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Cost-Effective Hydrogen Generation: Concurrent Optimization of Component Sizes and System Operation

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ABSTRACT

The attainment of cost-effective hydrogen production is pivotal for facilitating the increased utilization of hydrogen within future energy systems. This study proposes a mixed integer linear programming approach to simultaneously derive the optimal sizing and operation of hydrogen generation sites. The results showed that a 13.6% reduction in levelised cost of hydrogen can be obtained compared to benchmark solutions. The results highlight the intrinsic interconnection between optimal sizing and operation of hydrogen generation sites, emphasizing that they should not be treated as separate design phases.

Keywords: hydrogen generation, MILP, optimization, cost minimization, renewable energy resources.

NONMENCLATURE

Abbreviations	
LCOH	Levelised Cost of Hydrogen
PV	Photovoltaic
HHV	Higher Heating Value
Symbols	
k	Time [s]
SOC	State of Charge [-]
P	Power [W]
η	Efficiency [-]
$\dot{m}$	Mass flow rate [kg/s]
Q	Heat [W]
C	Capacity [Wh]
c	Cost [€]
S	Size [W]
Subscripts	
inv	Investment
op	Operational
m	Maintenance
c	Compressor
ch	Charging
disch	Discharging
e	Electrolyzer
b	Battery
imp	Imported
exp	Exported
nom	Nominal

1. INTRODUCTION

The increasing demand for clean and sustainable energy has driven the growing interest in hydrogen generation as a promising avenue for decarbonization. The European Commission has raised the ambition of renewable hydrogen production with the REPowerEU action plan from 5.6 Mton to 10 Mton domestic EU production and 10 Mton of hydrogen imports [1].

However, the cost-effectiveness of hydrogen supply remains a critical challenge that hinders its widespread adoption. The cost-effectiveness of hydrogen provision is directly influenced by the methods used for its generation. Traditional design methodologies typically involve sizing the key technologies utilized in hydrogen generation sites to fulfill a predefined hydrogen demand. For example, Minutillo et al. [2] studied a grid-connected PV plant integrated with a Proton Exchange Membrane (PEM) electrolyzer for different targeted hydrogen demands of 50, 100 and 200 kg/day. Levelised cost of hydrogen (LCOH) in the range 9.29 to 12.5 €/kg were calculated. Monthly averaged solar irradiation values for a specific location in Italy were considered and operational and maintenance costs were indicated as the main contributors to the calculated LCOH. Furthermore, Perna et al. [3] reported that, depending on the selected system configuration and location, the LCOH can be reduced to 5.64 €/kg.

However, the sizes selected in the mentioned studies are determined through rigorous energy and mass

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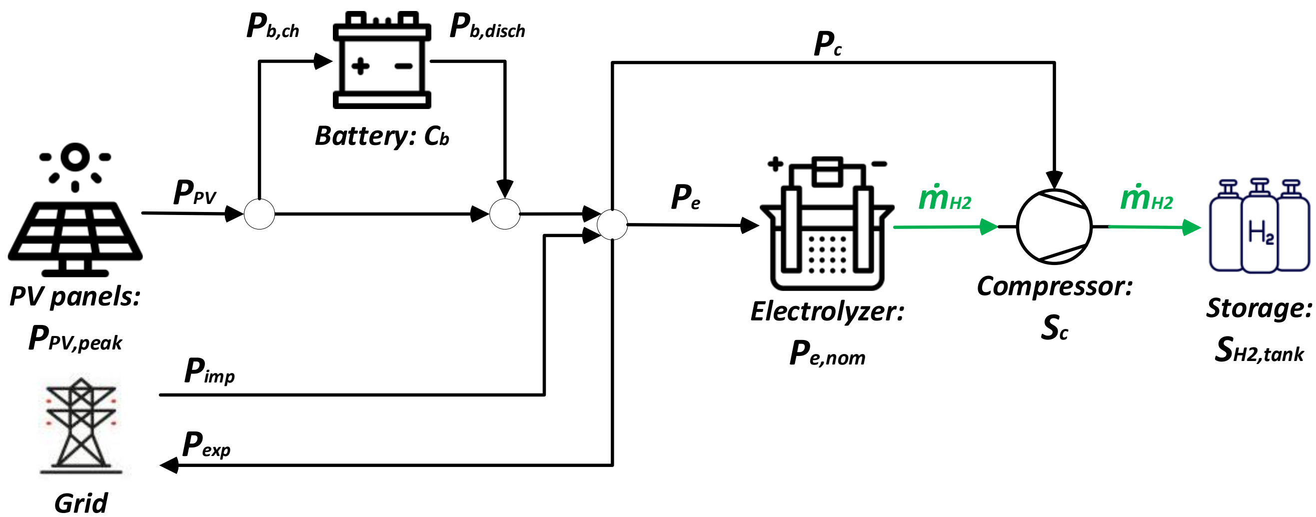


Figure 1 Schematic of the hydrogen generation site.

balance analyses of the system that adopts constant approximations of dynamic behaviors. Only in a second step, the operation of the hydrogen generation site with the selected component sizes is optimized [4].

This paper presents a novel numerical tool developed for the concurrent optimal sizing and operation of hydrogen generation sites. By simultaneously optimizing the sizes of key components and their operational parameters, our approach aims to achieve maximum efficiency while minimizing LCOH. A similar approach was implemented by Rioja et al. [5], although off-grid generation sites were considered and no mixed integer linear programming approach (MILP) was used.

The proposed method takes into account various factors such as site-specific conditions, technology choices, and energy inputs to deliver a comprehensive solution tailored to each unique hydrogen generation site.

2. ENERGY SYSTEM

The schematic of the considered hydrogen generation site is shown in Figure 1. The PEM electrolyzer is fed by a PV-battery source and by the grid. A compressor unit is considered to elevate the H_2 pressure from 10 bar to 820 bar [2], before feeding the generated hydrogen into a storage tank. The excess of electricity is sold to the grid. The use of by-products is disregarded in the study [6].

As detailed in the next section, the proposed methodology identifies the optimal sizes for PV panels, whereas predetermined sizes for batteries and electrolyzer are studied. Null sizes are allowed within the solution space. Consequently, the optimal layout emerging from the analysis may not encompass all the components depicted in Figure 1.

3. METHODOLOGY

The optimization problem formulated in this work determines the minimal operational and investment cost necessary to meet a desired hydrogen production of 100 kg/day, that ensures comparability with [2]. A MILP approach is adopted, similarly to [7].

3.1 Design variables

The optimization procedure returns, under defined boundary conditions, the optimal sizing and operational decision variables for the energy system specified in Section 2. These decision variables include:

(i) Size of PV system, $P_{PV,peak}$, and discretized size for battery, C_b, electrolyzer nominal power, $P_{e,nom}$, and compressor size, S_c.

(ii) At each time-step, *k*, the power consumed by the electrolyzer, $P_e\ (k)$, the compression power, $P_c\ (k)$, the battery discharging, $P_{b,disch}\ (k)$, and charging, $P_{b,ch}\ (k)$, power, and linked state of charge, $SOC\ (k)$.

(iii) At each time-step, the power exported, $P_{exp}\ (k)$, and imported, $P_{imp}\ (k)$, to/from the grid.

The design variables referring to the PV system size and battery capacity listed in (i) are allowed to be zero in the optimization framework. That is, the optimal configuration might not encompass all the technologies depicted in Figure 1.

3.2 Constraints

The amount of hydrogen generated per day, $m_{H2,day}$, is constrained as larger or equal to 100 kg/day [2]. The mass flow rate of generated hydrogen, $\dot{m}_{H2}$, is calculated as:

$$\dot{m}_{H2}(k) = P_e(k)\eta_e/HHV \tag{3.1}$$

Where the term η_e indicates the electrolyzer conversion efficiency and HHV is the higher heating value [5]. The energy balance for the considered energy system is ensured through the following inequality constraint:

$$\begin{aligned} P_e(k) + P_{b,ch}(k) + P_c(k) + P_{exp}(k) \\ \leq P_{PV}(k) + P_{b,disch}(k) + P_{imp}(k) \end{aligned} \tag{3.2}$$

The maximum power supplied to the electrolyzer is constrained by its nominal power, while its minimal operational load is set at 20% [5]: $P_e(k) \leq 0.2 \cdot P_e \cdot ely_{on}$. Where ely_{on} is a binary variable.

The battery SOC is constrained in the range 0 to 1, with the charging and discharging powers also constrained as follows:

$$P_{b,ch}(k) \leq {(1 - SOC(k))C_b}/{\Delta t\,\eta_b} \tag{3.3}$$

$$P_{b,disch}(k) \leq {\eta_b SOC(k) C_b}/{\Delta t} \tag{3.4}$$

Where η_b is the battery efficiency [5]. Besides, a big-M constraint is used to avoid simultaneous charging and discharging of the battery.

The compressor size, S_c, is determined by the electrolyzer size as follows:

$$S_c = \frac{\dot{m}_{H2,max}\, L_{is,c}}{\eta_c} \tag{3.5}$$

Where $\dot{m}_{H2,max}$ is the maximum hydrogen flow rate, calculated as per equation 3.1 for the electrolyzer nominal power. The term $L_{is,c}$ is the specific work of the compressor unit under the assumption of ideal gas, while η_c is the compressor efficiency, assumed as 0.75 in agreement to [2]. The power fed to the compressor at each time-step *k* is constrained by the compressor size, S_c, and proportional to the hydrogen flow rate:

$$P_c(k) = \frac{\dot{m}_{H2}(k)\, L_{is,c}}{\eta_c} \tag{3.6}$$

3.3 *Objective function*

The LCOH is considered as objective function of the minimization problem:

$$LCOH = \frac{c_{tot}}{m_{H2,year}} = \frac{c_{inv} + c_{op} + c_m}{m_{H2,year}} \tag{3.7}$$

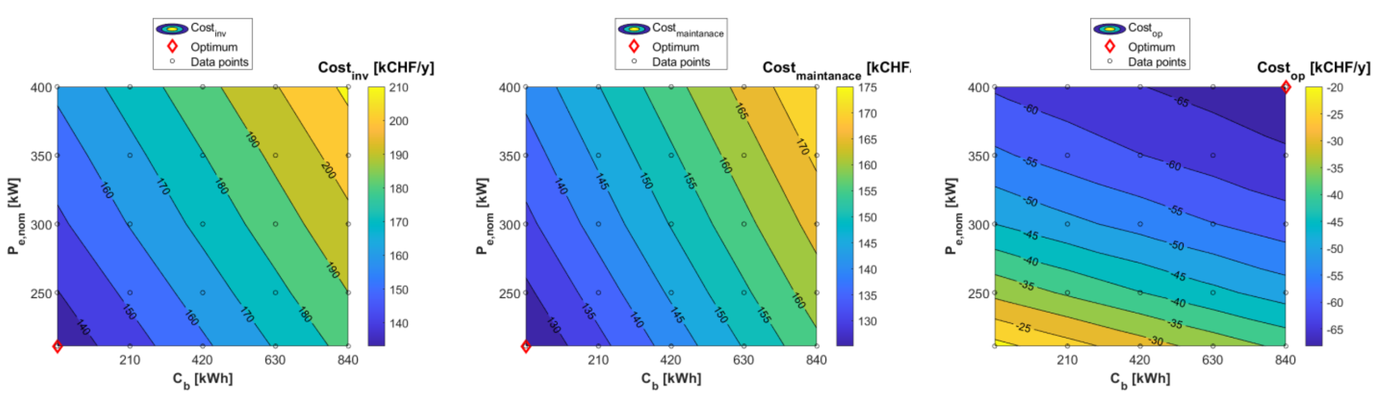
Start-up costs are also considered to penalize on-off behaviours [5], but are not accounted for in the final LCOH estimation. The annualized investment cost, $cost_{inv}$, operational cost, c_{op}, and maintenance cost, c_m, are estimated as follows:

$$c_{inv} = \sum_{i=1}^{\#components} S_i \cdot \frac{UP_i}{l_i} \tag{3.8}$$

$$c_{op} = \sum_{k=1}^{8760} (P_{imp}(k) \cdot c_{imp}(k) - P_{exp}(k) \cdot c_{exp}(k)) \tag{3.9}$$

$$c_m = \sum_{i=1}^{\#components} S_i \cdot UP_i \cdot c_{m,\%} \tag{3.10}$$

Where $c_{m,\%}$ represents the annual maintenance cost coefficient, expressed as a percentage of the initial investment cost [2]. The components considered for the



(a) (b) (c)

Figure 2. Cost breakdowns and the impacts of electrolyzer size and battery capacity variations: (a) annualized investment cost, (b) maintenance cost and (c) operational costs.

LCOH estimation are the following: PV, battery, electrolyzer, compressor, H_2 storage, dispenser and refrigerant. Given the constrained hydrogen production, the size for H_2 storage, dispenser and refrigerant are predetermined in the analysis and are selected in agreement to [2].

3.4 Input data

Fixed efficiencies are accounted for all the modelled components, values assumed as per the nominal points in [5]. Unit prices, components' lifetime and maintenance costs are assumed from [2,5]. The hydrogen generation site was assumed to be located in Dübendorf, Switzerland, and the year 2018 was assumed as reference year to determine the system boundary conditions. The optimization was solved with a 1-year horizon and hourly time-steps, with the irradiance values assumed from [8] and cost of electricity values from [9]. Figure 4 shows the boundary conditions adopted in this study.

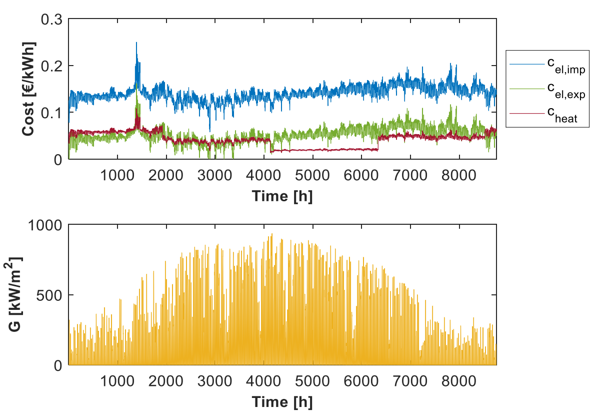


Figure 4. Boundary conditions (energy prices and solar irradiance) assumed for the analysis.

4. RESULTS AND DISCUSSION

The different cost categories versus the electrolyzer size and battery capacities, both considered as discrete values in the analysis, are depicted in Figure 2. Regarding annualized investment cost and maintenance costs, both categories are minimized for the smallest sizes considered in the design space and reduce with the components size, as expected. Regarding the operational costs, these are minimized in the instance of large electrolyzer size and battery capacity. Operational costs reduce with the battery capacity as larger fractions of cost-free energy (solar energy) can be stored during excess period and re-used in a later time. Similarly, the operational cost reduces with the electrolyzer size as larger sizes allow to use larger amounts of local solar energy during the day and thus reduces the amount of electricity imported from the grid.

The minimal LCOH cost is achieved as a trade-off of these three cost categories and, given the trends discussed above, the optimal point does not coincide with the minimal investment and maintenance cost one, as can be appreciated in Figure 5. Minimal LCOH is indeed achieved for a relatively large electrolyzer size of 300 kW. As a comparison, for the same targeted hydrogen demand of 100 kg/day, Minutillo et al. [2] selected and electrolyzer size of only 236 kW. Due to the large investment cost characterizing batteries, these do not pertain to the optimal configuration. Besides, regardless of the considered electrolyzer and battery sizes, the PV system size was always maximized (2193 kW_{peak}). That is, under the imposed market conditions, it is always beneficial to invest in PV.

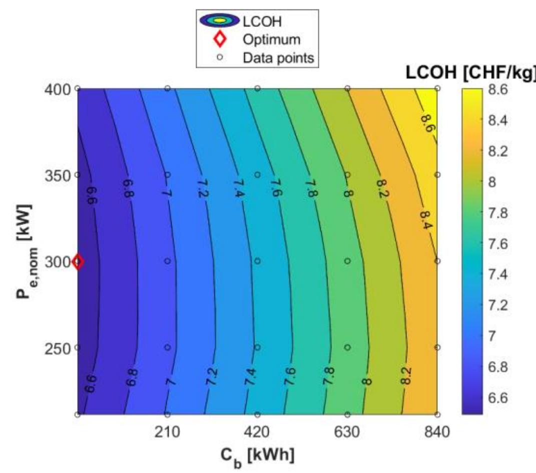


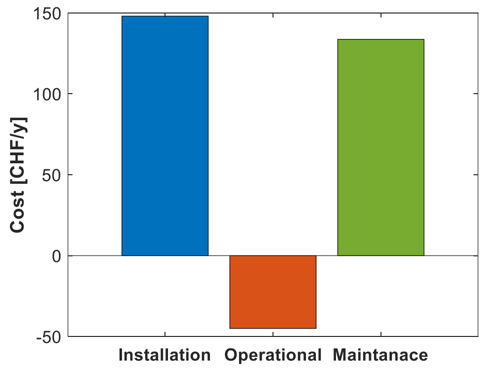
Figure 5 LCOH trend with electrolyzer size and battery capacity.

Table 1 Sizes for optimal point and benchmark [2].

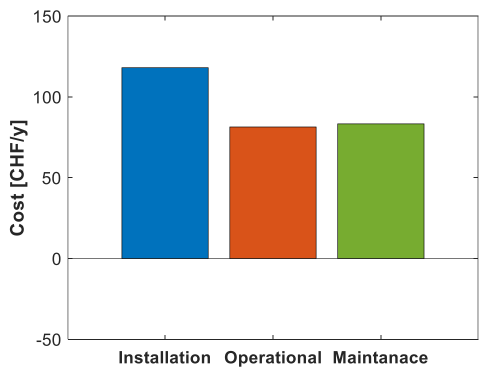
	Optimization results	***Benchmark* [2] *(with optimal operation)***
$P_{PV,peak}$ $[kW]$	2193.0	1422.0
$P_{e,nom}$ $[kW]$	300.0	236.0
C_b $[kWh]$	0.0	0.0
LCOH [CHF/kg]	6.68	7.74

4.1 Comparison with benchmark

The optimization results are compared with a benchmark solution in Table 1. The benchmark solution entails the sizes presented in [2], which were obtained through energy balances accounting for approximated constant operations. Thus, the system operation for the benchmark solution was optimized adopting the methodology presented in section 3 with components sizes constrained to the ones presented in [2].



(a)



(b)

Figure 6 Cost breakdowns for: (a) optimal solution and (b) benchmark solution with optimized operation.

In both solutions, no battery capacity was considered due to the large investment cost required. Nonetheless, the optimization results presented a doubled PV system size compared to the benchmark solution, that significantly reduced the operational cost of the system, as illustrated in Figure 6. Overall, the optimal solution presented in this work allows for a 13.6% reduction in LCOH. This reduction is obtained through a larger investment cost that enables for larger operational revenues through export during the plant lifetime.

5. CONCLUSIONS

In this work, a numerical tool for the simultaneous sizing and operation optimization of a hydrogen generation site was presented. Costs were minimized for a hydrogen production of 100 kg/day and LCOH reductions of 13.6% were obtained compared to a benchmark solution. It can be concluded that sizing and operational optimization are tightly interconnected and cannot be treated as separate steps during the design process. The optimal solution was characterized by a relatively large electrolyzer size of 300 kW and PV size of 2193 kW, which allowed for a larger amount of solar energy to be directly consumed during the day with a significant reduction of operational cost due to electricity imports during night.

In our future works, the modelling framework adopted in the analysis will be extended to account for off-design performance of each component and the system configuration will be varied to assess the benefits from waste heat recovery and to allow for the co-generation of both hydrogen and synthetic methane.

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