

How Much Technological Progress is Needed to Make Solar Hydrogen Cost-Competitive?

Jacob Schneidewind

Dedicated to Professor Matthias Beller on the occasion of his 60th birthday

Cost-effective production of green hydrogen is a major challenge for global adoption of a hydrogen economy. Technologies such as photoelectrochemical (PEC) or photocatalytic (PC) water splitting and photovoltaic + electrolysis (PV+E) allow for sustainable hydrogen production from sunlight and water, but are not yet competitive with fossil fuel-derived hydrogen. Herein, open-source software for techno-economic analysis (pyH2A) along with a Monte Carlo-based methodology for modelling of technological progress are developed. Together, these tools allow for the study of required technological improvement to reach a competitive target cost. They are applied to PEC, PC, and PV+E to identify required progress for each and derive actionable research targets. For PEC, it is found that cell lifetime improvements (>2 years) and operation under high solar concentration (>50-fold) are crucial, necessitating systems with high space-time yields. In the case of PC, solar-to-hydrogen efficiency has to reach at least 6%, and lowering catalyst concentration ($<0.2 \text{ g L}^{-1}$) by improving absorption properties is identified as a promising path to low-cost hydrogen. PV+E requires \approx two or threefold capital cost reductions for photovoltaic and electrolyzer components. It is hoped that these insights can inform materials research efforts to improve these technologies in the most impactful ways.

These technologies, however, cannot currently produce hydrogen at a cost that is competitive with hydrogen derived from steam reforming.^[6,7] Hence, the question arises what and how much technological progress is required to reach a point of competitiveness? Understanding these requirements can inform (materials) research efforts, focusing them on the areas that are most impactful for quickly improving green hydrogen production routes.

Techno-economic analysis (TEA) is a helpful tool in this regard: it allows for economic modelling of various (hypothetical) production processes, providing insight into how process parameters affect the levelized cost of hydrogen (LCOH₂, herein expressed using the unit $\$/\text{kg}(\text{H}_2)$). In the literature, various techno-economic studies of hydrogen production from solar energy can be found.^[6–12] Broadly speaking, they can be classified into three categories:

1. Introduction

Producing green hydrogen at a cost that is competitive with fossil fuel-derived hydrogen is one of the major challenges for transitioning to a hydrogen economy.^[1] There are promising technologies for converting solar energy and water to hydrogen, such as photoelectrochemical (PEC)^[2,3] and (particulate) photocatalytic (PC)^[4] water splitting as well as coupling of photovoltaic and electrolysis (PV+E)^[5] (see Figure 1).


1. Modelling of state-of-the-art technologies to obtain an estimate for the current LCOH₂^[6,11]
2. Modelling of hypothetical future technologies to obtain an estimate for a potential future LCOH₂^[13,14]
3. Learning curve analysis based on learning rates to model the decrease of LCOH₂ over time^[9,10]

Modelling of state-of-the-art or potential future technologies provides valuable single-point cost estimates and also reveals the impact of individual parameters through sensitivity analysis. However, they do not capture the trajectory of technological progress. Learning curve analysis does model the evolution of LCOH₂ over time but it faces two important limitations: first, historical data is often needed to derive reasonable estimates for the learning rates. It is therefore most reliable for mature technologies and challenging to apply for technologies which have not yet been widely deployed. Second, learning curves do not provide straightforward insight into which aspects of technological progress are actually responsible for the modelled LCOH₂ decrease.

Aside from these methodological aspects, there is also a major practical challenge encountered in the TEA literature: techno-economic models are often implemented in custom environments (e.g., Excel sheets or programming scripts which are not publicly available) due to the lack of standardized tools. This leads to reduced transparency and hinders

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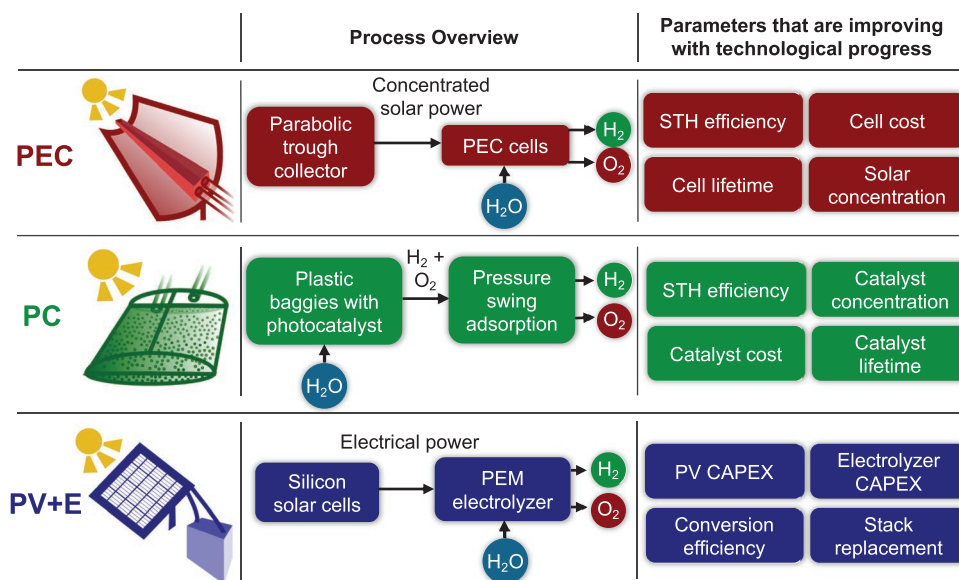


Figure 1. Overview of photoelectrochemical water splitting (PEC), photocatalytic water splitting (PC) and photovoltaic + electrolysis (PV+E) for green hydrogen production along with relevant parameters for technological progress. Abbreviations: “PEM” proton-exchange membrane, “CAPEX” capital expenditure, “STH” solar-to-hydrogen.

reproduction as well as comparison of literature results. It also creates overhead effort which goes into creation of these custom environments. Given this backdrop, the present study has three major goals:

1. Creation of the pyH2A open-source software as a transparent and reproducible tool for techno-economic modelling. Partly based on the H2A model developed by the U.S. Department of Energy,^[15] it allows for flexible modelling of various hydrogen production pathways.
2. Development of the Monte Carlo based development distance methodology to capture how technological progress affects the LCOH₂. Furthermore, this methodology can be used to determine which progress is required to reach cost-competitive hydrogen production. It is a new way to analyze techno-economic models and is inspired by the previous use of Monte Carlo for uncertainty quantification,^[6] and the use of contour plots to study how simultaneous change of multiple parameters impacts the LCOH₂.^[14]
3. Application of this methodology to PEC, PC, and PV+E, determining for each how much and which technological progress is needed produce hydrogen at a cost-competitive level. These insights are then used to derive actionable research targets for each technology.

2. Methodology

2.1. pyH2A Open-Source Software

pyH2A is an extensible framework for techno-economic analysis of hydrogen production, implemented in Python. It is open-source, with the source code available on GitHub (<https://github.com/jschneidewind/pyH2A>). Input parameters are provided in a plain text

file and different technologies are modelled by invoking plugins. These feed information into the central discounted cash flow calculation, from which the LCOH₂ is obtained. Any given techno-economic model can be interfaced with various analysis modules to perform cost breakdown, sensitivity, waterfall, or Monte Carlo analysis. A detailed description of the general pyH2A methodology is provided in Section S2 in the Supporting Information.

2.2. Hydrogen Production Technologies

This study focuses on photophysical/photochemical technologies for converting solar energy and water to hydrogen, namely photoelectrochemical (PEC) and photocatalytic (PC) water splitting as well as photovoltaic + electrolysis (PV+E). There are other promising solar hydrogen production pathways, such as those based on thermal^[16] or biological processes for water splitting^[17] or by utilizing biomass as a feedstock.^[18] While these routes are outside the scope of the present work, the described methodologies can also be applied to them.

For each selected technology, a hydrogen production plant with a design capacity of ≈1 metric ton(H₂)/day was modelled over its entire lifetime, obtaining the LCOH₂. The financial input parameters shared by all models can be found in Section S6.2 in the Supporting Information.

For photoelectrochemical (PEC) water splitting, hydrogen production is achieved by concentrating sunlight using parabolic trough collectors and focusing it on PEC cells, which are in a transparent enclosure with water. Irradiation of the PEC cells leads to hydrogen and oxygen production on opposite sides of cell, so that pure hydrogen can be obtained (see Figure 1, PEC). State-of-the-art properties of the PEC cells are based on devices by Kistler et al.^[2] and Khan et al.^[3] using a III–V absorber. The layout of the hydrogen production plant is based on Pinaud et al. (type 4 – PEC).^[13] A detailed description

of the process can be found in Section S3.1 (Supporting Information) and all input parameters are available in Section S6.3 in the Supporting Information.

In photocatalytic (PC) water splitting, a particulate photocatalyst is mixed with water and placed in plastic baggie reactors, which are exposed to sunlight.^[13,19,20] Action of the photocatalyst leads to production of a H_2/O_2 mixture, which is separated using pressure swing adsorption^[13] to obtain pure hydrogen (see Figure 1, PC). The CDot/ C_3N_4 photocatalyst reported by Liu et al.^[4] is used as a state-of-the-art reference and the plant layout is based on the “type 1 – single bed” design described by Pinaud et al.^[13] Section S4.1 (Supporting Information) contains a detailed process description and input parameters can be found in Section S6.4 in the Supporting Information.

Coupling of silicon solar cells with an off-grid proton-exchange membrane (PEM) electrolyzer is the basis for photovoltaic + electrolysis (PV+E). Electrical power from the solar cells is fed to the electrolyzer to produce pure hydrogen from water (see Figure 1, PV+E). The plant model is based on the one reported by Yates et al.^[6] A process description can be found in Section S5.1 (Supporting Information) and input parameters in Section S6.5 in the Supporting Information.

2.3. Monte Carlo/Development Distance Methodology

The aim of the Monte Carlo/development distance methodology is to model how simultaneous progress for multiple parameters of a technology affects the $LCOH_2$. For a given technology, this is accomplished in four steps (see also Section S2.4.4. in the Supporting Information):

1. Selection of parameters that improve with technological progress (selected parameters are shown for each technology in

Figure 1). For every parameter, a base value, which represents the state-of-the-art, is defined. Furthermore, a limit value is defined, which represents the limit which can possibly be achieved with future progress.

2. A large number (in this case 50 000) of random parameter value combinations are generated. Each parameter value is within its [base, limit] interval. This leads to 50 000 different instances of the original techno-economic model, each with random values for the selected parameters.
3. For each instance, the normalized distance of its parameter values to the base case is calculated. “Base case” means that all parameter values are equal to their base values (normalized distance is 0), while “limit case” means that all parameter values are equal to their limit value (normalized distance is 1). Details on the distance calculation can be found in Section S2.4.4.1 in the Supporting Information. This metric is herein referred to as “development distance”, since it is an indicator for the amount of technological development that is represented by a given instance.
4. The full discounted cashflow calculation is performed for every instance to obtain the corresponding $LCOH_2$.

With this methodology, a dataset of 50 000 instances for every technology model is obtained. Each instance has a unique combination of parameter values, an associated development distance and $LCOH_2$. Together, the datapoints map the entire trajectory from the state-of-the-art (base case) to future technologies (limit case). The Monte Carlo/development distance methodology is implemented in pyH2A.

The tables in Figure 2 show the base and limit values for the selected parameters of each technology. For PEC the parameters are: STH efficiency, solar concentration factor, cell cost ($\$/m^2$ (PEC cell)) and cell lifetime (in years). For PC, catalyst concentration ($g(\text{Catalyst}) L^{-1}$), catalyst cost ($\$/kg(\text{Catalyst})$),

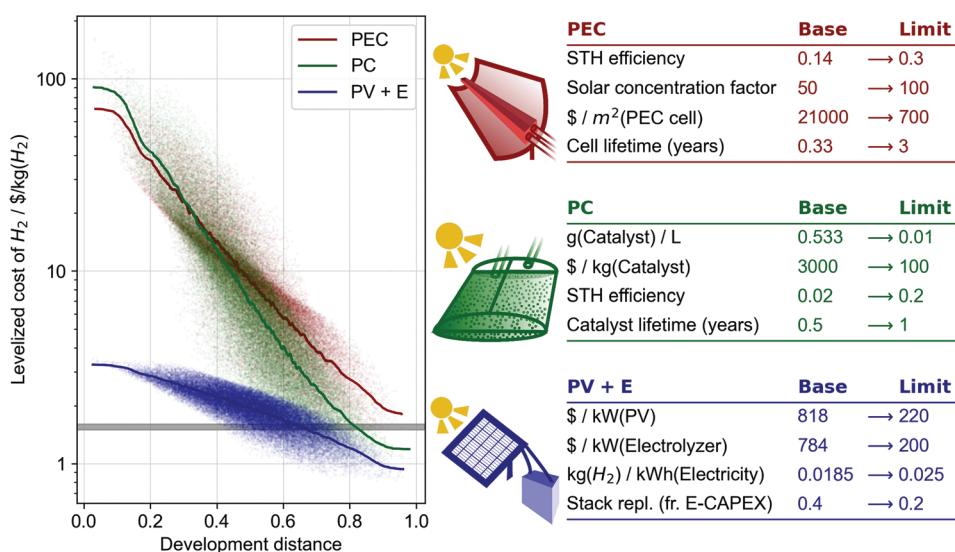


Figure 2. Relationship of development distance and $LCOH_2$ (log scale) for PEC, PC, and PV+E. The grey bar indicates the target cost range (1.5–1.6 $\$/kg(H_2)$). Savitzky–Golay smoothed trendlines are shown as solid lines. For each technology, parameters that constitute the respective development distance are shown on the right, along with their base and limit values. For details see Section S2.4.4.3 in the Supporting Information. “Stack repl. (fr. E-CAPEX)” stands for “Stack replacement cost (fraction of electrolyzer CAPEX)”.

STH efficiency and catalyst lifetime (in years) were selected. Selected PV+E parameters are: PV CAPEX (\$/kW(PV)), electrolyzer CAPEX (\$/kW(Electrolyzer)), conversion efficiency (kg(H₂)/kWh(Electricity)) and stack replacement cost (as a fraction of electrolyzer CAPEX). In the Supporting Information, sources/rationales for each selected base/limit value can be found (PEC: Section S3.1.4 (Supporting Information), PC: Section S4.1.4 (Supporting Information), PV+E: Section S5.1.3 (Supporting Information)).

2.4. Advantages and Limitations

The Monte Carlo/development distance methodology has several advantages compared to other analysis methods, which are commonly used in the literature. In comparison to sensitivity analysis,^[13] multiple instead of just one parameter are varied simultaneously. This gives a more realistic reflection of technological progress, which commonly involves simultaneous progress for multiple parameters (e.g., cost, efficiency, and lifetime improving together). Furthermore, by changing multiple parameters, interactions between changing parameters are captured, which is not possible with one-at-a-time methods such as sensitivity analysis. Contour plots^[14] address some of these shortcomings by plotting LCOH₂ as a function of two (or more, if the visualization allows) changing parameters. In this case, the techno-economic model is the mathematical function which provides an answer to the question: for these given parameters, what is the LCOH₂? Monte Carlo offers the powerful advantage of being able to reverse this question: for a given LCOH₂, what parameter values are needed to accomplish this LCOH₂? This is a question which is challenging to answer otherwise, because the techno-economic model is typically not an analytical function which can simply be solved for the parameters. Being able to solve the reversed question makes it easier to derive quantitative research targets to reach a given LCOH₂ target.

However, there are also several limitations for the methodology employed in this study

1. The limit values for the Monte Carlo/development distance modelling must be assumed since it is not possible to know which parameters values will actually be achieved in the future. The choice of limit values affects the development distance: choosing very optimistic limit values, for example, makes model instances with intermediate values appear at shorter development distances. This means that comparing the development distance values for different technologies is only valid if the limit values for each are equally “difficult” to achieve. As this notion is challenging to quantify, the development distance should always be seen in the context of the underlying base and limit values, especially when comparing technologies.

Importantly, however, the choice of limit values does not affect the analysis of the required parameter values to achieve a given cost target. In this case, the limit values only determine which part of the parameter space is explored.

Since selection of limit values is one of the central assumptions in the Monte Carlo/development distance methodology, the method(s) for choosing them should be carefully

considered. In this study, limit values are partly based on physical limits (e.g., for STH efficiency or catalyst concentration, Table S4.1–3 in the Supporting Information) and also on projected cost trends (e.g., see Table S5.1–3 in the Supporting Information). The estimation based on cost trends makes implicit assumptions about future deployments (see point 4) and can be prone to errors. Alternatively, expert elicitation surveys may be used to estimate realistic limit values. This approach can offer a different perspective independent of mathematical modelling, but is relies on carefully performed surveys to eliminate biases.

2. Even when choosing equally “difficult” limit values for different technologies, comparison of development distances between technologies can be challenging. This is because technologies may be at different stages of their development: for a rapidly evolving early-stage technology, going from a distance of 0 to 0.5 may be significantly easier/faster in comparison to an advanced technology which is already close to its limit. It may be possible to account for these differences by mapping development distance to time, which would reveal the different rates at which development distance progresses. However, establishing a distance/time correlation requires adequate historical data for calibration (see Section “Relating development distance to time”).
3. The present models only calculate the cost of hydrogen production, thus the cost for transport or storage is not considered.
4. For all calculations, the plant size (1 metric ton H₂/day) and location (Dagget, CA, USA) are fixed. Hence, plant scaling and geographical effects on the LCOH₂ are not considered. Although plant scaling effects are not considered, overall scaling effects due to increasing deployment are considered implicitly. Increasing deployment is one of the main driving forces for cost reduction (e.g., for PV^[9]), and modelling decreasing cost therefore includes an implicit assumption about scaled up deployment.
5. In this study, only a cost analysis of hydrogen production is performed. Other important aspects, such as modelling of life-cycle greenhouse gas emissions^[21] and net energy analysis^[22] are not included.

3. Results and Discussion

3.1. Development Distance and LCOH₂

The relationship between development distance and LCOH₂ provides an overview of technological progress’ impact on hydrogen cost. Figure 2 plots the development distance of each random model instance against its associated LCOH₂, along with a smoothed Savitzky–Golay trendline for each technology. The shown data reflects the entire trajectory from the current state-of-the-art (base case, development distance of 0) to the limit technologies (development distance of 1).

PEC and PC have a very high LCOH₂ for the base case in excess of 100 \$/kg(H₂). However, the LCOH₂ for both drops exponentially with increasing development distance, as indicated by the linear trend in the logarithmic plot. Such an exponential decrease points at a strong interaction between the

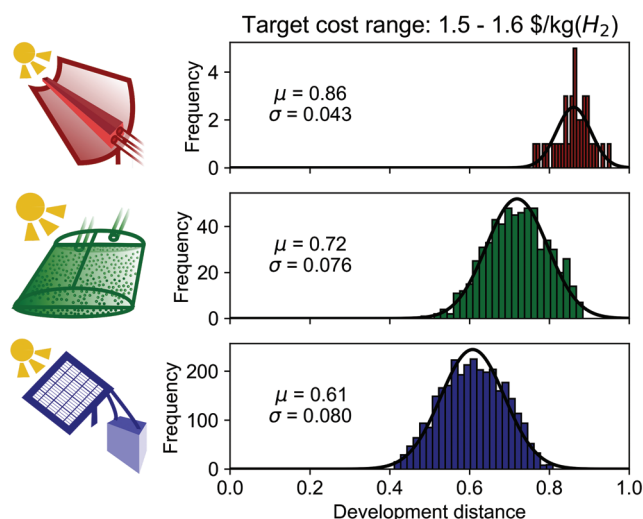


Figure 3. Histograms showing development distance distribution of model instances within the target cost range for each technology (top: PEC, middle: PC, bottom: PV+E). A fitted and scaled normal distribution is shown for each histogram (black line), with the corresponding mean (μ) and standard deviation (σ) shown as inlets. For details, see Section S2.4.4.4 in the Supporting Information.

selected parameters, leading to multiplicative effects. In case of PC, for example, improving both the STH efficiency and catalyst concentration produces a multiplicative cost reduction. It can also be seen that the LCOH₂ decreases more steeply for PC compared to PEC.

PV+E has a much lower LCOH₂ of around 3.6 \$/kg(H₂) for the base case. Increasing development distance, however, leads only to a roughly linear cost reduction (sublinear in logarithmic plot), indicative of weak interactions between selected parameters. In contrast to PEC and PC, parameter improvements (such as PV or electrolyzer CAPEX reductions) are largely independent of one another and do not produce multiplicative effects.

3.2. Model Instances in the Target Cost Range

To be cost-competitive on the global market, solar hydrogen has to reach the cost range of hydrogen derived from steam methane reforming (SMR), which is currently the dominant hydrogen production route.^[9] SMR hydrogen is produced at costs ranging from 1–2 \$/kg(H₂).^[9] For this study, we therefore defined the target cost range for cost-competitiveness as 1.5–1.6 \$/kg(H₂), which is indicated as a grey bar in Figure 2. It can be seen that PV+E crosses into the target cost range at the shortest development distance. PC also reaches it at somewhat longer distances while PEC seems to mostly level off above it. To gain insight into the requirements for cost-competitiveness, we turn to a more detailed analysis of the instances for each technology model that fall into the target cost range.

Figure 3 shows the development distance distribution of all instances with a LCOH₂ in the target cost range. From this analysis, we can obtain the mean development distances that are required to achieve cost-competitiveness. As already

indicated by Figure 2, PEC displays the longest mean development distance (0.86, standard deviation: 0.043) and only a very small number of instances actually reach the target cost range (low frequency values on the y axis). The high mean development distance means that almost all potential for technological improvement has to be exhausted in order to produce hydrogen at the defined target cost. PC shows a significantly shorter mean development distance of 0.72 with a relatively broad distribution of instances from 0.5 to 0.85 (standard deviation: 0.076). This implies that, while a significant amount of progress is required, the target cost can be achieved without having to use all of the innovation potential. In case of PV+E, the shortest mean development distance of 0.61 is observed with an equally broad distribution compared to PC (standard deviation: 0.080). Within the assumptions of this study, the shortest mean development distance indicates that PV+E requires the least amount of technological progress to reach cost-competitiveness.

3.3. Relating Development Distance to Time

It would be powerful to correlate development distance with time to obtain additional information on how long it may take to reach the derived distance targets. This can be done for technologies for which historical data on all parameters of the Monte Carlo analysis is available, and a suitable analysis method has been implemented in pyH2A (see Section S2.4.4.6 in the Supporting Information). Considering the technologies in this study, high quality historical data is available for PV+E (see Section S5.4 in the Supporting Information), allowing for a distance/time analysis for this technology.

Using historical PV and electrolyzer CAPEX data as well as a reasonable historical trend for electrolyzer efficiency, historical distance values from 2003 to 2020 were calculated (see **Figure 4**). Because historical parameter values are typically less advanced than the state-of-the-art base values, these distances are negative, covering a range from about –1 to 0. Interestingly,

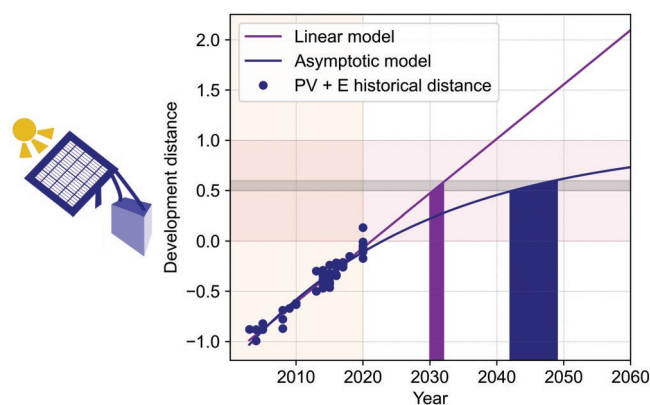


Figure 4. Relationship between development distance and time for PV+E based on historical data (2003–2020). Linear and asymptotic models are fitted to the historical distance values and extrapolated into the future. Distance region that enables cost-competitive hydrogen production (0.5–0.6) is highlighted in gray along with the corresponding timeframes of when these distances may be achieved (based on linear and asymptotic models). For details, see Sections S2.4.4.6 and S5.4 in the Supporting Information.

a linear relationship between distance and time is observed, with an annual distance increase of about 0.054. We can fit different functions to these historical datapoints, allowing us to extrapolate into the future and estimate when distance values between 0 and 1 may be achieved. For an optimistic scenario, a linear function was fitted, which assumes that the annual distance increase remains constant over time. In contrast, for a conservative scenario, an asymptotic function was used, which assumes that the annual distance increase goes down as the limit distance of 1 is approached.

Based on the extrapolated functions, we can estimate when PV+E will reach the distance region that enables cost-competitive hydrogen production (between 0.5 and 0.6): for the optimistic linear function, this region may be reached between 2030 and 2035, while for the conservative asymptotic function it may be reached between 2040 and 2050 (see Figure 4 and Figure S5.4-4 (Supporting Information)). Interestingly, these results are quite consistent with those obtained using learning curve analysis,^[10] despite being derived using a fundamentally different methodology which does not rely on learning rates.

It should be noted that the distance/time relationship derived for PV+E does not necessarily translate to PEC or PC: because these technologies are at a lower technology readiness level, progress is likely obtained at different timescales (see above, limitation number 2). Therefore, technology-specific distance/time relationships need to be established to account for technologies being at different stages of their development. The lack of high-quality historical data for PEC and PC prevents a distance/time analysis for them at this point. However, the methodology described herein may be applied to other technologies for which historical data is available.

3.4. Required Progress and Research Targets

Analysis of development distances provides an overall picture of (required) technological progress. To derive actionable insight, especially for informing research and development efforts, it is important to understand how much the underlying technological properties have to advance to achieve cost-competitive hydrogen production. To this end we can analyze the specific parameter values of model instances which reach the target cost range. In the following, the corresponding data will be visualized using colored scatter plots: each instance with an LCOH₂ in the target cost range is shown as a colored dot, with its (x, y) position and color determined by its parameter values (the fourth parameter which has been varied in the Monte Carlo simulation is not shown). For reference, the base case is also shown as a labelled and colored dot. From this visualization we can see which combinations of parameter values give rise to model instances with cost-competitive hydrogen production.

Figure 5 shows the colored scatter plot for PEC. Only a very small region of the parameter space gives rise to model instances in the target cost range, with this region being at the maximum distance from the base case. STH efficiency has to exceed 26%, cell cost has to be below 1500 \$/m² (PEC Cell) and cell lifetime has to exceed 2 years. The central challenge for PEC is that the PEC cells are the most expensive component of the plant for most model instances (see cost breakdown in

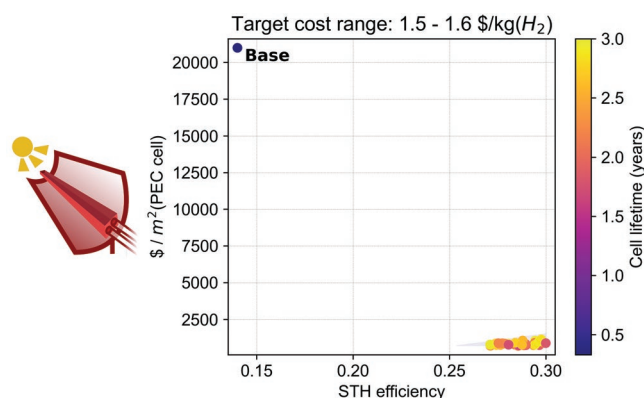


Figure 5. Colored scatter plot showing parameter values of PEC model instances within target cost range. For reference, the base case is shown in the top left. Light blue area illustrates largest possible region in which instances can lie (for details see Section S2.4.4.5 in the Supporting Information).

Figure S3.2-2 in the Supporting Information), but also have a short lifetime (especially compared to solar cells and electrolyzers).^[23] This is because various components of the cell are exposed to a reactive chemical environment.^[2] Since PEC cells are by definition highly integrated devices, most components have to be replaced together at the end of their lifetime, leading to high replacement costs (see Figure S3.2-1 in the Supporting Information) and thus a high LCOH₂. Based on our results, only a combination of high efficiency (small area of cells needed for a given H₂ production), low cost and long lifetime can overcome these challenges to reach the target cost range. It should also be noted that solar concentration is very likely necessary for low-cost H₂ production using PEC: modelling PEC without solar concentration shows that even for the limit case, LCOH₂ does not drop below 15 \$/kg(H₂) (see Section S3.4 in the Supporting Information). Solar concentrators will likely be significantly cheaper than PEC cells (per m²) for the foreseeable future. Hence, replacing PEC cell area with solar concentrator area enables effective cost reduction.^[24] In the limit case, however, solar concentrator cost actually becomes the dominant factor in PEC CAPEX (see Figure S3.3-2 in the Supporting Information). With respect to research targets these results imply the following: the lifetime of PEC cells has to be significantly improved (reaching on the order of years) to address the high costs resulting from regular replacements. Furthermore, PEC cells should be optimized to operate under high solar concentration factors (>50) to reduce the required cell area. This implies that highly active PEC materials (absorbers and electrocatalysts) are required which have a sufficient space-time yield to convert the high incoming energy flux (peak activity likely has to exceed 400 mol H₂ h⁻¹ m⁻² (PEC cell)). The importance of stability and efficiency are consistent with results from previous studies.^[13,14] While the important roles of solar concentration and high activity have also been identified in these studies, the previously assumed concentration factor (around 10)^[14] is much lower than what was found to be necessary in this study (50–100). It is uncertain if such progress for PEC is realistically achievable, especially to allow for it to compete with PV+E (see below).

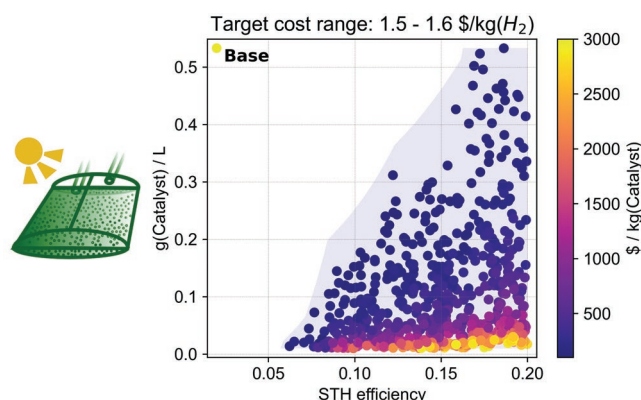


Figure 6. Colored scatter plot showing parameter values of PC model instances within target cost range. For reference, the base case is shown in the top left. Light blue area illustrates largest possible region in which instances can lie (for details see Section S2.4.4.5 in the Supporting Information).

For PC, a much larger region of the parameter space gives rise to model instances in the target cost range (see **Figure 6**). For cost-competitive hydrogen production, STH efficiency has to be at least 6%. Catalyst concentration can be as high as 0.5 g(Catalyst)/L, but concentrations below 0.2 g(Catalyst)/L open up much more flexibility with regards to efficiency and cost. For most cases, catalyst cost has to be below 1000 \$/kg(Catalyst), except when the catalyst concentration is very low (<0.05 g(Catalyst)/L). In all cases, the catalyst lifetime is relatively short (between 0.5 and 1 year), which necessitates regular catalyst replacements. In contrast to PEC, however, replacing the catalyst is straightforward because no other components have to be replaced with it: it can be removed from the water/catalyst mixture (e.g., by nanofiltration^[25]) and new catalyst is added. Looking at research targets, this data suggests that it is crucial to lower the catalyst concentration. Systems with low catalyst concentrations can tolerate lower STH efficiencies and higher catalyst costs, while reduction of the catalyst amount also reduces resource consumption for catalyst production. To achieve lower catalyst concentrations the main consideration is the absorption behavior of the photocatalyst: it needs to have a sufficiently high absorption cross section so that most sunlight is still absorbed even when lower concentrations are employed. The demands for catalytic activity are less stringent to enable low catalyst concentrations. Even for the limit case (highest efficiency, lowest concentration), peak catalytic activity does not have to exceed 7 mol H₂ g⁻¹ h⁻¹ (activities on the order of 1 mol H₂ g⁻¹ h⁻¹ have already been achieved^[26]), which corresponds to a turnover frequency of <1 s⁻¹ for a homogeneous catalyst (assuming a molar mass of 500 g mol⁻¹). Hence, light absorption performance is likely more important than highly active catalytic sites for H₂ and O₂ evolution. To identify effective paths to a cost-competitive system, it is insightful to look at the parameter values of the model instance with the shortest development distance that reaches the target cost range: with a distance of 0.48, this model instance has a STH efficiency of 17.5%, catalyst concentration of 0.01 g(Catalyst)/L, catalyst cost of 2950 \$/kg(Catalyst) and catalyst lifetime of 0.52 years. Hence, high catalyst cost and low lifetime can be tolerated

through the combination of high STH efficiency and low catalyst concentration. These characteristics point to the potential of homogenous photocatalysts, which can be used at low concentrations due to high molar absorptivity.^[27] Furthermore, it was recently shown that it is theoretically possible for homogeneous photocatalysts to achieve dual absorber STH efficiencies (>20%) with a single catalyst.^[28] With progress on catalyst concentration and STH efficiency, there is a pathway for PC to cost-competitive hydrogen production. Previously, the importance of improving STH efficiency for PC has been identified.^[13] However, catalyst concentration has so far largely been overlooked as a key parameter to enable cost effective hydrogen production using PC. Providing these new quantitative targets for catalyst concentration can hopefully help to inspire research efforts aimed at developing photocatalysts which can be used at lower concentrations.

Additionally, due to the simple plastic baggie reactor construction, PC has a low CAPEX (but rather high OPEX due to catalyst replacements, see Figures S4.2-1 and S4.3-1 in the Supporting Information), which is complementary to PV+E (high CAPEX, low OPEX, see Figure S5.2-1 in the Supporting Information) and could allow for easier construction of new plants. Safety issues due to generation of a H₂/O₂ mixture in the reactors have to be considered, but these risks were found to be manageable.^[29]

PV+E shows a well-defined region of the parameter space that gives rise to model instances with an LCOH₂ in the target cost range (**Figure 7**). The symmetry and gradients indicate that each parameter (PV CAPEX, electrolyzer CAPEX, conversion efficiency) has a roughly linear effect on LCOH₂ and there are no significant interactions between parameters (which was also shown by the linear development distance/LCOH₂ relationship). To reach the target cost range, PV CAPEX has to be below 650 \$/kW(PV) and electrolyzer CAPEX can be as high as 800 \$/kW(Electrolyzer) but only if the conversion efficiency approaches the theoretical maximum of 0.025 kg(H₂)/kWh(Electricity).^[6] Improving the conversion efficiency in general opens up possibilities to tolerate higher PV and electrolyzer CAPEX. However, the model instance with the shortest

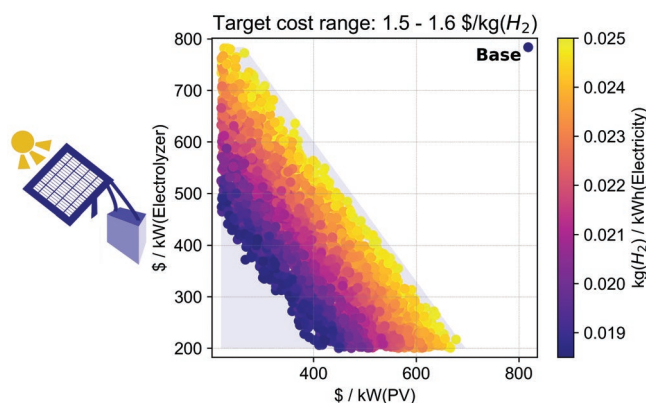


Figure 7. Colored scatter plot showing parameter values of PV+E model instances within target cost range. For reference, the base case is shown in the top right. Light blue area illustrates largest possible region in which instances can lie (for details see Section S2.4.4.5 in the Supporting Information).

development distance in the target cost range (distance of 0.41) has the base case conversion efficiency and stack replacement cost (0.0185 kg(H₂)/kWh(Electricity) and 40% of electrolyzer CAPEX), PV CAPEX of 300 \$/kW(PV) and electrolyzer CAPEX of 330 \$/kW(Electrolyzer). Hence, even without other improvements, it is possible to enable hydrogen production at the target cost by reducing PV and electrolyzer CAPEX two- or threefold each. These cost targets are consistent with previous findings on PV+E configurations which enable cost-competitive hydrogen production.^[9] Data from Figure 7 helps to map out the entire parameter space which realizes this goal.

The implication for research and development targets is that cost reductions are key, and efficiency improvements are not strictly necessary but open up possibilities to enable cost-competitive H₂ production even with more expensive components.

4. Conclusion

In summary, an open-source tool for transparent and reproducible techno-economic modelling of hydrogen production, called pyH2A, has been developed. Using pyH2A, a Monte Carlo-based methodology was conceived and implemented, which enables the study of how technological progress impacts the LCOH₂ using the new concept of “development distance.” With this methodology it also possible to dissect the influence of specific technological parameters and determine how much each has to advance to reach a defined target cost range.

The Monte Carlo/development distance method was then applied to the study of three solar hydrogen production routes: photoelectrochemical (PEC) and photocatalytic (PC) water splitting as well as photovoltaic + electrolysis (PV+E). For each, it was determined how much and which technological progress is needed to produce hydrogen at a cost level of 1.5–1.6 \$/kg(H₂) and the results were used to derive appropriate research targets.

For PEC, significant progress with respect to STH efficiency (>26%) and PEC cell stability is required, as lifetimes of at least 2 years are needed to alleviate the high costs resulting from cell replacements. Furthermore, solar concentration is a crucial component to enable low-cost hydrogen production using PEC and cells should be optimized to operate with high solar concentration factors (>50), necessitating highly absorbent semiconductors and highly active electrocatalysts.

For PC, STH efficiency has to exceed 6% and it is important to lower the catalyst concentration (<0.2 g(Catalyst)/L) by developing catalysts with large absorption cross sections. With a sufficiently high STH efficiency and low catalyst concentration, high catalyst cost (>2000 \$/kg(Catalyst)) and a short lifetime (≈0.5 years) can be tolerated, pointing towards the potential utility of homogeneous photocatalysts. Improvements of the photocatalyst open a path to cost-competitive H₂ production using PC, which could be a complementary technology to PV+E due to the low CAPEX of the plastic baggie reactor construction.

For PV+E, CAPEX reductions for both the photovoltaic and electrolyzer components are needed. The target cost can be reached by a two- or threefold cost reduction for each (300 \$/kW(PV) and 330 \$/kW(Electrolyzer) even without other technological improvements. Increasing the conversion

efficiency, however, opens up more flexibility for the cost of PV and electrolyzer systems.

It is our hope that these techno-economic insights inform materials research in the area of solar hydrogen production, so that research efforts can be directed to improve these technologies in the most impactful ways. Ultimately, these efforts will hopefully allow us to transition solar hydrogen into large scale applications, providing affordable green hydrogen on a global scale.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The author declares no conflict of interest.

Author Contributions

J.S. conceived and coordinated the project, developed the software, performed techno-economic modelling and data analysis, wrote the manuscript and curated the results for the supporting information and public repository.

Data Availability Statement

The data that support the findings of this study are openly available in GitHub at <https://github.com/jschneidewind/pyH2A>, <https://doi.org/10.5281/zenodo.6365957>.

Keywords

electrolysis, green hydrogen, photocatalysis, photovoltaics, techno-economic analysis, water splitting

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