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Optimal design of a renewable power-to-hydrogen system for the decarbonization of a semiconductor industry

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Abstract:

Hard-to-abate industries require significant amounts of hydrogen, which is mainly used as feedstock, reducing agent and gas carrier. Currently, most of this demand is met by fossil-based hydrogen produced on-site or delivered by trailers. There is therefore huge potential to decarbonize these industries by replacing conventional grey hydrogen supply with sustainable power-to-hydrogen systems that exploit renewable energy to produce green hydrogen through electrolysis. In this work, a semiconductors production plant was considered as a case study. Hydrogen is used as gas carrier in epitaxial silicon growth and the demand is about 110 tons per year. The goal is to explore the cost-effectiveness of on-site green hydrogen production. The power-to-hydrogen system includes a photovoltaic plant, a PEM electrolyzer, a compressor, a hydrogen tank, a grey hydrogen back-up system and the electrical grid connection. The optimal system sizing was carried out by adopting the Particle Swarm Optimization (PSO) algorithm able to identify the configuration that minimizes the Levelized Cost of Hydrogen (LCOH) while ensuring the coverage of the hydrogen demand over the entire year. For a detailed techno-economic assessment, size-dependent cost functions were applied, and the lifetime of the electrochemical component was estimated based on its operating hours during the year. Results show that the cost-optimal solution is the current scenario, where only grey hydrogen is employed (LCOH equal to 4 €/kg). Different decarbonization targets (i.e., grey hydrogen share constraint in the range 0-100%) were also investigated and the resulting LCOH ranges from 4 €/kg (full grey hydrogen scenario) to 10.85 €/kg (full green hydrogen scenario). The resulting Pareto front shows two distinct regions: the reduction of grey hydrogen share from 100% (current scenario) to 30% - corresponding to a decarbonization rate of 0% to 70% - follows a smooth trend with an LCOH increase from 4 to 6.2 €/kg (first region). Higher decarbonization rates (> 70%, second region) instead lead to a steeper increase in the LCOH, reaching 10.85 €/kg in the completely decarbonized scenario (0% grey hydrogen).

Keywords

Hydrogen, Electrolysis, Optimal sizing, Hard-to-abate, CO₂ savings

1. Introduction

Electronics manufacturing currently represents a niche industrial application of hydrogen. Specifically, high purity hydrogen (i.e., higher than 99.999%) is used as a gas carrier in the semiconductor industry for the epitaxial growth of the silicon wafers.

According to Rochlitz et al. [1], 16.5 million Nm³ of hydrogen are consumed annually by the around 500 epitaxy reactors across Europe. This demand is largely met by fossil-based hydrogen (i.e., grey hydrogen) that is delivered – either compressed or liquid – by trailers to the industrial plants, or alternatively produced on-site through Steam Methane Reforming (SMR). Thus, renewable power-to-hydrogen (P-t-H) systems can represent a promising low-carbon strategy for the hydrogen supply of the semiconductor industries. In fact, using green hydrogen in hard-to-abate sectors can effectively reduce CO₂ emissions in a cost-effective way. Gärtner et al. [2] investigated the integration of a power-to-hydrogen system in a German glass industry and found out that CO₂ emissions can be reduced by up to 60% through the use of renewable hydrogen. Marocco et al. [3] investigated the role of hydrogen in decarbonizing the high-temperature heat production in the steel sector. Moreover, they highlighted that lower Levelized Cost of Hydrogen (LCOH) values can be achieved by exploiting cheaper electricity, such as that generated by on-site Renewable Energy Sources (RES). Röben et al. [4] assessed the techno-economic feasibility of reducing direct CO₂ emissions in copper production by

installing a power-to-hydrogen system. They confirmed that the electricity price is a crucial parameter to achieve a cost-efficient decarbonization. In addition, they pointed out that exploiting the by-product oxygen can boost the profitability of this solution. Gu et al. [5] carried out a techno-economic analysis of a green methanol production plant and the results emphasized the impact of the carbon price on reaching the breakeven with the conventional process. However, no studies that specifically assess the cost-effectiveness of exploiting green hydrogen in the silicon wafers manufacturing were found in the literature. Thus, the present work aims at filling this gap by proposing a detailed techno-economic optimization study for a power-to-hydrogen application in the semiconductor industry. The optimal sizing of the RES-based hydrogen production system was performed by adopting the Particle Swarm Optimization (PSO) algorithm and the effects of different decarbonization targets on the LCOH were investigated by applying the ϵ -constrain method. The PSO algorithm was chosen because its robustness and good convergence speed make it ideal for the design of energy systems [6].

The structure of this work is as follows: Section 2 describes the design methodology and reports the main techno-economic input data, Section 3 outlines the case study, Section 4 shows the results and Section 5 summarizes the conclusions.

2. Methodology

2.1. System layout

The renewable power-to-hydrogen system consists of the following components: the photovoltaic panels (PV), the electrolyzer (EL), the compressor (CP), the pressurized hydrogen tank (HT), the grey hydrogen back-up system (HBS) and the national electrical grid (GR). The schematic layout of the system is shown in Figure 1.

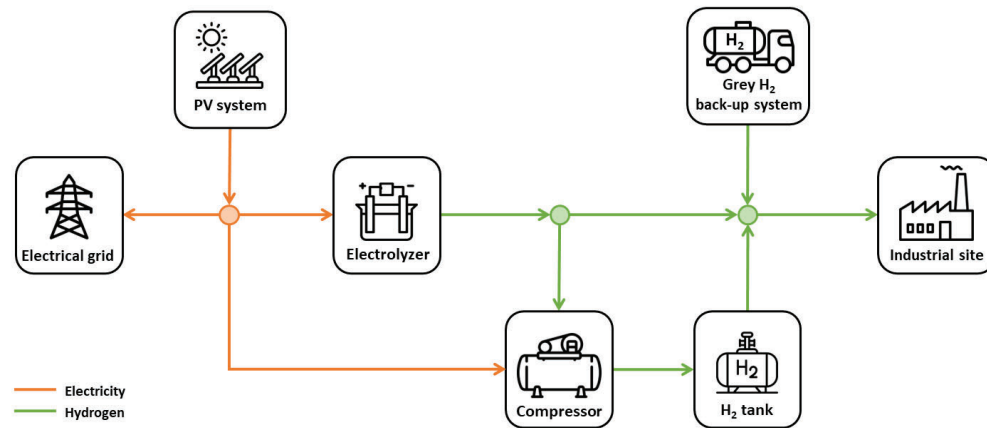


Figure 1. Schematic layout of the power-to-hydrogen system.

2.2. Modelling of the components

The modelling of the components of the power-to-hydrogen system is described below.

PV system

The PV power production was evaluated as follows [6]:

$$P_{PV}(t) = f_{PV} \cdot P_{PV,rated} \cdot \left(\frac{G_T(t)}{G_{STC}} \right) \cdot [1 + \alpha_P \cdot (T_c(t) - T_{c,STC})] \quad (1)$$

where P_{PV} (in kW) is the output power of the PV system, $P_{PV,rated}$ (in kW) is the rated power of the PV system, G_T (in kW/m²) is the incident solar radiation evaluated for the optimal configuration of tilt and azimuth angles, G_{STC} (in kW/m²) is the solar irradiance at Standard Test Conditions (STC), T_c (in °C) is the actual PV cell temperature during operation, $T_{c,STC}$ (in °C) is the cell temperature at standard test conditions, α_P (in 1/K) is the temperature coefficient of power, and f_{PV} is the derating factor.

The meteorological data for the estimation of the PV power production were extracted from the Photovoltaic Geographical Information System (PVGIS) tool considering the dataset for the Typical Meteorological Year (TMY) [7].

Electrolyzer

The Proton Exchange Membrane (PEM) technology was considered for the electrolyzer since it offers faster dynamic response and wider operating range than the alkaline technology, which results in better

performances when coupled with variable RES. The nominal efficiency of the PEM electrolyzer was assumed equal to 55% and the operating pressure was set to 30 bar. Moreover, a specific modulation range (10-100% of the rated power) was imposed to ensure safe and efficient operation of the electrolyzer [6]:

$$P_{EL,min} \leq P_{EL}(t) \leq P_{EL,rated} \quad (2)$$

where P_{EL} (in kW) is the electrolyzer operating power, $P_{EL,min}$ (in kW) is the minimum electrolyzer operating power and $P_{EL,rated}$ (in kW) is the electrolyzer rated power.

Hydrogen tank

A pressurized storage tank is required to cope with the fluctuations in hydrogen production and demand throughout the year. A Type-I tank (i.e., made of seamless aluminium or steel) with a maximum storage pressure of 200 bar was chosen. In addition, the minimum pressure of the tank was set to 20 bar according to the specific requirements of the industrial process.

The Level of Hydrogen (LOH) in the tank, which is defined as the ratio between the amount of hydrogen stored in the tank and its maximum capacity, was evaluated as follows:

$$LOH(t) = LOH(t-1) + \frac{P_{EL}(t-1) \cdot \Delta t \cdot \eta_{EL}}{LHV_{H_2} \cdot Cap_{H_2}} - \frac{\dot{m}_{H_2}(t-1) \cdot \Delta t}{Cap_{H_2}} \quad (3)$$

where Δt is the time resolution (i.e., 1 hour in this study), η_{EL} is the efficiency of the electrolyzer, LHV_{H_2} (in kWh/kg) is the lower heating value of hydrogen, Cap_{H_2} (in kg) is the rated capacity of the hydrogen tank, and \dot{m}_{H_2} (in kg/h) is the hydrogen flowrate sent to the industrial plant.

In order to guarantee the correct hydrogen supply to the industrial plant, at any time interval, the following constrain has to be met:

$$LOH_{min} \leq LOH(t) \leq LOH_{max} \quad (4)$$

The LOH_{min} can be evaluated as the ratio between the minimum and the maximum pressure storage, while LOH_{max} is set equal to 1.

Hydrogen compressor

A three-stage intercooled compressor was selected to increase the hydrogen pressure up to the storage tank value. The specific energy consumption to pressurize hydrogen from the operating condition of the electrolyzer (i.e., 30 bar) up to the maximum storage pressure (i.e., 200 bar) was assumed equal to 4 MJ/kg [8].

Grey hydrogen back-up system

A fossil-based back-up solution was also included in the system. Specifically, a tube trailer with pressurized grey hydrogen was considered.

2.3. Energy management strategy

In order to model the hourly operation of the power-to-hydrogen system over a reference year, an Energy Management Strategy (EMS) was implemented. The adopted control strategy sets the operating conditions of the system based on the hydrogen demand of the industrial plant and the availability of RES production.

The EMS starts with the evaluation of the hydrogen demand profile:

- If the hydrogen demand is higher than zero, the supply intervention has the following priority: first hydrogen from the electrolyzer (if electricity is available from RES), then green hydrogen from the pressurized storage tank and finally grey hydrogen from the fossil-based back-up system. Specifically, two sub-cases can occur:
 - o In case of hydrogen demand higher than zero and sufficient electricity from the PV, the electrolyzer can be switched on and operated within its modulation range, while the excess power – if any – can be exported to the electrical grid. The electrolyzer production can be fed directly to the industrial plant or, if the hydrogen demand is exceeded, it can be compressed and stored.
 - o In case of hydrogen demand higher than zero and power from the PV not available or not sufficient, the deficit must be covered first resorting to the green hydrogen storage and then to the grey hydrogen back-up system.
- If the hydrogen demand is zero, renewable electricity from the PV – if available – is converted into hydrogen, which is entirely stored. The excess power, if any, is then sold to the electrical grid.

2.4. Optimal design

The optimal design of the power-to-hydrogen system was performed by adopting the PSO algorithm and implementing a two-layer approach. According to this methodology, the sizing and dispatch problems are decoupled: in the outer loop a potential design solution (i.e., the sizes of the components) is iteratively generated by the PSO algorithm, while the operation of the power-to-hydrogen system is managed in the inner loop according to the rule-based EMS described in Section 2.2. The optimal design problem was formulated and solved in Matlab (r2022b) with a year-long time horizon and an hourly time-step resolution.

In the PSO algorithm, a population size of 100 was used and both the cognitive and social parameters were set to 1.9. The optimization procedure aims to identify the system configuration that minimizes the LCOH while satisfying the following constraints on the unmet hydrogen demand (UH_2) and the maximum share of grey hydrogen in the annual demand (GH_2):

$$UH_2 \leq UH_{2,target} \quad (5)$$

$$GH_2 \leq GH_{2,target} \quad (6)$$

Equation (5) represents the constraint on the system reliability and the target of unmet hydrogen demand ($UH_{2,target}$) was imposed to zero. Equation (6) defines the maximum share of grey hydrogen ($GH_{2,target}$) that can be used in the plant. The $GH_{2,target}$ term was varied between 100% and 0% to build up a Pareto front according to the ϵ -constrain method [6].

The LCOH (in €/kg), which represents the objective function to be minimized, is defined as follows:

$$LCOH = \frac{C_{NPC,tot}}{\sum_{n=1}^N \frac{M_{H_2}}{(1+d)^n}} \quad (7)$$

where $C_{NPC,tot}$ (in €) is the total Net Present Cost (NPC) of the system, M_{H_2} (in kg) is the annual hydrogen demand of the industrial site, d is the real interest rate (that includes both the nominal interest rate and the annual inflation rate) and N is the system lifetime (set equal to 20 years).

The NPC includes the capital expenditure, the operation and maintenance (O&M) costs and the replacement costs incurred over the whole lifetime of the system. The NPC was evaluated as (with $i = PV, EL, HT, CP$):

$$C_{NPC,tot} = \sum_i C_{inv,i} + \sum_{n=1}^N \left(\frac{\sum_i C_{O\&M,i,n} + \sum_i C_{rep,i,n} + C_{greyH_2,n} - C_{GR,sel,n}}{(1+d)^n} \right) \quad (8)$$

where $C_{inv,i}$ (in €) is the investment cost (i.e., CAPEX) of the i -th component incurred at the beginning of the project, $C_{O\&M,i,n}$ (in €) is the operation and maintenance cost of the i -th component during the n -th year, $C_{rep,i,n}$ (in €) is the replacement cost of the i -th component incurred at the n -th year (if required), $C_{greyH_2,n}$ (in €) is the annual cost due to the purchase of the fossil-based hydrogen and $C_{GR,sel,n}$ (in €) is the annual revenue for selling the surplus electricity to the grid.

The specific CAPEX of the PV system was assumed equal to 800 €/kW which is in line with the cost of the utility-scale projects in Europe [9].

The specific investment cost $c_{inv,EL}$ (in €/kW) of the PEM electrolyzer was estimated by using a modified power law that considers both the plant capacity and the maturity of the technology [10]:

$$c_{inv,EL} = \left(k_0 + \frac{k}{P_{EL,rated}} \cdot (P_{EL,rated})^\alpha \right) \cdot \left(\frac{V}{V_0} \right)^\beta \quad (9)$$

where k_0 and k are the fitting parameters, $P_{EL,rated}$ (in kW) is the rated power of the electrolyzer, α is the scaling factor, β is the learning factor, V and V_0 are the plant installation year and the reference year, respectively. For a more detailed techno-economic assessment, the lifetime of the electrolyzer stack was evaluated based on the actual number of operating hours during the year.

The specific CAPEX of the pressurized tank was set at 500 €/kg, which is in good agreement with the costs of Type-I tanks with storage pressure below 250 bar [11]. The specific investment cost of the compressor was assumed equal to 1600 €/kW [8]. Finally, a cost of 4 €/kg was considered for the fossil-based back-up solution [1]. The main techno-economic input data are summarized in Table 1.

Table 1. Techno-economic input data.

Parameter	Value	Ref.
PV		
f_{PV}	86%	[6]
α_p	-0.003 1/K	[6]
CAPEX	800 €/kW	[9]
O&M (annual)	2% (of the CAPEX)	
Lifetime	20 yr	
Electrolyzer (PEM)		
Efficiency (η_{EL})	55%	[3]
Modulation range	10-100% (of the rated power)	[3]
Operating pressure	30 bar	[3]
Stack lifetime	40,000 h	[6]
Balance of plant lifetime	20 yr	[6]
α	0.622	[10]
β	-158.99	[10]
k_0	585.85	[10]
k	9458.2	[10]
V_0	2020	[10]
O&M (annual)	3% (of the CAPEX)	[6]
Stack replacement cost	26.7% (of the CAPEX)	[6]
Hydrogen tank		
Maximum pressure	200 bar	[3]
CAPEX	500 €/kg	[11]
O&M (annual)	2% (of the CAPEX)	[3]
Lifetime	20 yr	[3]
Hydrogen compressor		
Specific energy consumption	4 MJ/kgH ₂	[8]
CAPEX	1600 €/kW	[8]
O&M (annual)	2% (of the CAPEX)	[3]
Lifetime	20 yr	[3]
Grey hydrogen		
Emission factor for SMR	9.5 kgCO ₂ /kgH ₂	[12]
Cost	4 €/kg	[1]
Other assumptions		
Discount rate	4.9%	
Revenue for exported electricity	0.0363 €/kWh	
System lifetime	20 yr	

3. Case-study

A semiconductor production plant located in Southern Europe was considered as a case study. The real hourly demand profile over one reference year was used in this analysis. The plant operates continuously throughout the year with an average hydrogen demand of about 12.5 kg/h (which is in agreement with other literature

sources [1]) and a maximum consumption of around 15.5 kg/h. Further details on the demand profile are omitted for confidentiality reasons. The total annual hydrogen demand amounts to 110 tons and is currently met by a conventional fossil-based solution (i.e., grey hydrogen purchased externally and delivered by trailer).

4. Results and discussion

The optimal sizing was first performed without imposing any constraint on the $GH_{2,target}$ and the LCOH resulted in 4 €/kg, confirming that fossil-based hydrogen is currently the cheapest solution. However, adopting this strategy exhibits severe environmental drawbacks since the production of 110 tons of grey hydrogen generates 1045 tons of CO₂ emissions per year.

In order to assess the effect of the different decarbonization targets on the LCOH, the design of the energy system was then carried out by imposing a constraint on the annual grey hydrogen share, which was gradually reduced from 100% to 0%. The main sizing results and economic performance indicators are summarized in Table 2.

By reducing the amount of grey hydrogen that can be used by the industrial plant, the sizes of PV and electrolyzer increase significantly. Specifically, the rated capacities of PV and EL rise respectively from 0.68 MW and 0.27 MW (with 90% grey hydrogen share) to 11.96 MW and 3.3 MW (in the 100% RES-based configuration with 0% grey hydrogen share). Despite the considerable increase in the PV size (up to 11.96 MW), the corresponding footprint is consistent with the available space in the industrial site and the surrounding areas.

Furthermore, the results clearly show that the installation of a hydrogen storage (including hydrogen tank and compressor) is not economically convenient for scenarios with a grey hydrogen share higher than 70%. The size of the pressurized tank is relatively small (between 19 and 644 kg) when the grey hydrogen share is between 70% and 10%, and then sharply increases to 4930 kg when only green hydrogen is considered (0% grey hydrogen share).

Table 2. Main sizing results and economic performance indicators.

Grey H ₂ share [%]	PV [MW]	EL [MW]	HT [kg]	CP [kW]	LCOH [€/kg]	CO ₂ emissions [ton/y]
100%	0	0	0	0	4.00	1045
90%	0.68	0.27	0	0	4.46	940
80%	1.32	0.55	0	0	4.77	836
70%	1.98	0.83	19	7	5.07	731
60%	2.62	1.10	59	12	5.37	627
50%	3.23	1.39	101	22	5.66	522
40%	3.87	1.66	153	30	5.94	418
30%	4.62	1.94	201	35	6.23	313
20%	5.63	2.25	369	41	6.67	209
10%	7.29	2.75	644	50	7.50	104
0%	11.96	3.30	4930	60	10.85	0

As shown by the Pareto front in Figure 2, the cost of hydrogen ranges from 4 to 10.85 €/kg. Green hydrogen appears to be more expensive than fossil-based alternatives, but this solution can be beneficial from an environmental perspective since it allows the CO₂ emissions to be considerably reduced (up to 1045 ton/y of CO₂ emissions can be avoided).

It is worth noting that the LCOH increases evenly up to a grey hydrogen share of 30% – which corresponds to a decarbonization rate of 70% – with an LCOH of 6.2 €/kg (Figure 2). In this region, reducing the annual consumption of grey hydrogen by e.g., 50%, leads to a saving of 522 tons of CO₂ per year and an increase in the LCOH (compared to the 100% grey hydrogen scenario) of 41%. At higher decarbonization rates (> 70%), the Pareto front shows a steeper slope and increase in LCOH: the transition to a complete decarbonization of the energy system (0% grey hydrogen share) indeed leads to an increase in the LCOH of about 170%.

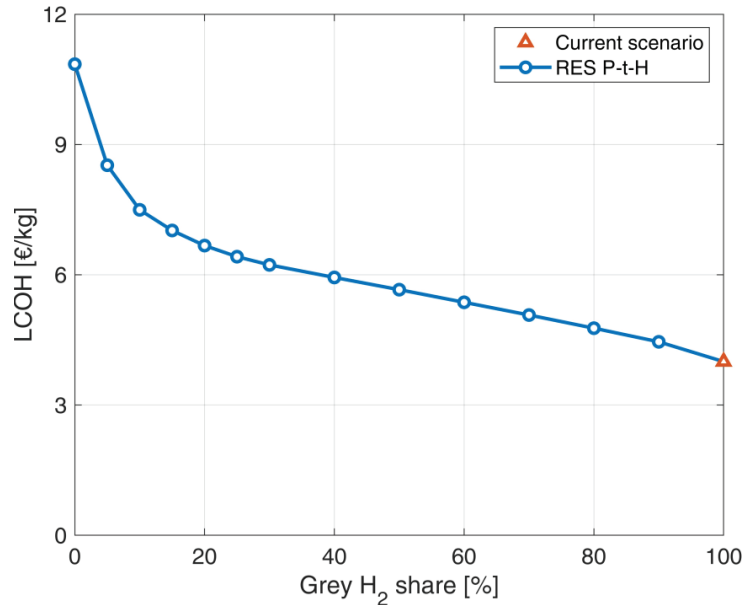


Figure 2. Pareto front between the levelized cost of hydrogen and the grey hydrogen share.

Figure 3 shows the breakdown of the NPC for different values of grey hydrogen share. For values above 50%, the purchase of fossil-based hydrogen represents the largest cost contribution (yellow area in Figure 3), while for the other scenarios the PV and EL costs have the largest impact. Moreover, it is evident that with the transition to lower values of grey hydrogen share, the revenues associated with the surplus electricity exported to the grid increase significantly (“Grid export” area in Figure 3) because of the sharp increase in the PV size. Finally, it is noteworthy that the storage system is an important cost contribution (20%) in the fully decarbonized scenario (0% grey hydrogen share), in which a large tank (4930 kg) is required to ensure a reliable supply of green hydrogen throughout the year.

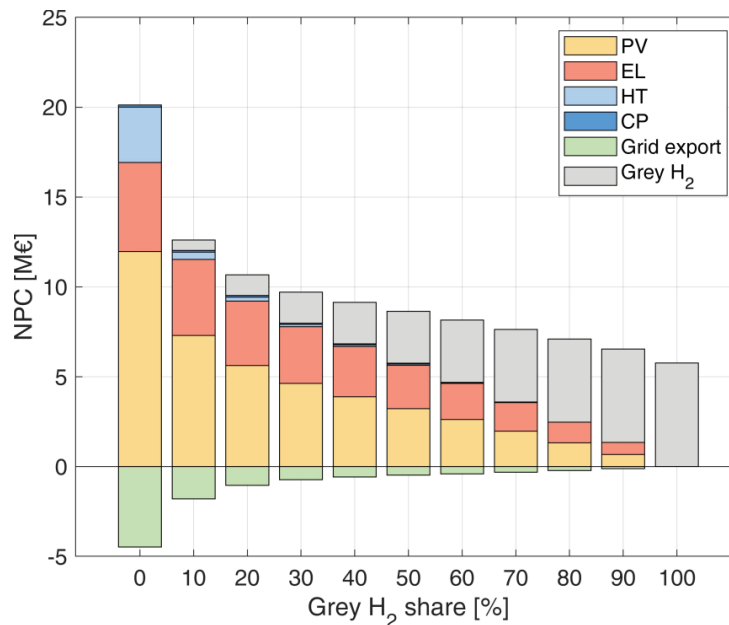


Figure 3. NPC breakdown for different annual grey hydrogen share.

5. Conclusions

This study aimed at assessing the techno-economic feasibility of decarbonizing a semiconductor industry by exploiting green hydrogen. The optimal sizing of the renewable power-to-hydrogen system was carried out by adopting the PSO algorithm in a two-layer optimization approach. Different decarbonization targets (i.e., 0% to 100%) were investigated and the LCOH resulted in the range between 4 and 10.85 €/kg. Producing green hydrogen proved to be more expensive than conventional fossil-based solutions but it can effectively reduce CO₂ emissions. The resulting LCOH- $GH_{2,target}$ Pareto front shows two distinct regions: the reduction of grey hydrogen share from 100% (current scenario) to 30% - corresponding to a decarbonization rate of 0% to 70% - follows a smooth trend with an LCOH increase from 4 to 6.2 €/kg (first region). Higher decarbonization rates (> 70%, second region) instead lead to a steeper increase in the LCOH, reaching 10.85 €/kg in the completely decarbonized scenario (0% grey hydrogen). In the scenarios with a grey hydrogen share above 50%, the purchase of grey hydrogen represents the main contribution of the NPC, while in the other scenarios PV and EL provide the largest shares. In the fully decarbonized configuration, the size of the storage system increases significantly, as it has to ensure the supply of green hydrogen throughout the entire year and reaches a share of 20% share of the overall NPC.

In conclusion, renewable power-to-hydrogen system does not represent the most cost-competitive solution, from an economic point of view, to provide hydrogen to the industrial plant. However, the profitability of the RES-based configuration can be significantly boosted when considering also the environmental benefits (i.e., CO₂ emission savings) generated by replacing the conventional grey hydrogen supply with the low carbon one. In addition, both the costs of photovoltaic and electrolyzer technologies are expected to decrease in the coming years, and this reduction could enhance the competitiveness of green hydrogen for industrial applications. In a future work, a sensitivity analysis on the main economic parameters will be carried out in order to identify the conditions in which green hydrogen can achieve the cost-parity with the current fossil-based supply.

Nomenclature

CAPEX	Capital Expenditures
CP	Compressor
EL	Electrolyzer
EMS	Energy Management Strategy
GR	Grid
HBS	Hydrogen Back-up System
HT	Hydrogen Tank
LCOH	Levelized Cost Of Hydrogen
LOH	Level of Hydrogen
NPC	Net Present Cost
O&M	Operation and Maintenance
PEM	Proton Exchange Membrane
PSO	Particle Swarm Optimization
P-t-H	Power-to-Hydrogen
PV	Photovoltaic
RES	Renewable Energy Sources
SMR	Steam Methane Reforming
TMY	Typical Meteorological Year

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