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Optimizing the Operation of an Electrolyzer with Hydrogen Storage Using Two Different Methods: A Trade-Off Between Simplicity and Precision in Minimizing Hydrogen Production Costs Using Day-Ahead Market Prices

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Abstract: The potential for hydrogen is high in industrial processes that are difficult to electrify. Many companies are asking themselves at what cost they can produce hydrogen using water electrolysis with hydrogen storage. This article presents a user-friendly and less computationally intensive method (called method 1 in the following) for determining the minimum of the levelized cost of hydrogen (LCOH) by optimizing the combination of electrolyzer size and hydrogen storage size and their operation, depending on electricity prices on the day-ahead market. Method 1 is validated by comparing it with a more accurate and complex method (called method 2 in the following). The methods are applied to the example of a medium-sized industrial company in the mechanical engineering sector with a total natural gas demand of 8 GWh per year. The optimized LCOH of the analyzed company in method 1 is 5.00 €/kg. This is only slightly higher than in method 2 (4.97 €/kg). The article shows that a very good estimate of the LCOH can be made with the user-friendly and less computationally intensive method 1. For further validation of the methods, they were applied to other companies and the results are presented below.

Keywords: optimization methods; hydrogen; electrolyzer; hydrogen storage; companies; hydrogen production costs; electricity market; LCOH

Citation: Saars, L.; Madsen, M.; Meyer, J. Optimizing the Operation of an Electrolyzer with Hydrogen Storage Using Two Different Methods: A Trade-Off Between Simplicity and Precision in Minimizing Hydrogen Production Costs Using Day-Ahead Market Prices. *Energies* **2024**, *17*, 5546. https://doi.org/10.3390/en17225546

Academic Editor: Giovanni Esposito

Received: 9 October 2024
Revised: 31 October 2024
Accepted: 5 November 2024
Published: 6 November 2024

1. Introduction

At the Climate Conference in Paris in December 2015, 197 countries agreed on a unified climate protection agreement with the overarching goal of limiting global warming to "well below" two degrees Celsius compared to pre-industrial levels [1]. On 24 June 2021, the German government passed a new Climate Protection Act. The act includes raising Germany's greenhouse gas reduction target for 2030 to a 65 percent reduction compared to 1990 levels. Additionally, greenhouse gases are to be reduced by 88 percent by 2040, with binding achievement of greenhouse gas neutrality by 2045. Furthermore, the revised act also tightened the requirements in individual sectors. As a result, among others the climate policy pressure on the sector industry is increasing [2].

The industrial sector is the second-largest emitter of emissions in absolute terms in Germany (155 million tons of CO_2 equivalent in 2023 [3]), after the energy sector, which places increasing responsibility on the industrial sector to meet the climate targets [4]. Electrolyzers will be important not only for the energy industry but also for the industrial sector, as they enable the decarbonization of processes that are difficult to electrify. Particularly in industries such as chemicals, steel, and cement, the use of green hydrogen, produced via electrolysis from renewable electricity, can significantly reduce the reliance on fossil fuels [5–7].

The expansion of power plant capacities in the field of wind and solar energy will result in electricity generation becoming more volatile compared to conventional nuclear and coal power plants [8,9]. Solar radiation and wind availability are dictated by nature and cannot be adjusted to the European energy demand [10]. As a result, the increased expansion of renewable energies will lead to more frequent situations in the energy market where electricity production exceeds conventional demand, resulting in a negative residual load [11,12]. With increasingly fluctuating prices on the day-ahead market, the ability to store energy is also becoming more economically interesting [13,14]. There is scientific consensus that an energy supply with high shares of renewable energy will not be feasible without short- and long-term storage solutions [15,16]. In this context, chemical storage systems are expected to play a crucial role in the energy system of the future. Additionally, hydrogen (up to certain volume percentages) can be injected into the natural gas grid without restriction [17,18].

Water electrolysis using electricity from renewable energy sources with a hydrogen storage system will play a central role in future energy markets, as it provides a method for the short-, medium-, and long-term storage and utilization of electricity from renewable energy sources [19–21]. Through electrolysis, electricity from renewable sources such as wind and solar energy can be used to split water (H_2O) into hydrogen (H_2) and oxygen (O_2). Hydrogen can serve as a clean energy carrier in various sectors, including transportation and industry, enabling the decarbonization of these sectors [22–25].

This article presents a user-friendly method that can be used to make a good estimate of the levelized cost of hydrogen (LCOH) in an industrial setting and compares it with a precise and complex method to validate it. Two methods for modeling and optimizing the operation of an electrolyzer with hydrogen storage are therefore presented and compared. This article shows that a simple dynamic surface can provide a preliminary estimate of the optimal size of electrolyzer and hydrogen storage, depending on the hydrogen demand profile and electricity prices on the day-ahead market. The methods are applied to different companies and industries. The validation is described in the text using the example of a medium-sized industrial company in the mechanical engineering sector with a total natural gas demand of 8 GWh per year. The results for further companies can be found in Appendix A. The aim of both methods is to identify the optimal constellation of electrolyzer and hydrogen storage size and their operation to minimize the LCOH by taking advantage of the best prices on the day-ahead market.

Since flexible operation is essential for the electrolyzer considered in the model, alkaline water electrolysis (AEL) technology and solid oxide electrolysis (SOEL) technology are not further considered due to their high operating temperatures and the associated longer start-up times [26–28]. The focus of this article is therefore on the modeling and optimization of a proton exchange membrane (PEM) electrolyzer, which is particularly distinguished by its flexible operation. Table 1 below shows that PEM electrolysis compared to AEL and SOEL technology has great potential for flexibility electricity markets.

Table 1. Overview of electrolysis types and their potential for flexibility markets [26].

Electrolysis Technology	Reaction Time (Cold Start)	Frequency Containment Reserve (FCR) Full Offer Power: 30 s Min. Size: 1 MW Provision: 4 h	Automatic Frequency Restoration Reserve (aFRR) Full Offer Power: 5 min Min. Size: 1 MW Provision: 15 min	Manual Frequency Restoration Reserve (mFRR) Full Offer Power: 12.5 min Min. Size: 1 MW Provision: 15 min
Alkaline water electrolysis	1 min–10 min	Yes—with restrictions	Yes—with restrictions	Yes
Proton exchange membrane electrolysis	1 s to 5 min	Yes—with restrictions	Yes	Yes
Solid oxide electrolysis	<60 min	No	No	No

Hydrogen storage is typically classified into physical and metal-based categories [29]. Small-scale hydrogen storage ranges from a few grams to 10 kg of hydrogen, suitable for laboratory use and portable applications. Medium-scale storage extends from 10 kg to several tons, ideal for industrial applications and local distribution. Large-scale storage encompasses several tons to 100 tons of hydrogen, typically used for regional energy systems [30]. Therefore, for the modeling of an electrolyzer with hydrogen storage in industrial companies, the focus is on medium-scale hydrogen storage. Medium-scale hydrogen storage generally involves either compressed hydrogen stored in high-pressure tanks or liquefied hydrogen stored in cryogenic tanks [30,31]. To liquefy hydrogen, it must be cooled to a temperature below −253 °C, which is not only time-consuming but also consumes nearly 40% of the hydrogen's energy content [32]. Therefore, liquid hydrogen is more suited for long-distance transport and aviation. Liquid hydrogen can be transported on a large scale using trailers or specialized ships equipped with appropriate tanks for intercontinental hydrogen transport [30,33]. For industrial applications, a medium-sized high-pressure storage system that stores hydrogen in a gaseous state under high pressure is therefore appropriate. In the context of the modeling, it is assumed that a high-pressure storage system will be installed at the industrial site, with its size determined through optimization.

The existing models for optimizing the operation of an electrolyzer with hydrogen storage are not developed on a corporate level, but rather focus on the participation of the electrolyzer in the electricity market and the associated energy system-supporting operation.

The doctoral thesis by Martin Kopp, which was submitted to the Department of Electrical Engineering/Computer Science at the University of Kassel in 2018, focuses on the optimization of the operation of a concrete electrolyzer with a nominal electrical output of 6 MW as part of the "Energiepark Mainz" project [34]. In the model, there is no condition that specifies a hydrogen demand that must be covered. The optimization of the operation cannot be applied to companies from industry. The methods of Martin Kopp therefore differ fundamentally in two aspects from the methods presented here: (1) The methods cannot be applied at a corporate level and do not take into account a predetermined fixed hydrogen demand that must be covered, and (2) no user-friendly and less computationally intensive simulation tool is developed that enables users to obtain an initial estimate of the hydrogen production costs.

The article "A multi-stage stochastic dispatching method for electricity-hydrogen integrated energy systems driven by model and data" by Yang et al. proposes a multi-stage coordinated dispatching framework of "day-ahead deterministic dispatching—online security monitoring—intra-day flexible correction" [35]. The article uses a stochastic approach and combines deterministic models with deep learning and stochastic optimization to monitor and adjust uncertainties in real time. In the article presented here, uncertainties only play a role insofar as they influence electricity prices on the day-ahead market. Here, flexibility is achieved through the behavior of the electrolyzer and the use of hydrogen storage, but without machine learning methods for uncertainty forecasting. The main difference between the two articles is that on the one hand a comprehensive and multi-level optimization model for a hybrid energy supply is developed, while on the other hand a cost-efficient optimization of hydrogen production on a daily basis is achieved, aiming at user-friendliness and low computational requirements.

Hydrogen has a very low volume-related energy density and a high mass-related energy density compared to fossil fuels, which would result in extremely large hydrogen storages [36,37]. Compressing hydrogen to a high pressure is not only necessary in order to store a large amount of energy but is also very energy-intensive. The compression work in this model is calculated by first determining the equation of state and the caloric equation of the gas to be compressed. A simplification for calculating the energy used for compression is to assume an isentropic and adiabatic process [38].

$$W = \int_{V_1}^{V_2} p\,dV \tag{1}$$

Assuming that the hydrogen to be compressed behaves like an ideal gas, the following formula is obtained [38].

$$W_{\Delta S=0,\text{ideal}} = \frac{\gamma}{\gamma - 1} RT_1 \left[\left(\frac{p_2}{p_1} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right], \tag{2}$$

with T_1 and p_1 as temperature and pressure before compression, and with the simplified assumption: $\gamma = \frac{c_p}{c_v} = 1.4$ [38]. The actual compression is not reversible, so that the energy actually required is usually determined as follows using an isentropic compression efficiency η_{adiabat} [39]:

$$W = \frac{W_{\Delta S=0,\text{ideal}}}{\eta_{\text{adiabat}}} \tag{3}$$

where η_{adiabat} usually has values in the range of 0.75–0.90 [38,40,41]. The limited efficiency of an electric drive of 0.90–0.98 is then multiplied by this efficiency so that the required power or energy input can be calculated in kWh [38,40]. The actual compression can also be described as an interpolation of the above ideal compression and isothermal compression. Depending on the equation of state, the isothermal compression can be determined as follows [38,39].

$$W_{\Delta T=0,\text{ideal}} = RT\ln\frac{V_2}{V_1} \tag{4}$$

The interpolation of ideal and isothermal compression is used in this article to determine the electricity demand of the compressor that compresses the hydrogen to a high pressure for the high-pressure storage in the model. The pressure of the hydrogen storage can then be freely selected in the dynamic tool. The electricity used to compress the hydrogen from the initial pressure p_1, i.e., the operating pressure of the electrolyzer, to the final pressure p_2, i.e., the pressure in the hydrogen storage, is then taken into account in the model.

2. Methods

For the transferability of the results to all constellations of nominal electrolyzer output and storage size, the unit (electrolyzer) full load hours are introduced below. For example, if an electrolyzer can produce 1 kg of hydrogen per hour, an associated storage system with a storage capacity of 10 kg of H_2 corresponds to a storage capacity of 10 full load hours.

The basis for optimizing the size of the electrolyzer and hydrogen storage is a natural gas demand profile from an industrial company, provided with hourly resolution. Additionally, an oxygen and heat demand profile can be supplied to the tool. Waste heat with a temperature level of approximately 70 °C is generated during the electrolysis process and can be used too [38–43]. In the model presented in this article, the optimization of the electrolyzer and hydrogen storage system is focusing on the production and use of hydrogen. The model can also take into account the by-products oxygen and waste heat that can have a positive impact on the LCOH if they are used on site, but the consideration of by-products is not part of this article and will be analyzed in another publication. The use and sale of oxygen and waste heat can have a significant influence on the result of the LCOH calculation.

The example company from the mechanical engineering sector which is used in both methods has a natural gas demand of 8 GWh per year. The natural gas demand profile of the example company from 2023 is shown in the following Figure 1.

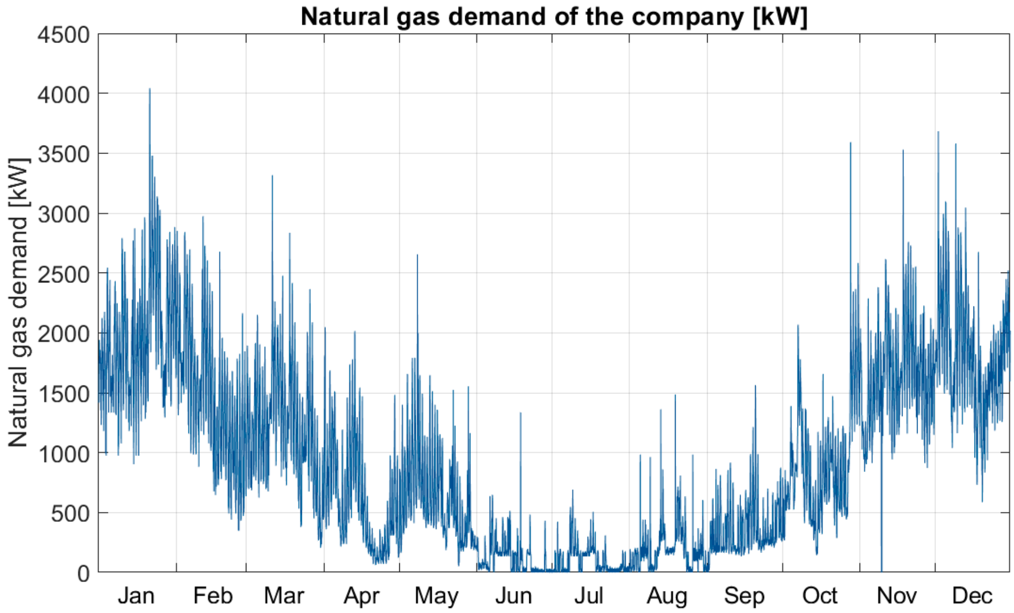


Figure 1. Natural gas demand profile of the example company from 2023 used in the model.

The hourly resolved electricity market prices on the day-ahead market are exported from the "Energy-Charts" website of the Fraunhofer Institute for Solar Energy Systems ISE and used in the model [42]. Since electricity deliveries are traded for each hour of the following day on the day-ahead market, it is assumed that the forecast period for electricity procurement in the industrial company is 24 h. The electricity prices from the day-ahead market that go into the optimization model are therefore always considered 24 h in advance. The forecast period can also be made variable in the model. The electricity prices on the day-ahead market in 2023 are shown in the following Figure 2. The largest outliers in the electricity price data set were adjusted. The assumptions made regarding other ancillary electricity costs such as levies and taxes are shown below.

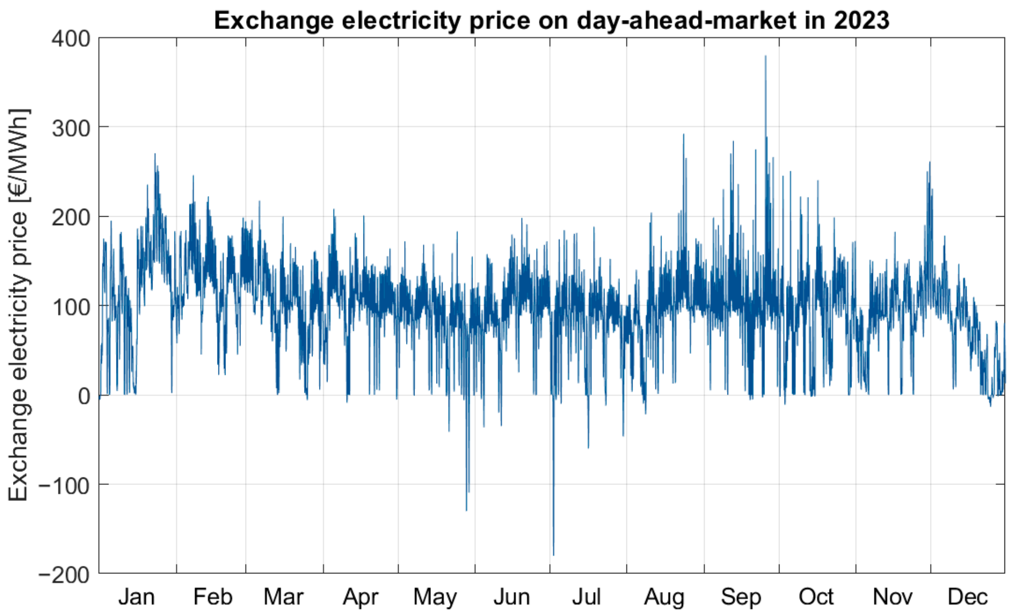


Figure 2. Exchange electricity prices on the day-ahead market from 2023 used in the model.

The problem is formulated in both methods as a nonlinear programming (NLP) optimization problem to determine the cost-optimal operation of the electrolyzer with hydrogen storage. The described optimization problem represents an NLP because the objective function is nonlinear. This means that the mathematical relationships between the variables cannot be represented by linear equations or inequalities [43]. The LCOH is to be minimized through optimization. The objective function in the model is therefore the following [44,45]:

$$\mathrm{LCOH} = \min \frac{I_0(x,y) + \sum_{t=1}^{\overline{T}} \frac{A_t(x,y) + \min J_t\left(c^T L\right)}{(1+i)^t}}{\sum_{t=1}^{\overline{T}} \frac{m_{H2}(x,y)}{(1+i)^t}} \text{ with} c = f(x,y), \tag{5}$$

$$\text{and } J = \min_L c^T L,\ c \in \mathbb{R}^n, L \in \mathbb{Q}[0 \le L \le 1]^n, \tag{6}$$

with the following constraints for the variable parameters: $x \in \mathbb{Q}[0 \le x \le 10]$, $y \in \mathbb{Q}[0 \le y \le 24]$.

In addition, x represents nominal electrical power of electrolyzer [MW], y represents hydrogen storage size [electrolyzer full load hours], I_0 represents investment at time t = 0 (CAPEX) [€], A_t represents annual operating costs (OPEX, excluding electricity costs) in year t [€/a], J_t represents electricity costs in year t [€/a], m_{H2} represents quantity of hydrogen produced in year t [kg/a], c^T represents hourly exchange electricity prices (transposed) [€/MWh], L represents load electrolyzer, I represents internal rate of return of the company [%], $\overline{T}$ represents number of periods of the investment, t represents time interval, and n represents number of hours in the year times the number of constraints.

The method for calculating the hydrogen production costs in a dynamic economic efficiency calculation is described in detail below. The limitations of the variable parameters for electrolyzer and hydrogen storage size are therefore as follows:

- The power of the electrolyzer is limited in the model and should vary between 0 MW and a maximum of 10 MW: $0 \le P_{Ely,elektr.} \le 10$;
- The size of the hydrogen storage is limited in the model taking into account the forecast period. The forecast period is 24 h, so that the hydrogen storage should not exceed 24 electrolyzer full load hours. The hydrogen storage size should therefore vary between 0 electrolyzer full load hours and the number of hours in the forecast period in electrolyzer full load hours: $0 \le K_{storage} \le 24$.

2.1. Dynamic Profitability Analysis and Calculation of LCOH

In the dynamic profitability analysis, all cash flows are differentiated over time. The LCOH is calculated as part of the profitability analysis. The calculation is dynamic, so that the costs are set in relation to the amount of hydrogen converted over the entire lifetime:

$$\mathrm{LCOH} = \frac{I_0(x,y) + \sum_{t=1}^{\overline{T}} \frac{A_t(x,y)}{(1+i)^t}}{\sum_{t=1}^{\overline{T}} \frac{M_{H2}(x,y)}{(1+i)^t}}, \tag{7}$$

with x: nominal electrical power of electrolyzer, y: hydrogen storage size, I_0: investment at time t = 0 (CAPEX), A_t: annual operating costs (OPEX, including electricity costs) in year t, M_{H2}: quantity of hydrogen produced in year t, i: internal rate of return of the company, $\overline{T}$: number of periods of the investment, and t: time interval.

The precise and reliable assumption of component investments in the model is essential for the dynamic profitability analysis, as it forms the basis for well-founded decisions on profitability and long-term planning. As part of this article, comprehensive literature research was carried out and cost functions for the electrolyzer and compressor were established. The following two figures (Figure 3) show the cost functions for the electrolyzer and compressor used in the model to calculate the LCOH [46–54].

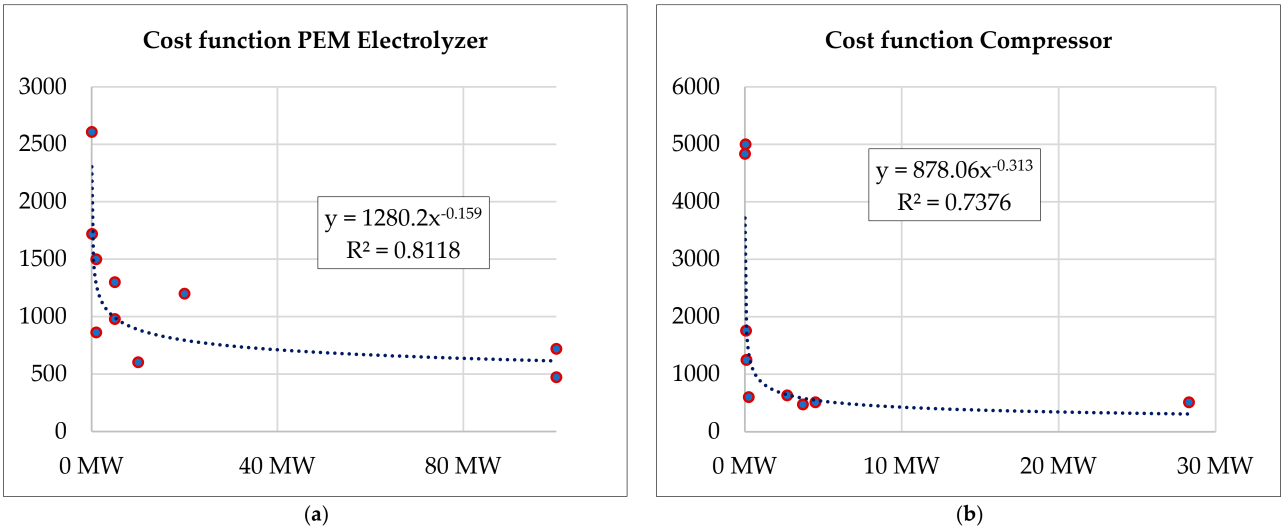


Figure 3. (**a**) Cost function for PEM electrolyzer [46–51]; (**b**) cost function for compressor [47,52–54].

The cost functions presented in this subsection are transferred to the model and provide a reliable and literature-based basis for the dynamic profitability analysis at the example company. For the hydrogen storage, which stores hydrogen in a gaseous state at high pressure as described above, the model assumes a fixed value for the specific costs in € per kg of hydrogen of 579 €/kg [55,56].

To calculate the LCOH, assumptions are made regarding the electrolyzer, the hydrogen storage, the compressor, the dynamic profitability analysis, and the ancillary electricity costs, which are presented below in Tables 2–6. Ranges for key figures were determined from the literature, from which the corresponding assumptions are then defined. The assumptions can be easily adjusted in the model.

Table 2. Overview of the assumptions made for the PEM electrolyzer in the model.

Position	Model	Research	Source
Investment [€/kW]	See cost function		
Operating temperature [degrees Celsius]	60	50–60	[47,57–61]
Operating pressure [bar]	50	20–80	[47,57–59,61–63]
Lifetime stacks [years]	40,000	30,000–100,000	[47,48,58–63]
System efficiency electrical [%]	63	46–83	[49,50,58–60,64–69]
Amortization period [years]	20	20	[60,62,63]
Funding rate [%]	40%	-	
Annual operating costs [% of investment]	3%	3–5	[37,48,58,60,62,63]
Stack replacement costs [€/kW]	800	420–1.060	[37,48,62,63]
Water requirement [l/kg]	12	9–25	[70,71]

Table 3. Overview of the assumptions made about hydrogen storage in the model.

Position	Model	Research	Source
Pressure level [bar]	500	150–950	[30,59,72,73]
Amortization period [years]	20	-	-
Investment [€/kg]	579	515–579	[56,59,74]
Funding rate [%]	40	-	-
Annual operating costs [% of investment]	6	4–6	[50]

Table 4. Overview of the assumptions made about the compressor in the model.

Position	Model	Research	Source
Investment [€/kW]	See cost function		
Output pressure p_1 (operating pressure of the electrolyzer) [bar]	50	20–80	[47,57–59,61–63]
Temperature before compression T_1 [K]	293.15	-	-
Amortization period [years]	20	-	-
Funding rate [%]	0	-	-
Annual operating costs [% of investment]	6	4–6	[50]
Isentropic efficiency [%]	88	0.75–0.90	[38,40,41]
Efficiency electr. drive [%]	98	0.90–0.98	[38,40]
Isentropic exponent Kappa	1.40	1.40	[38]
Specific gas constant R [J/kgK]	4124	4124	[38,75]

Table 5. Overview of the assumptions made in the dynamic profitability analysis.

Position	Model
Period under review [a]	20
Calculatory interest rate [%]	4.50
Cost surcharge electricity price through trading on the exchange (purchasing) [%]	10
Other one-off investment costs (planning, feasibility study, expert report, etc.) [% of total investment]	15
Water costs [€/m^3]	4.5

Table 6. Overview of the assumptions made regarding ancillary electricity costs.

Position	Model
Grid fees [€/MWh]	0
Electricity tax [€/MWh]	0
Concession charge [€/MWh]	1.10
Electricity Network Charges Ordinance levy [€/MWh]	0
Other fees [€/MWh]	0
Value-added tax (VAT) [%]	0

The model makes the simplified assumption that the electricity used for electrolysis is exempt from almost all ancillary electricity costs. With the delegated act, presented by the EU Commission in February 2023 on the definition of renewable hydrogen, this assumption would also correspond to reality, on the assumption that green hydrogen is produced [76]. It is therefore assumed that only the concession charge has to be paid.

2.2. Method 1—Calculation of LCOH with Approximate Schedules (Focus on Simplicity)

Method 1 presented in this article can also be easily implemented in Excel (version 14.0 or higher) using for example the evolutionary algorithm (EA). The method is significantly less computationally intensive and user-friendly. First, the hydrogen demand in electrolyzer full load hours for each hour of the year is determined. Additionally, the hydrogen demand in electrolyzer full load hours for the next 24 h (or an alternative forecast period) is calculated for each hour. Subsequently, the corresponding lowest electricity prices on the day-ahead market are identified for each hour based on the determined hydrogen demand for the next 24 h. For example, if the hydrogen demand over the next 24 h is 14 electrolyzer full load hours, the 14th lowest-priced hour within the next 24 h is identified. The operation of the electrolyzer and hydrogen storage is then dependent on several factors. Whether the electrolyzer only meets the hydrogen demand in the respective hour or operates at full load depends on several constraints, which are described below.

Economic constraint—comparison of electricity market prices: The electrolyzer will only be operated at full load if the electricity market price in the considered hour is lower than the identified price during the forecast period. The forecast period encompasses the future hours for which demand is projected. First, the hydrogen demand is determined in electrolyzer full load hours at time $t_{forecast}$:

$$H_{forecast}(t) = \sum_{t}^{t+t_{forecast}} H(t), \tag{8}$$

where $H_{forecast}(t)$ is the hydrogen demand during the forecast period as a function of time t and $H(t)$ is the hydrogen demand at time t. The determined electrolyzer full load hours in the forecast period are then assigned an electricity price on the day-ahead market. The model compares the electricity price at time t with the lowest price identified during the forecast period. This constraint can be formalized as follows:

$$Pr(t) < Pr(H_{forecast}(t)), \tag{9}$$

where $Pr(t)$ is the current electricity market price and $Pr(H_{forecast}(t))$ is the lowest price identified during the forecast period.

Capacity constraint—availability of capacities in the hydrogen storage system: Another constraint for operating the electrolyzer at full load is the availability of sufficient storage capacity in the hydrogen storage. The current filling level of the storage must be less than the maximum capacity of the storage. This constraint can be formalized as:

$$L_{storage} < K_{storage}, \tag{10}$$

where $L_{storage}$ is the current storage level, and $K_{storage}$ is the maximum capacity of the hydrogen storage.

Cover demand—securing the hydrogen demand: The third constraint is that the hydrogen demand must be covered every hour. The electrolyzer must be operated in such a way that the hydrogen demand of the industrial company under consideration is completely covered every hour. This constraint can be formalized as follows:

$$H_{2demand,t} \leq H_{2production,t} + H_{2storage,t} \tag{11}$$

where $H_{2demand,t}$ is the hydrogen demand in hour t, $H_{2production,t}$ is the hydrogen production of the electrolyzer in hour t, and $H_{2storage,t}$ is the hydrogen available from storage in hour t.

By defining the constraints described above, a generation profile for the electrolyzer and a profile for the filling level of the hydrogen storage are obtained in hourly resolution as a function of the electrolyzer size and hydrogen storage size. The optimized results can then be used to calculate the LCOH.

2.3. Method 2—Calculation of LCOH with Ideal Schedules (Focus on Precision)

In order to evaluate the simplified method 1, the electrolyzer schedule in method 2 is first determined hourly over the year with a solver in a subordinate optimization. The objective is to reduce electricity costs by identifying the optimal time periods for consumption. As in method 1, the same forecast period is applied for each hour. The ideal sizes of the electrolyzer and the storage system (with ideal operation of the electrolyzer) are then determined in a higher-level optimization (as described above). The second and third constraints from method 1 also apply.

Referring to traveling salesman problems [77], a similar approach is used. The function is formulated with the following:

$$A \cdot L \leq b,\ A \in [-1, 0, 1]^{n \times n},\ b \in \mathbb{R} \tag{12}$$

whereby n represents the number of hours h in the forecast period. As already described above, the binary decision vector is noted as L with length of the forecast period and c contains the hourly exchange electricity prices. Inequality constraints of this integer nonlinear program can be passed to the solver as A and b. Because the inequality constraints specify that A·L is less than or equal to b, the contents of A and b are negated in the following to invert the constraints. For the first period, A_1 is filled with −1 as the lower triangular matrix. The vector b_1 contains the cumulative hydrogen demand d_h of the respective hours.

The constraints A_1 and b_1 ensure that the hydrogen demand is always covered. As an example, a time period of 3 (instead of 24) hours is shown in the representation of the constraints.

$$h = 1 \quad 2 \quad 3 A_1 = \begin{pmatrix} -1 & 0 & 0 \\ -1 & -1 & 0 \\ -1 & -1 & -1 \end{pmatrix} b_1 = \begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix} \tag{13}$$

The following example shows the fictitious case where hydrogen is only required in hour 2. Constraints A_2 and b_2 ensure that the hydrogen storage has a finite capacity. In hour 0 at the start of optimization, the hydrogen storage is empty. In this example, the storage has a capacity of 10 electrolyzer full load hours and each 1 full load hour of hydrogen is required in hour 2 and 3 of the period. Accordingly, the storage system may produce a maximum of 10 full load hours of hydrogen within the initial period and a maximum of 12 full load hours after 3 h.

$$h = 1 \quad 2 \quad 3 A_2 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix} b_2 = \begin{pmatrix} 10 \\ 11 \\ 12 \end{pmatrix} \tag{14}$$

A_1 and A_2 are concatenated vertically to A, and vectors b_1 and b_2 to b, respectively, to hand A and b over to the solver. This subordinate optimization results in the most favorable electrolyzer operation for a given storage size and electrolyzer size.

A higher-level optimization then varies the electrolyzer and storage sizes, identifies the optimal electrolyzer schedule with the lower-level optimization in each case, and determines the ideal electrolyzer and storage size by minimizing the total costs (described in the subsection before) without additional constraints.

The difference between the two methods is illustrated using the example of a 10 h schedule in the following Table 7. From hour 5 to hour 7 three electrolyzer full load hours of hydrogen are needed (see column 3). The constraint is that the hydrogen demand must be covered every hour. In method 1, the three most favorable prices (60, 70, and 85 €/electrolyzer full load hour) are determined over the ten hours (forecast period in the example). The electrolyzer does not run in hour 2 because the price of 90 €/electrolyzer full load hour is not one of the three identified prices. In method 1, the optimizer therefore does not know that the electrolyzer will have to be operated at an even higher price in hour 7 in order to cover the hydrogen demand. In an ideal schedule as shown in method 2, the electrolyzer would run in hour 2. As the example in Table 7 shows, the difference in the result of the two methods (255 € compared to 245 €) is not great, but nevertheless the computing time is significantly higher and the user-friendliness lower in method 2.

Table 7. Difference between the two methods illustrated with an example of 10 h.

Hour	Electricity Costs [€/Electrolyzer Full Load Hour]	H_2 Demand [Electrolyzer Full Load Hour]	Electrolyzer Runs Method 1, On/Off [Full Load Hours]	Electrolyzer Runs Method 2, On/Off [Full Load Hours]
1	100	0	0	0
2	90	0	0	1
3	100	0	0	0
4	85	0	1	1
5	100	1	0	0
6	70	1	1	1
7	100	1	1	0

Table 7. *Cont.*

Hour	Electricity Costs [€/Electrolyzer Full Load Hour]	H_2 Demand [Electrolyzer Full Load Hour]	Electrolyzer Runs Method 1, On/Off [Full Load Hours]	Electrolyzer Runs Method 2, On/Off [Full Load Hours]
8	60	0	0	0
9	100	0	0	0
10	100	0	0	0
	Electricity costs with schedule from method 1:			**255.00 €**
	Electricity costs with schedule from method 2:			**245.00 €**

3. Results

To validate the methods described above, natural gas demand profiles are used in hourly resolution from industrial companies in various sectors. The hourly gas demand profiles are transferred to the dynamic tool. All companies do not have any potential for oxygen utilization and waste heat utilization. Therefore, in the calculation there is not any positive income considered. Since the optimization is based on the gas demand profile, the fact that there is only a gas demand does not negatively impact the validation of the methods. After the gas demand profile has been transferred to the tool, the parameters are set as described above to determine an electrolyzer production profile and a profile for the hydrogen storage fill level.

First, the results are presented using the example of a mechanical engineering company with method 1. As described above, the company is a medium-sized company in the mechanical engineering sector. The company has a natural gas demand of 8 GWh per year. The optimization with method 1 for the mechanical engineering company results in a nominal electrical power output for the PEM electrolyzer of 4.52 MW and a hydrogen storage capacity of 902.36 kg. The compressor is designed in the tool based on the maximum hydrogen volume to be compressed in any hour of the year. The nominal electrical power of the compressor in the optimal configuration is 93.47 kW. When comparing the annual electricity costs of the electrolyzer without hydrogen storage to the optimal combination of electrolyzer and hydrogen storage sizes, it becomes clear that the use of hydrogen storage can achieve electricity cost savings of 296,906.74 € per year. Taking into account the funding rates, the investments amount to 2,731,793.57 € for the electrolyzer, 313,478.54 € for the hydrogen storage, and 172,338.87 € for the compressor.

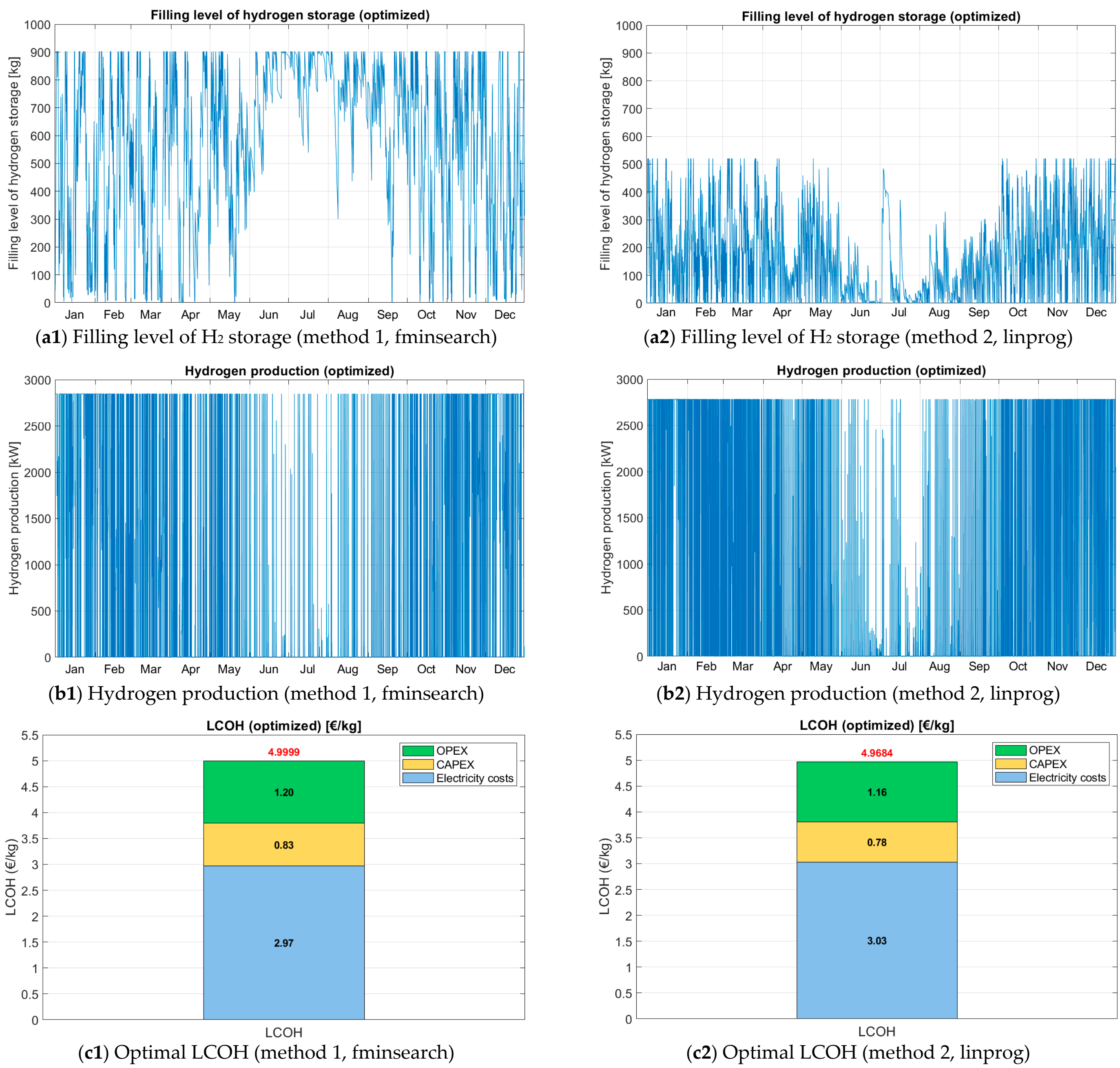
The following Table 8 shows the results of the two methods. Method 1 uses the function fminsearch and method 2 uses the function linprog in Matlab (version R2024b).

Table 8. Results and comparison of the methods using the example company.

Result	Method 1 (Fminsearch in Matlab)	Method 2 (Linprog in Matlab)
Nominal electrical power electrolyzer [MW]	4.52 MW	4.42 MW
Hydrogen storage size [kg]	902.36 kg	520.40 kg
Nominal electrical power compressor [kW]	93.47 kW	91.35 kW
Saved electricity costs with hydrogen storage [€/a]	296,372.10 €/a	280,904.00 €/a
Optimal LCOH [€/kg]	5.00 €/kg	4.97 €/kg

The following figures (Figure 4) show the hydrogen storage fill level and the hydrogen production profile of the modeled electrolyzer in hourly resolution over the year and the results for the LCOH in both methods for the example company.

The results show that an initial estimate can be made using the simplified method 1 which can also be implemented with the evolutionary algorithm in Excel. The production costs are only slightly higher in method 1, so that this method enables an estimate of the prices at which hydrogen can be produced at the industrial site. Method 1 therefore offers great potential to provide industrial companies with an Excel tool to estimate the hydrogen production costs in the company. Depending on the electricity prices on the day-ahead market, it can be estimated whether a switch to hydrogen is an economical alternative.



(**a1**) Filling level of H_2 storage (method 1, fminsearch) (**a2**) Filling level of H_2 storage (method 2, linprog)

(**b1**) Hydrogen production (method 1, fminsearch) (**b2**) Hydrogen production (method 2, linprog)

(**c1**) Optimal LCOH (method 1, fminsearch) (**c2**) Optimal LCOH (method 2, linprog)

Figure 4. Comparison of methods: (**a1**,**a2**) Filling level of hydrogen storage; (**b1**,**b2**) hydrogen production profile; (**c1**,**c2**) LCOH.

It is noticeable that the electrolyzer is operated less frequently in method 1, but then at a higher output than in method 2. In both methods, the optimizer tries to design the electrolyzer to be as small as possible, as the electrolyzer is particularly expensive. Due to the higher level of detail in the calculation in method 2, it is possible to design the hydrogen storage system smaller and still take advantage of favorable electricity prices.

The following Figure 5 shows the LCOH in method 1 as a function of the electrolyzer and hydrogen storage size.

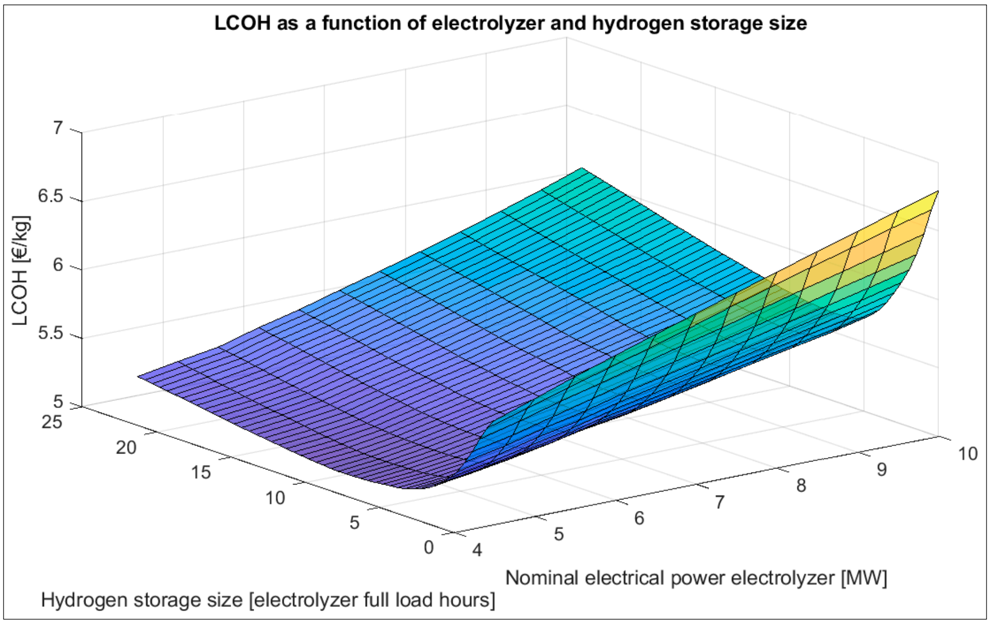


Figure 5. LCOH in method 1 as a function of electrolyzer and hydrogen storage size.

4. Discussion

The results show that the simplified method 1 can be used to estimate the LCOH, but the electrolyzer and hydrogen storage system are larger and the electricity cost savings are therefore greater than in method 2. The LCOH in method 1 (5.00 €/kg) is only slightly higher than in method 2 (4.97 €/kg). Method 1, which requires significantly less computing time and is very user-friendly, can therefore be used as a first approximation. In the example company from the mechanical engineering sector, the flexible operation of the electrolyzer with hydrogen storage and the associated use of favorable electricity prices on the day-ahead market means that hydrogen can be produced for approx. 5.00 €/kg. This corresponds to 15 cents per kWh. At around 3.50 cents per kWh at the beginning of 2024, wholesale prices for natural gas are still slightly above the pre-crisis level due to the war in Ukraine [78]. The purchase price for natural gas for the example company is around 6 to 8 cents per kWh of natural gas. A switch to hydrogen as an energy source with self-generation through electrolysis is therefore not currently economical. If the exchange electricity prices on the day-ahead market become even more volatile and the electrolyzer can be operated even more at times with negative electricity prices, the LCOH can be further reduced. There is therefore a need for further research to create suitable scenarios for the energy supply of the future and to investigate the effects on the LCOH.

In addition, essential parameters such as assumptions regarding investments in electricity costs have a significant impact on the results. Sensitivity analyses can provide further insight. Figure 6 below illustrates the influence of the parameters on the result of the LCOH calculation with and without funding of the electrolyzer. The electricity costs and the investment for the electrolyzer have a significant influence on the result. If the costs for the individual components of the electrolyzer can be reduced through technical progress, this has a strong positive influence on the LCOH. In addition, the impact of the funding rate for the electrolyzer on the result is shown to illustrate that funding has a significant influence that must definitely be taken into account. As the reduction in electricity costs through even larger storages is not significantly higher, an increase in the specific costs for the storage only has a minor effect on the result. Figure 6 also shows the company's purchase price for natural gas (7.5 cents per kWh). This shows the large gap between the purchase price of natural gas and the company's own hydrogen production costs. The gap could be closed long-term by increasing electricity price fluctuations, rising natural gas prices, or falling investment in the electrolyzer. There is a need for further research to draw up corresponding scenarios and compare them to find out which parameters need to change in order for companies to produce their own hydrogen economically.

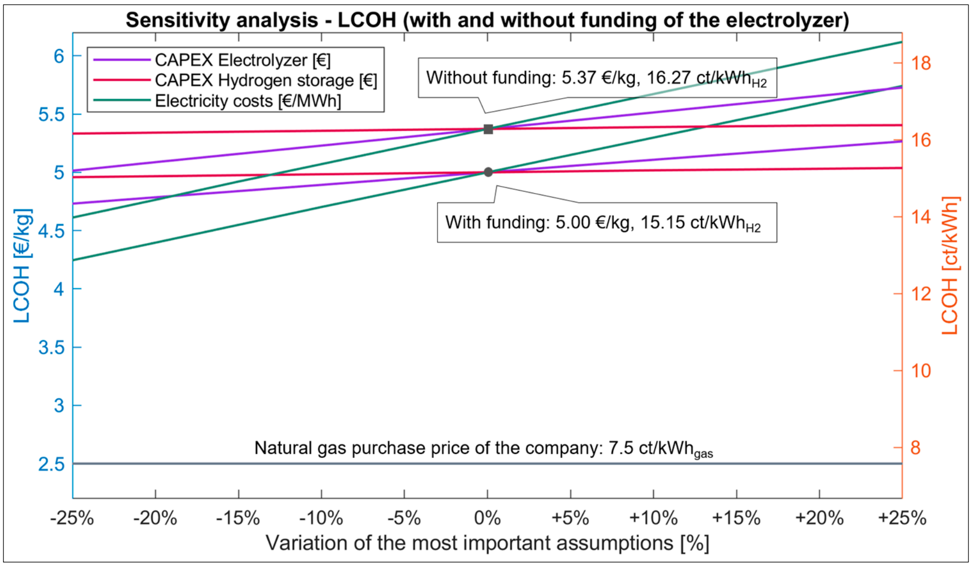


Figure 6. Sensitivity analysis—LCOH (with and without funding of the electrolyzer).

If the example company has the potential to purchase or sell the by-products oxygen and heat, this can have a significant influence on the result of the calculation. The example company has no oxygen demand and cannot use the waste heat generated. It is therefore difficult to make a realistic assumption about the oxygen and heat prices at this point. In order to nevertheless be able to analyze the influence of the use of by-products on the hydrogen production costs, it is assumed that the example company can sell the oxygen for 2 cents per kilogram and the waste heat for 4 cents per kWh. The sale of oxygen in the optimization model leads to a reduction in the LCOH of 0.10 €/kg and the sale of waste heat leads to a reduction in the LCOH of 0.51 €/kg.

Furthermore, the fact that future natural gas grids will contain different natural gas–hydrogen mixtures requires in particular an adaptation of systems and peripherals at the end consumer in order to guarantee reliable operation should not be neglected in the future. The change in fuel composition due to the use of hydrogen has a considerable influence on the heating gas composition (proportion of water, nitrogen oxides, oxygen, etc.) in the systems. The main difficulties with H_2 concentrations above 50% by volume include noise emissions due to resonance at the burner head and overheating of the gas nozzle in the burner head [78]. As the hydrogen content increases, the flame shape, flame position, and flame color change. With a hydrogen content of 90% by volume and higher, the reaction zones become significantly more discrete and compact. This is due to the increased reactivity of hydrogen, which manifests itself in a higher flame speed and a shorter ignition delay time [79]. However, the retrofitting of equipment and peripherals to ensure hydrogen capability is disregarded in this article, simplifying the assumption that the natural gas demand measured by the energy provider in hourly resolution in the industrial company can be substituted by hydrogen. Therefore, the retrofitting of equipment and the associated costs have no influence on the hydrogen production costs determined in the model. Further research is needed to investigate the hydrogen compatibility of equipment and processes, particularly in terms of the costs associated with conversion.

Although the optimization model delivers robust and practical results, it must be emphasized that the assumptions and parameters are highly dependent on current electricity price forecasts and advancements in electrolyzer technology. A central issue remains the uncertainty in electricity price developments. Long-term planning is therefore associated with a certain degree of uncertainty, which can be mitigated through additional scenario analyses. Another critical element concerns the scalability of the methodology presented here. While its application has been successfully validated for individual companies, it remains open to what extent this methodology can also be applied to larger industrial clusters. This may require further investigation to examine the viability of the method on a larger scale. Additionally, the developed optimization model could be expanded to include an oxygen and/or heat storage system. If oxygen and heat demand profiles are also supplied to the model, the optimization could determine the ideal size for an oxygen and/or heat storage system. This is beyond the scope of this article, indicating a need for further research, allowing the presented model to be expanded accordingly.

In the long term, decarbonization and the associated fight against climate change will only be successful if short-, medium-, and long-term storage options are implemented that make a significant contribution to grid stability and security of supply. The methods presented here for developing an optimization model can help to support the transformation towards climate neutrality. Since the presented method 1 is less computationally intensive and complex, the optimization model can be used by companies shortly after publication of the article and thus make an important contribution to combating climate change.

Author Contributions: Conceptualization, L.S. and J.M.; methodology, L.S. and M.M.; validation, L.S., M.M. and J.M.; formal analysis, L.S.; investigation, J.M.; writing—original draft preparation, L.S.; writing—review and editing, L.S., M.M. and J.M.; visualization, L.S.; supervision, J.M.; project administration, L.S. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in the study are included in the article, further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

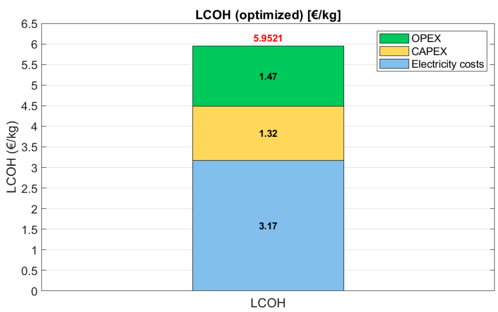
Appendix A

The results of other companies are presented below.

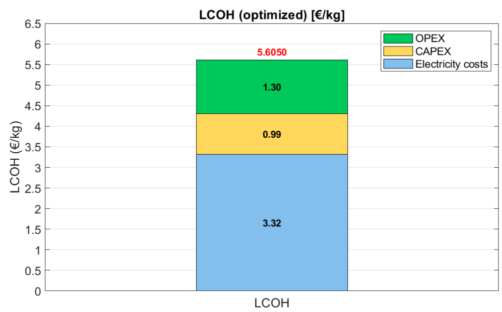
Appendix A.1. Company 2: Manufacturing Company with an Annual Natural Gas Demand of 1.57 GWh

Table A1. Overview of the most important results and comparison of the methods in Company 2.

Result	Method 1 Fminsearch Matlab	Method 2 Linprog Matlab
Nominal electrical power electrolyzer [MW]	1.15 MW	0.78 MW
Hydrogen storage size [kg]	187.33 kg	216.86 kg
Nominal electrical power compressor [kW]	23.85 kW	16.08 kW
Saved electricity costs thanks to the hydrogen storage system [€/a]	50,105.33 €/a	41,105.78 €/a
Optimal LCOH [€/kg]	5.95 €/kg	5.61 €/kg

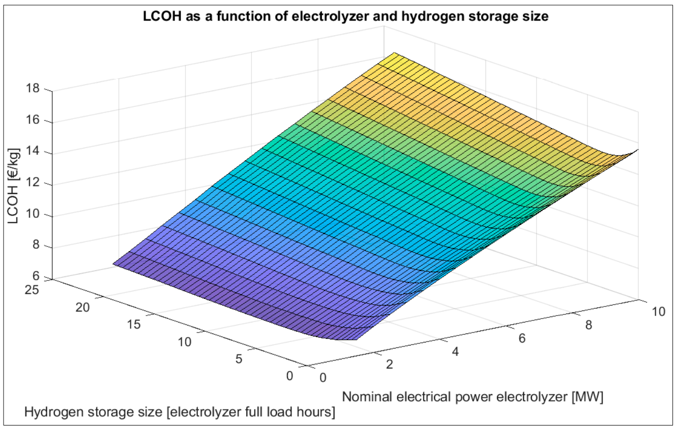


(**a1**) Optimal LCOH Company 2 (method 1, fminsearch)



(**a2**) Optimal LCOH Company 2 (method 2, linprog)

Figure A1. *Cont.*



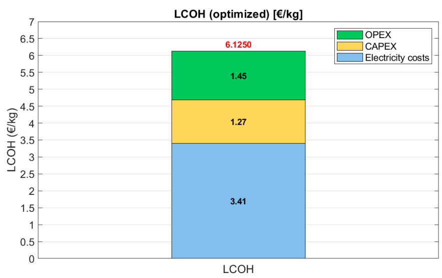
(**b**) Optimal LCOH Company 2 in method 1 as a function of the electrolyzer and storage.

Figure A1. Comparison of methods in Company 2: (**a1**,**a2**) LCOH; (**b**) LCOH in method 1 as a function of the electrolyzer and storage.

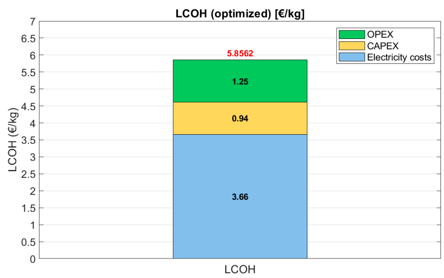
Appendix A.2. Company 3: Manufacturing Company with an Annual Natural Gas Demand of 3.40 GWh

Table A2. Overview of the most important results and comparison of the methods in Company 3.

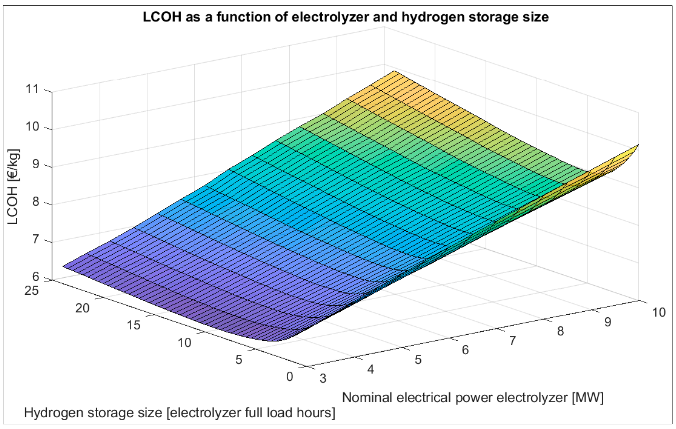
Result	Method 1 Fminsearch Matlab	Method 2 Linprog Matlab
Nominal electrical power electrolyzer [MW]	2.77 MW	1.99 MW
Hydrogen storage size [kg]	452.21 kg	228.52 kg
Nominal electrical power compressor [kW]	57.35 kW	41.09 kW
Saved electricity costs thanks to the hydrogen storage system [€/a]	123,627.54 €/a	90,113.45 €/a
LCOH [€/kg]	6.12 €/kg	5.86 €/kg



(**a1**) LCOH Company 3 (method 1, fminsearch)



(**a2**) LCOH Company 3 (method 2, linprog)



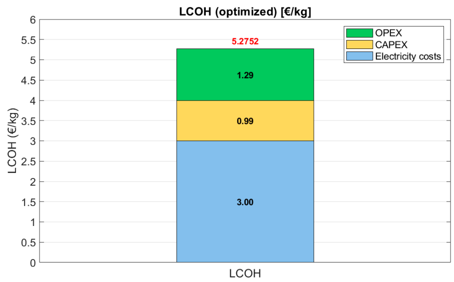
(**b**) LCOH Company 3 in method 1 as a function of the electrolyzer and storage.

Figure A2. Comparison of methods in Company 3: (**a1**,**a2**) LCOH; (**b**) LCOH in method 1 as a function of the electrolyzer and storage.

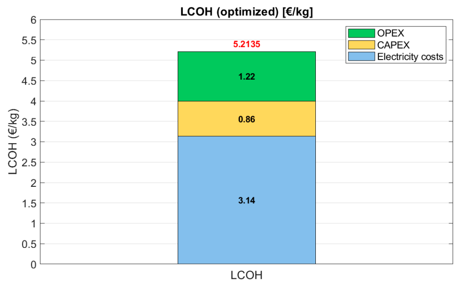
Appendix A.3. Company 4: Spirits Manufacturer with an Annual Natural Gas Demand of 1.28 GWh

Table A3. Overview of the most important results and comparison of the methods in Company 4.

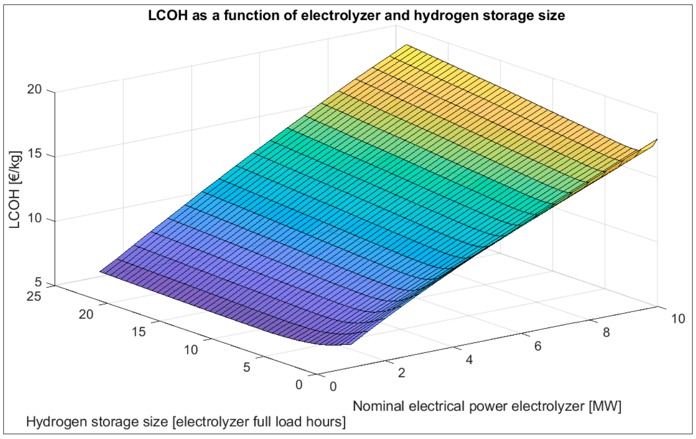
Result	Method 1 Fminsearch Matlab	Method 2 Linprog Matlab
Nominal electrical power electrolyzer [MW]	0.63 MW	0.52 MW
Hydrogen storage size [kg]	122.88 kg	142.09 kg
Nominal electrical power compressor [kW]	16.62 kW	10.73 kW
Saved electricity costs thanks to the hydrogen storage system [€/a]	51,014.71 €/a	44,459.73 €/a
LCOH [€/kg]	5.28 €/kg	5.21 €/kg



(**a1**) Optimal LCOH Company 4 (method 1, fminsearch)



(**a2**) Optimal LCOH Company 4 (method 2, linprog)



(**b**) LCOH Company 4 in method 1 as a function of the electrolyzer and storage.

Figure A3. Comparison of methods in Company 4: (**a1**,**a2**) LCOH; (**b**) LCOH in method 1 as a function of the electrolyzer and storage.

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