuming 30% efficiency = 21,000 $/m2. 30-fold cost reduction analogous to 30-fold cost reduction for photocatalyst in photocatalytic model.
Lifetime (years)	3.0	9-fold lifetime increase relative to base case (0.33 years).
Length (m)	6	Based on sizing in Pinaud 2013.
Width (m)	0.3	Based on sizing in Pinaud 2013.

Land Area Requirement

Name	Value	Comment
Cell Angle (degree)	35	Used for total land area calculation.
South Spacing (m)	6.71	
East/West Spacing (m)	17.3	

Direct Capital Costs - Water Management

Name	Value	Path	Comment
Water pump ($)	213.0	None	Based on Pinaud 2013.
Water Manifold Piping ($ per cell)	11.58	PEC Cells > Number > Value	
Water Collection Piping ($ per cell)	1.502	PEC Cells > Number > Value	
Water Column Collection Piping ($ per cell)	1.1015	PEC Cells > Number > Value	
Water Final Collection Piping ($ per cell)	0.231	PEC Cells > Number > Value	

Direct Capital Costs - Gas Processing

Name	Value	Path	Comment
Condenser ($)	7,098.0	None	Based on Pinaud 2013.
Manifold Piping ($ per cell)	11.58	PEC Cells > Number > Value	
Collection Piping ($ per cell)	1.502	PEC Cells > Number > Value	
Column Collection Piping ($ per cell)	1.1015	PEC Cells > Number > Value	
Final Collection Piping ($ per cell)	0.231	PEC Cells > Number > Value	

Direct Capital Costs - Control System

Name	Path	Value	Comment
PLC ($)	None	3,000.0	Based on Pinaud 2013.
Control Room Building ($)	None	17,527.0	
Control Room Wiring Panel ($)	None	3,000.0	
Computer and Monitor ($)	None	1,500.0	

Name	Path	Value	Comment
Labview Software ($)	None	4,299.0	
Water Level Controllers (cost per cell, $)	PEC Cells > Number > Value	50.0	
Pressure Sensors (cost per cell, $)	PEC Cells > Number > Value	3.333	
Hydrogen Area Sensors (cost per cell, $)	PEC Cells > Number > Value	73.42	
Hydrogen Flow Meter ($)	None	5,500.0	
Instrument Wiring (cost per cell, $)	PEC Cells > Number > Value	0.252	
Power Wiring (cost per cell, $)	PEC Cells > Number > Value	0.1256	
Conduit (cost per cell, $)	PEC Cells > Number > Value	3.759	

Direct Capital Costs - Installation Costs

Name	Path	Value	Comment
Piping Installation (per cell, $)	PEC Cells > Number > Value	5.65	Based on Pinaud 2013.
Reactor Installation (per m2 of solar collection area)	Non-Depreciable Capital Costs > Solar Collection Area (m2) > Value	22.0	
Pump Installation (% of pump cost)	Direct Capital Costs - Water Management > Water pump ($) > Value	30%	
Gas processing installation (% of gas processing cost)	Direct Capital Costs - Gas Processing > Summed Total > Value	30%	
Control system installation (% of control system cost)	Direct Capital Costs - Control System > Summed Total > Value	30%	

Indirect Capital Costs

Name	Path	Value	Comment
Engineering and Design (% of total direct capital costs)	Direct Capital Costs > Total > Value	7%	Based on Pinaud 2013.
Process Contingency (% of total direct capital costs)	Direct Capital Costs > Total > Value	20.0%	
Up-Front Permitting Costs (% of total direct capital costs)	Direct Capital Costs > Total > Value	0.5%	
Site Preparation (% of total direct capital costs)	Direct Capital Costs > Total > Value	1%	

Non-Depreciable Capital Costs

Name	Value	Comment
Cost of land ($ per acre)	500.0	Land cost based on Pinaud 2013.

Fixed Operating Costs

Name	Full Name	Value	Comment
area	Area per staff (m2)	60,000	Based on Pinaud et al. 2013, smaller area per staff compared to PV+E and photocatalytic model due to smaller size of individual units, more connections and sensors.
supervisor	Shift supervisor	1	
shifts	Shifts	3	
hourly labor cost	Burdened labor cost, including overhead ($ per	50.0	

Name	Full Name	Value	Comment
	man-hr)		

Other Fixed Operating Costs

Name	Full Name	Path	Value	Comment
g&a	G&A rate (% of labor cost)	Fixed Operating Costs > Labor Cost > Value	20.0%	Based on Pinaud 2013.
property tax	Property tax and insurance rate (% of total capital investment per year)	Total Capital Costs > Inflated > Value	2.0%	
repairs	Production Maintenance and Repairs (% of direct capital costs)	Direct Capital Costs > Total > Value	0.5%	
fees	Licensing, Permits and Fees ($ per year)	None	1000.0	

Utilities

Name	Usage per kg H2	Usage Unit	Cost	Cost Unit	Price Conversion Factor	Price Conversion Factor Unit	Comment
Industrial Electricity	0.16	kWh/kg H2	pyH2A.Lookup_Tables. Utility_Cost~Industrial_ Electricity_AEO_2017_ Reference_Case.csv	GJ	0.0036	GJ/kWh	Electricity usage based on Pinaud 2013.
Process Water	2.369	gal/kg H2	0.0023749510945008	$(2016)/gal	1.	None	Seawater reverse osmosis cost ca. 0.6 $/m3 (equal to ca. 0.0023 $/gal), based on Kibria 2021 and Driess 2021.

Unplanned Replacement

Name	Full Name	Path	Value	Comment
unplanned replacement	Total Unplanned Replacement Capital Cost Factor (% of total direct depreciable costs/year)	Depreciable Capital Costs > Inflated > Value	0.5%	Based on Pinaud 2013.

Sensitivity_Analysis

Parameter	Name	Type	Values
Solar-to-Hydrogen Efficiency > STH (%) > Value	STH efficiency	value	15%; 40%
PEC Cells > Cell Cost ($/m2) > Value	PEC cell cost ($/m^{2})	value	350; 1,400
PEC Cells > Lifetime (years) > Value	PEC cell lifetime (years)	value	1.5; 6

6.5 Photocatalytic Water Splitting (Photocatalytic/PC)

Workflow

Name	Type	Description	Position
Hourly_Irradiation_Plugin	plugin	Plugin to calculate solar irradiation from typical meteorological year data	0
Photocatalytic_Plugin	plugin	Computes number of required baggies, cost of baggies and catalyst cost	2
Catalyst_Separation_Plugin	plugin	Computes cost of catalyst separation	2
Multiple_Modules_Plugin	plugin	Modelling of multiple plant modules, adjustment of labor requirement	3

Display Parameters

Name	Value
Name	Photocatalytic
Color	darkgreen

Technical Operating Parameters and Specifications

Name	Value	Path	Full Name
Operating Capacity Factor (%)	90.0%		
Plant Design Capacity (kg of H2/day)	1,111		
Maximum Output at Gate	90%	Technical Operating Parameters and Specifications > Plant Design Capacity (kg of H2/day) > Value	% of plant design capacity, reduction due to loss in H2/O2 separation.
Plant Modules	10	None	10 identical modules, only affects labor requirement calculation.

Construction

Name	Full Name	Value
capital perc 1st	% of Capital Spent in 1st Year of Construction	100%

Hourly Irradiation

Name	Value	Comment
File	pyH2A.Lookup_Tables.Hourly_Irradiation_Data~tmy_34.859_-116.889_2006_2015.csv	Location: Dagget, CA, USA

Irradiance Area Parameters

Name	Value	Comment
Module Tilt (degrees)	0	Flat baggies on the ground.
Array Azimuth (degrees)	0	Flat baggies on the ground.
Nominal Operating Temperature (Celsius)	45	
Mismatch Derating	98%	
Dirt Derating	98%	Values taken from Chang 2020, analogues to silicon PV.

Name	Value	Comment
Temperature Coefficient (per Celsius)	0.0%	No decrease on photocatalyst activity with higher temperature assumed.

Solar Input

Name	Value	Comment
Mean solar input (kWh/m2/day)	Hourly Irradiation > Mean solar input no tracking (kWh/m2/day) > Value	Solar irradiation for baggies on flat ground without tracking.
Hourly (kWh/m2)	Hourly Irradiation > No Tracking (kW) > Value	

Solar-to-Hydrogen Efficiency

Name	Value	Comment
STH (%)	2.0%	Kang 2015, C3N4/CDot catalyst, 2% STH.

Catalyst

Name	Value	Comment
Cost per kg ($)	3,000	CatCost Model of Urea/Melamine derived catalyst, 5% mass yield, 0.5% wt% Ruthenium as cost placeholder for CDots (Kang 2015 uses 0.48% wt% CDots on C3N4), 60 kWh electricity per kg(catalyst) due to electrochemical CDot synthesis, process template "Metal on Metal Oxide - Strong Electrostatic Adsorption" used in CatCost Model, 5 t/a production scale, estimated cost: 890 $/kg, increased to 3,000 $/kg.
Concentration (g/L)	0.533	Kang 2015: 2% STH, 80 mg C3N4/CDot catalyst in 150 ml, 1150 umol H2 after 6h, 9 cm^2 irradiation area (2266 J/h incident irradiation), ca. 2.395 mmol H2/h/g; Tremblay 2020: 3.4% STH (200 W m^-2), 30 mg C3N4 + catalase in 20 ml, 47.49 umol H2/h, ca. 1.583 mmol H2/h/g (ca. 5 cm2 irradiation area gives reported STH); Zhao 2021: 1.16% STH (100 mW/cm^2), 0.64 cm^2 irradiated area, 11.25 umol H2 h^-1, 40 mg catalyst, 0.281 mmol H2/g/h, activity 420 nm irradiation: 65 umol H2/h, 40 mg, 1.625 mmol H2/g/h.
Lifetime (years)	0.5	Kang 2015, 45 days continuous irradiation, 200 days with recycling
Molar Weight (g/mol)	500	Assumption for calculation of hypothetical homogeneous water splitting catalyst.
Molar Attenuation Coefficient (M^-1 cm^-1)	8000	Assumption for calculation of hypothetical homogeneous water splitting catalyst.

Reactor Baggies

Name	Value	Comment
Height (m)	0.05	Optimal height depends on absorption coefficient of material/complex and catalytic activity (TOF or mol H2/h/g). Height of 5 cm based on experimental set-up used in Kang 2015 (shown in Kang 2015 SI).
Length (m)	323.0	Baggie parameters based on Pinaud 2013.
Width (m)	12.2	
Cost Material Top ($/m2)	0.54	
Cost Material Bottom ($/m2)	0.47	
Number of ports	12	Number of ports per baggie.
Cost of port ($)	30	Cost per port.
Other Costs ($)	610.7	Other costs per baggie.
Markup factor	1.5	Markup factor of baggies.

Name	Value	Comment
Additional land area (%)	30.0%	Land area required in addition to area occupied by baggies.
Lifetime (years)	5	Lifetime of reactor baggies.

Catalyst Separation

Name	Value	Comment
Filtration cost ($/m3)	0.24	Cost of nanofiltration per m3 of water based on Costa 2006. Nanofiltration as a proxy for cost of actual catalyst separation.

Direct Capital Costs - Equipment

Name	Value	Path	Comment
Baggie roll system ($)	37,000.0	None	Equipment costs based on Pinaud 2013.
Forklift ($)	18,571.0		
Water pump ($)	213.0		
Water pipes ($ per baggie)	39.9	Reactor Baggies > Number > Value	

Direct Capital Costs - Gas Processing

Name	Value	Path	Comment
Compressor ($)	526,302.0	None	Cost estimate based on Pinaud 2013. Fixed cost of compressor for plant design output (1 ton H2/day).
Condenser ($)	13,765.0		
Intercooler-1 ($)	15,103.0		
Intercooler-2 ($)	15,552.0		
Pressure Swing Adsorption ($)	107,147.0		
Reactor Outlet Pipe ($ per baggie)	3.17	Reactor Baggies > Number > Value	
Main Collection Pipe ($ per baggie)	329.6	Reactor Baggies > Number > Value	
Final Collection Pipe ($ per baggie)	23.7	Reactor Baggies > Number > Value	

Direct Capital Costs - Control System

Name	Path	Value	Comment
PLC ($)	None	2,000.0	Control system cost based on Pinaud 2013
Control Room Building ($)	None	8,000.0	
Control Room Wiring Panel ($)	None	3,000.0	
Bed Wiring Panel ($ per baggie)	Reactor Baggies > Number > Value	146.0	
Computer and Monitor ($)	None	1,500.0	
Labview Software ($)	None	4,299.0	
Water Level Controllers ($ per baggie)	Reactor Baggies > Number > Value	50.0	
Pressure Sensors ($ per baggie)	Reactor Baggies > Number > Value	345.0	

Name	Path	Value	Comment
Hydrogen Area Sensors ($ per baggie)	Reactor Baggies > Number > Value	7,600.0	
Gas Flow Meter ($)	None	5,500.0	
Instrument Wiring ($ per baggie)	Reactor Baggies > Number > Value	22.7	
Power Wiring ($ per baggie)	Reactor Baggies > Number > Value	7.6	
Conduit ($ per baggie)	Reactor Baggies > Number > Value	142.4	

Direct Capital Costs - Installation Costs

Name	Path	Value	Comment
Excavation ($ per baggie)	Reactor Baggies > Number > Value	2570.0	Installation costs based on Pinaud 2013.
Baggie Reactor Startup (% of baggie cost)	Direct Capital Costs - Reactor Baggies > Baggie Cost ($) > Value	5%	
Baggies installation ($ per baggie)	Reactor Baggies > Number > Value	800.0	
Gas processing installation (% of gas processing cost)	Direct Capital Costs - Gas Processing > Summed Total > Value	30%	
Control system installation (% of control system cost)	Direct Capital Costs - Control System > Summed Total > Value	30%	

Indirect Capital Costs

Name	Path	Value	Comment
Engineering and Design (% of total direct capital costs)	Direct Capital Costs > Total > Value	7%	Indirect capital costs based on Pinaud 2013.
Process Contingency (% of total direct capital costs)	Direct Capital Costs > Total > Value	20.0%	
Up-Front Permitting Costs (% of total direct capital costs)	Direct Capital Costs > Total > Value	0.5%	
Site Preparation (% of total direct capital costs)	Direct Capital Costs > Total > Value	1%	

Non-Depreciable Capital Costs

Name	Value	Comment
Cost of land ($ per acre)	500.0	Land cost based on Pinaud 2013.

Fixed Operating Costs

Name	Full Name	Value	Comment
area	Area per staff (m2)	405,000	Labor cost based on Pinaud 2013, solar collection area that can be overseen by one staff member.
supervisor	Shift supervisor	1	Number of shift supervisors.
shifts	Shifts	3	Number of shifts per day.
hourly labor cost	Burdened labor cost, including overhead ($ per man-hr)	50.0	

Other Fixed Operating Costs

Name	Full Name	Path	Value	Comment
g&a	G&A rate (% of labor cost)	Fixed Operating Costs > Labor Cost > Value	20.0%	Other fixed operating costs based on Pinaud 2013.
property tax	Property tax and insurance rate (% of total capital investment per year)	Total Capital Costs > Inflated > Value	2.0%	
repairs	Production Maintenance and Repairs (% of direct capital costs)	Direct Capital Costs > Total > Value	0.5%	
fees	Licensing, Permits and Fees ($ per year)	None	1000.0	

Utilities

Name	Usage per kg H2	Usage Unit	Cost	Cost Unit	Price Conversion Factor	Price Conversion Factor Unit	Comment
Industrial Electricity	3.29	kWh/kg H2	pyH2A.Lookup_Tables. Utility_Cost~Industrial_ Electricity_AEO_2017_ Reference_Case.csv	GJ	0.0036	GJ/kWh	Electricity usage based on Pinaud 2013.
Process Water	2.637	gal/kg H2	0.0023749510945008	$(2016)/gal	1.	None	Seawater reverse osmosis cost ca. 0.6 $/m3 (equal to ca. 0.0023 $/gal), based on Kibria 2021 and Driess 2021.

Unplanned Replacement

Name	Full Name	Path	Value	Comment
unplanned replacement	Total Unplanned Replacement Capital Cost Factor (% of total direct depreciable costs/year)	Depreciable Capital Costs > Inflated > Value	0.5%	Based on Pinaud 2013.

Sensitivity_Analysis

Parameter	Name	Type	Values
Solar-to-Hydrogen Efficiency > STH (%) > Value	STH efficiency	value	1%; 4%
Catalyst > Cost per kg ($) > Value	Catalyst cost ($/kg)	value	1500; 6000
Catalyst > Lifetime (years) > Value	Catalyst lifetime (years)	value	0.25; 1
Catalyst > Concentration (g/L) > Value	Catalyst concentration (g/L)	value	0.25; 1.0
Direct Capital Costs - Gas Processing > Compressor ($) > Value	Compressor cost ($)	value	250,000; 1,000,000

Monte_Carlo_Analysis

Name	Value	Comment
Samples	50,000	Number of samples in Monte Carlo simulation.
Target Price Range ($)	1.5; 1.6	

Name	Value	Comment
Input File	./Photocatalytic/Base/Monte_Carlo_Output.csv	

Parameters - Monte_Carlo_Analysis

Parameter	Name	Type	Values	File Index	Comment
Solar-to-Hydrogen Efficiency > STH (%) > Value	STH efficiency	value	20%; Base	0	Maximum theoretical STH efficiency ca. 28% for two-absorber system, Schneidewind 2021.
Catalyst > Concentration (g/L) > Value	g(Catalyst) / L	value	Base; 0.01	1	Model calculation for homogeneous photocatalyst: molar mass 500 g/mol, molar attenuation coefficient of 10,000 M^-1 cm^-1, water height of 5 cm, at a concentration of 0.01 g/L gives an absorbance of 1 (10% transmittance).
Catalyst > Cost per kg ($) > Value	$ / kg(Catalyst)	value	100.0; Base	2	CatCost model catalyst cost drops to 140 $/kg at 100 t/a production scale, estimating lower bound of catalyst cost at 100 $/kg.
Catalyst > Lifetime (years) > Value	Catalyst lifetime / years	value	Base; 1	3	Doubling lifetime of 6 months to 1 year.

6.6 Photovoltaic + Electrolysis (PV+E)

Workflow

Name	Type	Position
Hourly_Irradiation_Plugin	plugin	0
Photovoltaic_Plugin	plugin	0
Multiple_Modules_Plugin	plugin	3

Display Parameters

Name	Value
Name	PV + E
Color	darkblue

Hourly Irradiation

Name	Value	Comment
File	pyH2A.Lookup_Tables.Hourly_Irradiation_Data~tmy_34.859_-116.889_2006_2015.csv	Location: Dagget, CA, USA

Irradiance Area Parameters

Name	Value	Comment
Module Tilt (degrees)	Hourly Irradiation > Latitude > Value	Module tilt equal to latitude of location.
Array Azimuth (degrees)	180	
Nominal Operating Temperature (Celsius)	45	
Mismatch Derating	0.98	Based on Chang 2020.
Dirt Derating	0.98	Based on Chang 2020.
Temperature Coefficient (per Celsius)	-0.4%	Based on Chang 2020.

Irradiation Used

Name	Value	Comment
Data	Hourly Irradiation > Horizontal Single Axis Tracking (kW) > Value	Single axis tracking based on Chang 2020.

Technical Operating Parameters and Specifications

Name	Value	Comment
Plant Modules	10	Modelling of 10 modules for calculation of staff cost to facilitate comparison with PEC and photocatalytic model.

Construction

Name	Full Name	Value
capital perc 1st	% of capital spent in 1st year of construction	100%

CAPEX Multiplier

Name	Value	Full Name
Multiplier	1.0	CAPEX multiplier for every 10-fold increase of system size.

Electrolyzer

Name	Value	Comment
Nominal Power (kW)	5,500.0	Production of ca. 1 t of H2 per day to compare with PEC and photocatalytic models.
CAPEX Reference Power (kW)	1,000.0	
Power requirement increase per year	0.3%	Based on Chang 2020
Minimum capacity	10.0%	Based on Chang 2020, minimum capacity for electrolyzer to operate.
Conversion efficiency (kg H2/kWh)	0.0185	Based on Chang 2020
Replacement time (h)	80,000.0	Based on Chang 2020, operating time after which electrolyzer stacks have to be replaced.

Photovoltaic

Name	Value	Path	Comment
Nominal Power (kW)	1.5	Electrolyzer > Nominal Power (kW) > Value	Optimal PV oversize ratio, same as Chang 2020
CAPEX Reference Power (kW)	1,000.0		
Power loss per year	0.5%	Based on Chang 2020	
Efficiency	22%	None	Only used for area calculation.

Direct Capital Costs - PV

Name	Value	Path	Comment
PV CAPEX ($/kW)	818.0	Photovoltaic > Nominal Power (kW) > Value ; Photovoltaic > Scaling Factor > Value	Based on Chang 2020, Chiesa 2021 Middle East PV installation cost, Shah 2021.

Direct Capital Costs - Electrolyzer

Name	Value	Path	Comment
Electrolyzer CAPEX ($/kW)	784.0	Electrolyzer > Nominal Power (kW) > Value ; Electrolyzer > Scaling Factor > Value	Based on Chang 2020, IRENA 2020 Green Hydrogen (PEM System CAPEX 700 - 1400 $/kg), Shah 2021.

Non-Depreciable Capital Costs

Name	Value	Comment
Cost of land ($ per acre)	500.0	Same as PEC and Photocatalytic model, based on Pinaud 2013.

Fixed Operating Costs

Name	Full Name	Value	Comment
area	Area per staff (m2)	405,000	Same as photocatalytic model, solar collection area that can be overseen by one staff member.
supervisor	Shift supervisor	1	Same as PEC and photocatalytic model, number of shift supervisors.
shifts	Shifts	3	Same as PEC and photocatalytic model, number of shifts per day.
hourly labor	Burdened labor cost, including	50.0	Same as PEC and photocatalytic model.

Name	Full Name	Value	Comment
cost	overhead ($ per man-hr)		

Other Fixed Operating Costs

Name	Value	Path	Comment
Electrolyzer OPEX (% of CAPEX)	2%	Direct Capital Costs - Electrolyzer > Electrolyzer CAPEX ($/kW) > Value	Based on Stolten 2020, Shah 2021.
PV OPEX (% of CAPEX)	2%	Direct Capital Costs - PV > PV CAPEX ($/kW) > Value	Based on Stolten 2020.

Utilities

Name	Usage per kg H2	Usage Unit	Cost	Cost Unit	Price Conversion Factor	Comment
Process Water	10	L/kg H2	0.0006	$/L	1.	Seawater reverse osmosis cost ca. 0.6 $/m3 (equal to 0.0006 $/L), based on Kibria 2021 and Driess 2021.

Planned Replacement

Name	Cost ($)	Path	Comment
Electrolyzer Stack Replacement	40%	Direct Capital Costs - Electrolyzer > Electrolyzer CAPEX ($/kW) > Value	Based on Chang 2020

Sensitivity_Analysis

Parameter	Name	Type	Values
Planned Replacement > Electrolyzer Stack Replacement > Cost ($)	Stack repl. cost (% of E-CAPEX)	value	20%; 80%
Direct Capital Costs - PV > PV CAPEX ($/kW) > Value	PV CAPEX ($/kW)	value	400; 1600
Direct Capital Costs - Electrolyzer > Electrolyzer CAPEX ($/kW) > Value	Electrolyzer CAPEX ($/kW)	value	400; 1600
Electrolyzer > Conversion efficiency (kg H2/kWh) > Value	Electrolyzer efficiency (kg H_{2}/kWh)	value	0.015; 0.025
Photovoltaic > Power loss per year > Value	PV power loss per year	value	0.25%; 1.0%
Electrolyzer > Power requirement increase per year > Value	Electrolyzer power increase per year	value	0.15%; 0.6%

Waterfall_Analysis

Parameter	Name	Type	Value	Show Percent
Direct Capital Costs - PV > PV CAPEX ($/kW) > Value	$/kW(PV)	value	220	
Direct Capital Costs - Electrolyzer > Electrolyzer CAPEX ($/kW) > Value	$/kW(Electro- lyzer)	value	200	
Electrolyzer > Conversion efficiency (kg H2/kWh) > Value	kg(H_{2})/ kWh(Electricity)	value	0.025	
Planned Replacement > Electrolyzer Stack Replacement > Cost ($)	Stack replacement (%E-CAPEX)	value	20%	True

Monte_Carlo_Analysis

Name	Value	Comment
Samples	50,000	Number of samples in Monte Carlo simulation.
Target Price Range ($)	1.5; 1.6	
Input File	./PV_E/Base/Monte_Carlo_Output.csv	

Parameters - Monte_Carlo_Analysis

Parameter	Name	Type	Values	File Index	Comment
Direct Capital Costs - PV > PV CAPEX ($/kW) > Value	$ / kW(PV)	value	Base; 220	0	Based on Waldau 2021 PV CAPEX projection for 2050 (PV module learning rate of 25%, BOS learning rate of 7.5%, base PV growth scenario).
Direct Capital Costs - Electrolyzer > Electrolyzer CAPEX ($/kW) > Value	$ / kW(Electrolyzer)	value	Base; 200	1	CAPEX reduction to 200 $/kW in 2050 based on IRENA Green Hydrogen 2020, learning curve model Waldau 2021 (using their cost reduction factor of ca. 4-5 until 2050 due to learning).
Electrolyzer > Conversion efficiency (kg H2/kWh) > Value	kg(H_{2}) / kWh(Electricity)	value	Base; 0.025	2	Maximum efficiency: 0.02538 kg H2/kWh, Chang 2020 (based on reaction enthalpy).
Planned Replacement > Electrolyzer Stack Replacement > Cost ($)	Stack repl. (% E-CAPEX)	value	Base; 20%	3	Decreasing stack replacement cost to 20% of electrolyzer CAPEX.

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