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Techno-Economics Optimization of H_2 and CO_2 Compression for Renewable Energy Storage and Power-to-Gas Applications

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Abstract: The decarbonization of the industrial sector is imperative to achieve a sustainable future. Carbon capture and storage technologies are the leading options, but lately the use of CO_2 is also being considered as a very attractive alternative that approaches a circular economy. In this regard, power to gas is a promising option to take advantage of renewable H_2 by converting it, together with the captured CO_2, into renewable gases, in particular renewable methane. As renewable energy production, or the mismatch between renewable production and consumption, is not constant, it is essential to store renewable H_2 or CO_2 to properly run a methanation installation and produce renewable gas. This work analyses and optimizes the system layout and storage pressure and presents an annual cost (including CAPEX and OPEX) minimization. Results show the proper compression stages need to achieve the storage pressure that minimizes the system cost. This pressure is just below the supercritical pressure for CO_2 and at lower pressures for H_2, around 67 bar. This last quantity is in agreement with the usual pressures to store and distribute natural gas. Moreover, the H_2 storage costs are higher than that of CO_2, even with lower mass quantities; this is due to the lower H_2 density compared with CO_2. Finally, it is concluded that the compressor costs are the most relevant costs for CO_2 compression, but the storage tank costs are the most relevant in the case of H_2.

Keywords: power to gas; methanation; hydrogen; carbon conversion; CO_2 utilization; CCU

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1. Introduction

The utilization of renewable resources is imperative to decarbonize all energy-related sectors, including power, industry, heat, transport, and desalination, thereby achieving global emissions targets and avoiding the effects of climate change. Decarbonization is a very challenging target for humanity due to high capital investment, the competition among energy sectors, the necessity of environmental policies, and public acceptance [1]. International regulations try to drive initiatives and plans to reach these goals. In Europe, the "EU Reference Scenario 2016. Energy, transport and GHG emissions. Trends to 2050" quantifies the contribution of renewable net electricity generation at 44% by 2030 and 56% by 2050 [2].

To achieve these objectives and properly manage electricity production from renewable sources, the implementation of large energy storage systems is essential. Current energy storage technologies present weak points when applied at a large scale, as for example the limited storage potential. Nevertheless, there are several technologies that have been proposed to overcome the drawback of actual energy storage options. The more generic alternative is Power to X, which includes options for converting renewable energy into liquids or gases [3]. These can be stored, distributed, or converted into valuable products with low environmental impact that mainly depend on the electricity source and the methodological concept of CO_2 [4]. Among these options, energy storage through Power to Fuels [5] or, in particular, Power to Methane, is the most preferable pathway [3]. This technology also could have positive socio-economic impacts in a circular economy scenario [6].

In this technology, excess energy is used to produce a synthetic fuel. The most common fuel is hydrogen, but it also could be synthetic natural gas (SNG), methanol, and others. In particular, when methane is produced, power-to-gas (PtG) is one of the most versatile energy storage technologies and it converts surplus renewable electricity into synthetic natural gas by combining H_2 from water electrolysis with CO_2 through methanation reaction. This technology has also been proposed for carbon utilization using captured CO_2 to produce a 'CO_2 neutral' natural gas [7]. Under certain design configurations, where synthetic fuels are used in the same installation where the CO_2 is captured (industry or power plant), the CO_2 could be effectively recycled [8]. It allows the temporal displacement (storage) in the use of renewable energy. The CO_2 source could also be through direct air capture (DAC) [9], and in this case environmental impacts are clearly minimized. In a PtG process renewable electrical energy is converted into CH_4 through two processes: (i) electrolysis of water, which produces H_2 and O_2 (Reaction 1); and (ii) conversion of H_2 into CH_4 with an external source of CO_2 through methanation, according to the Sabatier reaction (Reaction 2).

$$H_2O \leftrightarrow H_2 + \frac{1}{2}O_2 \qquad \Delta H_{298K} = +285.8\ \mathrm{kJ/mol} \tag{1}$$

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O \qquad \Delta H_{298K} = -164.9\ \mathrm{kJ/mol} \tag{2}$$

The methanation implies an enrichment in energy density, while H_2 has an energetic density of 12.7 MJ/m^{3}N; in turn, the energetic density of CH_4 is 40 MJ/m^{3}N [10]. Furthermore, the CH_4 produced can be injected directly into the natural gas grid as a storage structure or used as a substitute for fossil fuels. In the case of H_2 and CO_2, which are the inputs for the reaction, it would be necessary to have storage vessels to manage the renewable production (H_2) and the utilization of carbon emissions (CO_2).

The necessity of these storage vessels opens a new research line about the feasible operational variables that minimize the energy requirements and system costs, to help carry out multi-criteria optimization of this energy storage design. This work is an attempt to address this problem. The objective of this research is to find the feasible layout and storage pressure that minimize the capital and operation cost of H_2 and CO_2 gas compression and storage vessels.

Regarding H_2 compression and storage, the main research has focused on the thermodynamic analysis of filling hydrogen storage tanks and the influence of temperature evolution. The effects of heat losses and filling rate optimization for a refuelling gaseous fuel tank was studied by Ruffio et al. [11]. Their objective was to compare the temperature and pressure evolutions coming from different equations of state and from thermodynamic tables. They optimized the filling rate to minimize heat losses in a tank up to 270 bar. A similar analysis was developed elsewhere [12,13]. In this work [12], a parametric study was performed to analyse the effect of the initial conditions on the exergy destruction and efficiency of the filling processes. The focus was on the transient filling process and determined temperature and pressure changes inside the storage tank during filling. The final pressure was 350 bar and the initial pressure varied between 5 and 20 bar. Similar objectives were showed by Johnson et al. [13]. Bourgeois et al. reviewed the research on the H_2 filling procedure [14], which is a hot topic for the H_2 and electrolyser industry. The compression work input for different compression processes were previously analysed by Jensen et al. [15]. The percentage of LHV for hydrogen compression varies between 5 and 20% for pressures up to 600 bar, depending on an ideal isothermal or adiabatic compression. This huge variation, 400% in energy requirement, emphasizes the necessity of a particular study for each H_2 application where the process compression configuration was also studied.

CO_2 compression was mainly investigated in relation to Carbon Capture and Storage (CCS) applications. Romeo et al. [16] studied the power requirements for CO_2 compression and the minimization of energy requirements through intercooling compression. These power requirements could be as much as 100 kWe per tonne CO_2 and it is a key issue for the feasibility of this system. They proposed the integration of intercooling CO_2 compression into the low-pressure part of a steam cycle to take advantage of the intercooling heat and analysed the energetic and economical results, finding a reduction in the compression power requirement of around 40%. Several researches have also work on this topic for CCS. Fu and Gundersen [17] made a theoretical approach and analysed the heat and work integration and its application to CCS. Sunku et al. [18] developed an advanced exergy analysis of a CO_2 pressurization strategy. Fu et al. [19] studied the utilization of compression heat with regenerative steam Rankine cycles and Pei et al. [20] with Organic Rankine Cycle (ORC) to minimize the energy requirements.

As in the case of H_2, the analysis of CO_2 compression depends strongly on the final application. For CCS applications, the objective is gas transportation from the source to the storage site. Generally, the gas is transported in supercritical conditions or condensed below its critical point. Jackson and Brodal [21] made a comparison of the energy consumption associated with compression process alternatives. The main finding was that the performance advantages claimed for improved CO_2 compression process schemes are often optimistic. It requires a detailed simulation of the process with performance data provided by a commercial CO_2 compressor manufacturer, analysis of transient performance [22], and include the limitations caused by composition, safety, and transportation options (pipelines and ships) [23].

With these precedents regarding the importance of application when analysing H_2 and CO_2 compression to find the proper design and feasible operational variables, the objective of this work is to carry out a techno-economic analysis of H_2 and CO_2 compression and storage for power-to-gas applications. Several compression configurations were considered, with the aim to determine the storage pressure that minimize the economic annual costs (including CAPEX and OPEX) of the overall system.

2. Methodology

2.1. Process Simulation

This section details the hypothesis and procedures used in the simulation of the gas compression and storage system using the software Engineering Equation Solver (EES), which is an equation-solving program that can numerically solve non-linear algebraic and differential equations and includes high accuracy thermodynamic and transport property databases [24]. The aim of this section is to present a base case process simulation and detail the cost calculations. For the sake of clarity and understanding, the output pressure maintains a constant value of 20 bar. This base case only illustrates the effect of the process configuration, varying the number of serial compressor stages with the objective of assessing the power consumption and equipment costs (CAPEX and OPEX). Two gases have been considered in the simulations: CO_2 and H_2. For each gas different scenarios were analysed, varying the number of intercooling-compression stages (k = 1–5).

Each stage is composed of three main industrial equipment: a centrifugal gas compressor and two heat exchangers, similar to [16]; Figure 1. These two heat exchangers make up the intermediate cooling stage between compressors. They have been considered because of the high gas temperatures at the compressor outlet. In the first heat exchanger, part of the thermal energy resulting from the compression phase can be used (H_u). In the second heat exchanger, it is considered that the thermal energy coming from the temperature difference between the inlet and outlet is not enough to be used (H_{nu}). Therefore, this second heat exchanger simply reduces the temperature of the gas with levels close to ambient temperature and cutting down the compressor power-specific consumption.

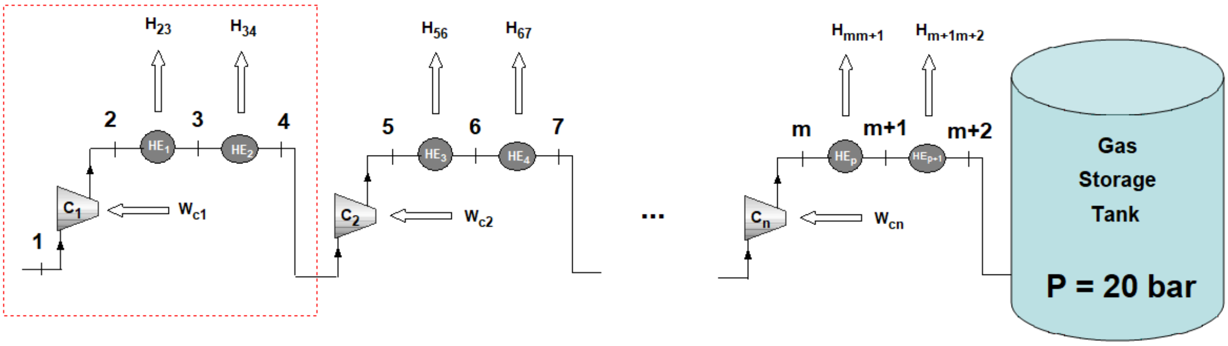

Figure 1. General scheme of the simulation.

It was assumed that CO_2 mass flow is the equivalent to convert the H_2 produced by a 1 MW electrolyser into CH_4 in a methanation installation, meaning, 0.055 kg/s. A similar assumption is for the H_2 that comes from a 1 MW electrolyser plant, obtaining a hydrogen mass flow of 0.0058 kg/s. For both gases, it was assumed that the plant compresses the gases for maximum storage of 48 h per week in intermittent periods and is stored in pressurized tanks. Both gases were assumed under real fluid conditions and the compressor isentropic efficiency varied from 70% to 95% (with increments of 5%). The thermodynamic gas properties were obtained for each point of Figure 1. Table 1 shows the hypothesis used in the calculations

Table 1. Simulation hypothesis.

	Carbon Dioxide		Hydrogen	
	Value	**Unit System**	**Value**	**Unit System**
Methane Power	1000	kW	-	-
LHV Methane	50,030	kJ/kg	-	-
Methane mass	0.02	kg/s	-	-
Carbon dioxide mass	0.055	kg/s	-	-
Days per week	2	day	2	day
Compression ratio	1–4	-	1–4	-
Hydrogen power	-	-	1000	kW
Electrolyser efficiency	-	-	70	%
LHV Hydrogen	-	-	120,000	kJ/kg
Hydrogen mass	-	-	0.0058	kg/s
Inlet gas pressure	1 bar			
Storage pressure	20 bar			
Temperature between serial heat exchangers	60 °C			
Inlet gas temperature	30 °C			
Isentropic efficiency	85%			

2.2. Cost Analysis

As is well-known, working with configurations that offer very low power consumption does not imply that they are the most economically feasible. For that reason, this subsection covers the analysis of the costs associated with the process of compression and storage of the two working gases. The aim of this analysis is to obtain mathematical expressions for the cost of the equipment involved in the process as well as for the operational costs. It must be mentioned that the storage pressure again keeps a constant value of 20 bar to evaluate the different cost expressions in the first instance.

There are several methodologies to estimate the investment needed for the whole system. However, in this research the methodology used is based on a percentage of the procurement costs of the equipment needed. This investment method was selected due to it being used in preliminary cost estimations where little cost-related data are available.

For that reason, it should be mentioned that the uncertainty associated with this method is approximately 20% to 30% [25], which is usual for economic analyses in the literature.

The additional elements involved in the initial investment are estimated on a percentage average of the equipment costs, as shown in Table 2 and Equation (3) [25], where f_i are factors that represent piping, electric costs, control equipment, etc. The average percentages were obtained from Peters et al. [25], for the calculation of industrial plant costs where the whole process involves fluid-type components. Provided the industrial equipment cost varies in time and considering that this study has been developed in October 2021, an update rate, based on the variation in the Chemical Engineering Plant Cost Index [26], was considered to actualize the overall costs.

$$\text{CAPEX} = \sum(E + f_1 E + f_2 E + \ldots + f_n E) = E \sum(1 + f_1 + f_2 + \ldots + f_n) \tag{3}$$

Table 2. Investment estimation based on a percentage of the equipment acquisition costs.

Cost Description Study Case	Unit	Value
FIXED COSTS		
E, Main equipment cost (compressors and heat exchangers)	(%)	100
Equipment installation	(%)	20
Instrumentation and control systems	(%)	16
Gas piping	(%)	34
Electrical systems	(%)	5
Industrial warehouse	(%)	5
Service centre	(%)	10
TOTAL FIXED COSTS	(%)	190
VARIABLE COSTS		
Engineering and supervision	(%)	5
Building costs	(%)	10
Legal costs	(%)	3
Administrative fees	(%)	2
Contingencies	(%)	10
TOTAL VARIABLE COSTS	(%)	30
CAPEX	(%)	220

For the compressors, heat exchangers, pressure storage vessels, and equipment procurement costs the following equipment cost expressions were used [25]:

$$Cost_C(W) = -0.1288 * W^2 + 500.04 * W + 43.997 \tag{4}$$

$$Cost_{HE}(H) = -0.038 * H^2 + 149.18 * H + 12.849 \tag{5}$$

$$\begin{aligned} Cost_T(V,\ M,\ P) &= VF * MF * PF \\ &= \left(0.0811 *\ V^2 + 167.42 * V + 13529\right) *\ (0.0365 * P + 1.227) \end{aligned} \tag{6}$$

$$E_i = (n_C * Cost_C + n_{HE} *\ Cost_{HE} + n_T * Cost_T) \tag{7}$$

For the operational costs, a fixed energy cost price was assumed (Iberian Electricity Market) [27]. For electricity, an average cost of 0.106 €/kWh was assumed as representative and 0.0351 €/kWh for natural gas. To calculate the value of the operational cost and the savings for the utilization of the waste energy in the heat exchangers the following expressions were used:

$$\text{OPEX} = \left(W_n\ [kW] * COE \left[\frac{€}{kWh}\right] * T_o \left[\frac{h}{year}\right]\right) - U_e \left[\frac{€}{year}\right] \tag{8}$$

$$U_e = \frac{H_r}{\eta_{HE}}[kW] * COG\left[\frac{€}{kWh}\right] *\ T_o\left[\frac{h}{year}\right] \tag{9}$$

where we considered an operational time of 48 h/week, meaning (T_o) 2496 h/year, and a 10% heat losses in the heat exchangers (90% efficiency, η_{HE}) to calculate the incomes for the utilization of intercooling energy (U_e) that comes from the first heat exchanger of every single stage. We considered that the price savings from the reused heat is equivalent to the cost of energy price (using natural gas as a fuel) that must be delivered to reach the same difference in temperatures.

Then, for the total investment estimation, an annual temporal base was set to obtain the annual costs required for each gas and configuration. The economic assumption considers for the whole compression and storage plant a service life of 20 years, and the investment is calculated with an interest rate of 3%. In that case, the expression for the calculating the annual cost (a) of the equipment depends on CAPEX, annual interest (i), and service life (n), and is shown in Equation (10):

$$a = CAPEX * \frac{i * (1+i)^n}{(1+i)^n - 1} \tag{10}$$

Once the costs are presented in a suitable time base they can be added, and they are covered under the variable TAC (Total Annual Costs), whose expression is shown hereunder, Equation (11):

$$TAC \left[\frac{€}{year}\right] = a + \mathrm{OPEX} \tag{11}$$

2.3. Case Study Results

Since the process is made up of different stages in series, the calculation process is iterative for the different scenarios. The main variables that influence power consumption and thermal energy that can be utilized are the inlet gas compressor temperature, number of intercooling–compression stages, isentropic efficiency, inlet gas pressure, and working gas.

To evaluate the influence of gas temperature at the compressor inlet, this parameter was modified from 50 °C to 100 °C using a single compression stage. The results of this single scenario show a reduction of 13.85% in the specific work required by the compressor using lower inlet temperatures. Therefore, the lower the temperature at the compressor inlet, the lower the power consumption. Hence, this idea justifies the necessity of placing intermediate heat exchangers between compressors to minimize specific power consumption.

Another parameter that has direct influence on global consumption is the number of intercooling compression stages used to reach a certain storage pressure. In this research different scenarios were studied—ranging from one to five intercooling compression stages keeping a constant pressure of 20 bar to see the differences in consumption between scenarios. Then, if the two scenarios that differ in the number of compression stages are compared (3 and 4 stages), the results show a decrease in consumption of 2.98% using 4 compression stages (base case). Therefore, scenarios with a higher number of stages in series offer lower consumptions. This is a key result to be considered in the optimization procedure due to the higher number of stages implying an increase in equipment costs. Thus, the optimal scenario will have to consider low consumption without compromising the global costs. Table 3 illustrates the net power requirements, heat to be used, and heat to be discarded due to a low temperature level with different compressor–intercooling stages for CO_2 and H_2 as the operating gas.

Table 3. Net power required, and the heat used and discarded considering a storage pressure of 20 bar: CO_2 (left); H_2 (right).

K	W_{net} (kJ/kg)	H_u (kJ/kg)	H_{nu} (kJ/kg)	W_{net} (kJ/kg)	H_u (kJ/kg)	H_{nu} (kJ/kg)
1	15.23	14.60	1.64	40.72	38.15	2.52
2	12.86	10.77	3.12	32.19	27.11	5.04
3	12.13	8.56	4.58	29.86	22.26	7.55
4-SC	11.77	6.72	6.06	28.77	18.65	10.07
5	11.56	5.03	7.54	28.15	15.51	12.58

For scenarios with a higher number of compressors, the power required by each compressor is lower than the case with few compressors. Working with less compressor stages leads to higher temperatures in the compressor outlet and, therefore, the specific power requirements are higher than in the case of more stages. In designs that include a lower number of stages, more heat is transferred in the heat exchangers and could be used elsewhere. In contrast, when increasing the number of compression stages, the heat not reused is getting higher due to the increasing number of stages. These effects are well-described in the literature [16,20,21].

In reference to the whole system, the inlet gas pressure has a considerable effect on the target variable. Several inlet gas pressures (1–3 bar) were tested given a different number of compression stages (k = 1–5), and the results indicate that for a fixed storage pressure, the higher the gas pressure at the inlet, the lower the consumption as has been validated elsewhere [28]. This is justified because the difference between the inlet pressure and storage pressure is reduced and, as a consequence, the work required by the compressor drops, too.

Finally, the working gas is the variable that has a larger influence on global consumption due to the intrinsic properties of each gas (Table 3). For compressing low-density gases, there is work required by the compressors; therefore, the consumption is higher than for high-density gases. A comparison was set between the two working gases in this paper and it has shown a huge difference in consumption due to H_2 having a much lower density than CO_2.

To summarize, the two variables that facilitates minimum power consumption are: low gas temperatures at compressor inlet and using multiple compression stages. However, this statement implies a direct increase in the CAPEX needed for the whole installation since more equipment is needed. On the other hand, working with high isentropic efficiencies and elevated inlet gas pressure favours the decrease in consumption. Nevertheless, it must be noted that equipment with higher efficiencies implies higher acquisition costs, so optimization is required to take into account all these variables. Finally, it must be highlighted that the most important dependency in consumption is the density of the working gas.

For economic calculations a base case with 4 compressor intercooling stages has been chosen. Under this configuration compression and storage process is composed of 4 compressors, 8 heat exchangers and one high pressure gas storage tank. Table 4 show the CAPEX and variable cost description for economic calculations, and Tables 5 and 6 the main economic variable varying the number of stages.

Table 4. Detailed description of CAPEX considering a storage pressure of 20 bar. Base case.

Cost Description Study Case	Cost CO_2 (€)	Cost H_2 (€)
FIXED COSTS		
E, Main equipment cost (Compressors and heat exchangers)	460,303	747,072
Equipment installation	92,061	149,414
Instrumentation and control systems	73,648	119,532
Gas piping	156,503	254,004
Electrical systems	23,015	37,354
Industrial warehouse	23,015	37,354
Service centre	46,030	74,707
TOTAL FIXED COSTS	874,576	1,419,437
VARIABLE COSTS		
Engineering and supervision	23,015	37,354
Building costs	46,030	74,707
Legal costs	13,809	22,412
Administrative fees	9206	14,941
Contingencies	46,030	74,707
TOTAL VARIABLE COSTS	138,091	224,122
CAPEX	**1,012,667**	**1,643,558**

Table 5. Summary of the costs per scenario considering a storage pressure of 20 bar, CO_2.

K	TAC (€/Year)	CC (€)	HEC (€)	TC (€)	E (€)	CAPEX (€)	a (€/Year)	OPEX (€/Year)
1	40,117	51,582	14,058	173,737	253,435	557,557	37,477	2640
2	49,941	47,208	13,366	173,737	321,617	707,557	47,559	2382
3	60,196	46,016	13,176	173,737	390,839	859,846	57,795	2401
4-SC	70,551	45,467	13,087	173,737	460,303	1,013,000	68,067	2484
5	80,945	45,152	13,036	173,737	529,861	1,166,000	78,353	2592

Table 6. Summary of costs per scenario considering a storage pressure of 20 bar, H_2.

	TAC (€/Year)	CC (€)	HEC (€)	TC (€)	E (€)	CAPEX (€)	a (€/Year)	OPEX (€/Year)
1	87,816	64,144	15,867	449,650	545,527	1,200,000	80,670	7147
2	96,130	52,012	14,045	449,650	609,856	1,342,000	90,182	5948
3	106,067	48,961	13,589	449,650	678,069	1,492,000	100,269	5797
4-SC	116,331	47,587	13,384	449,650	747,072	1,644,000	110,473	5858
5	126,717	46,808	13,268	449,650	816,367	1,796,000	120,720	5997

The results highlight the greater influence of CAPEX than OPEX in the economic calculations and its variation according the number of stages considered. The cost of the equipment is clearly higher when working with a higher number of compression stages. It also can be observed that there is a minimum in OPEX that emerges because of the difference between the scenarios in terms of the heat reused, not reused, and the work required. Therefore, an optimization study must be carried out, to obtain the right balance between consumption and costs.

3. Optimization of Annual Costs

Previous calculations were done for a fixed final pressure in the storage tank. Evidently, if this pressure is modified then the final results of the cost and consumption will change, and other process configuration may minimize the cost. There are several variables that could influence the results. On the one hand, the cost expression of the gas storage tank depends on the internal pressure, gas volume, and material from which the tank is constructed. The higher the gas storage pressure (compressor cost increases), the lower the volume required to store it (storage tank cost decreases), but the tank material must be stronger to withstand high pressures (storage tank cost increases). Thus, the inverse influence of these variables in the expression of the tank cost makes this optimization study essential. Equation (6) show the cost dependency on volume and pressure. Increasing gas pressure causes an increment in density and a reduction in (specific) volume. As these two variables are multiplying in Equation (6), the pressure that minimizes the capital cost is not evident. Pressure and volume are related through the density and the pressure that minimizes the cost depends on the variation in gas density with pressure. On the other hand, the work required by the equipment (overall consumption) also plays an important role in the optimization study, since it is directly related to costs. For example, if the number of compression stages in series increases, the compressor's consumption decreases. Therefore, operating costs decrease. However, it must be considered that the greater the number of stages in series, the greater the number of equipment that needs to be purchased; therefore, the total cost increases. This is another dichotomy that justifies the optimization study.

The aim of this section is to do an optimization analysis of the different scenarios previously shown. For each gas (CO_2 and H_2) an optimization problem was solved. As a result, the optimal configuration or scenario was selected—for each gas—based on the input hypotheses showed in Table 7.

Table 7. Boundary conditions for the optimization study.

	Carbon Dioxide		Hydrogen	
	Value	**Unit System**	**Value**	**Unit System**
Methane mass	0.02	kg/s	-	-
Carbon dioxide mass	0.055	kg/s	-	-
Days per week	2	day	2	day
Compression ratio	1–4	-	1–4	-
Hydrogen mass	-	-	0.0058	kg/s
Inlet gas pressure	1 bar			
Temperature between serial heat exchangers	60 °C			
Inlet gas temperature	30 °C			
Isentropic efficiency	85%			
Compression ratio	1–4			

The objective function is to minimise the TAC, which include the yearly investment cost calculated with CAPEX, interest rate, and amortization years (Equations (4)–(7), (10), and (11)). This variable takes into account the influence of pressure on the compressor, the number of stages, and the storage tank costs. It also includes the energy consumption to pressurize CO_2 or H_2 to the storage tank pressure. A similar analysis can be found in [29]. Constraints include mass and energy balances in the compressors and heat exchangers and the variables included in Table 7. So, the problem is formulated according Equation (12):

$$\begin{array}{ll} \text{Objective function:} & \text{Minimize TAC} \\ \text{Constraints:} & \text{Subject to: Energy balances} \\ & \text{Equipment costs} \\ & \text{Number of stages (discrete variable)} \end{array} \tag{12}$$

Two optimization methods (Golden Section Search and Quadratic Approximations) were used and both agrees at the storage pressure. Using CO_2 as the working gas, the optimized configuration is the one with four intercooling compression stages. In this optimal scenario, the storage pressure that minimises the TAC—with a value of 60.068 €/year—is 72.47 bar. This value is just below the supercritical pressure. Increasing the pressure above this value increase the compressor, installation, and operational cost without reducing significantly the storage tank value and cost. For the first three scenarios it can be observed how the compressor ratio is over the boundary imposed (1–4), and that is why those scenarios are not considered as technically feasible (Table 8). Although the storage pressure is very similar between Scenarios 4 and 5, it must be noted, in Table 8, the final cost increment from 56,966 to 67,223 €/year economically when working with a larger number of stages. The columns related to the cost of the compressor, heat exchangers, and tank are unitary costs.

Table 8. Optimization results for the different scenarios, CO_2.

K	P (bar)	V (m^3)	Cr	TAC (€/Year)	CC (€)	HEC (€)	TC (€)	E (€)	CAPEX (€)	a (€/Year)	OPEX (€/Year)
1	72.40	-	72.40	-	-	-	-	-	-	-	-
2	72.45	-	8.51	-	-	-	-	-	-	-	-
3	72.46	-	4.17	-	-	-	-	-	-	-	-
4-SC	72.47	15.49	2.92	60,068	46,114	13,378	93,749	385,231	847,505	56,966	3102
5	72.48	15.49	2.36	70,397	45,640	13,265	93,749	454,597	1,000,000	67,223	3174

In the case of hydrogen, the optimal configuration to minimise TAC is the one with three intercooling compression stages (Table 9). This is achieved for a hydrogen storage pressure of 67.64 bar and a related TAC of 83,734 €/year. For the reasons explained before, in this case the first two scenarios were considered as not valid.

Table 9. Optimization results for the different scenarios, H_2.

K	P (bar)	V (m^3)	Cr	TAC (€/Year)	CC (€)	HEC (€)	TC (€)	E (€)	CAPEX (€)	a (€/Year)	OPEX (€/Year)
1	57.27	-	57.27	-	-	-	-	-	-	-	-
2	65.41	-	8.09	-	-	-	-	-	-	-	-
3	67.64	193.70	4.00	83,734	51,446	13,958	271,669	509,756	1,121,000	75,380	8354
4-SC	68.66	191	2.88	93,677	49,325	13,641	271,332	577,765	1,271,000	85,437	8240
5	69.24	189.5	2.33	103,879	48,140	13,465	271,156	646,506	1,422,000	95,602	8278

If we compare both gases, it is clear that the difference in costs between them is mainly due to density variances. While comparing the results between both gases, the difference in mass flow rate must be highlighted. Due to the low density of hydrogen, the global costs would increase when working with a higher mass flow rate.

Sensitivity Analysis

Due to the influence of some key variables on the final results, the next sub-section provides a sensitivity analysis regarding variations in the price of electricity and operational hours for the optimised scenarios shown before.

Firstly, the price of electricity considering both was modified—an increase and decrease of 15% in the cost of energy. This has been performed for the optimal scenario for each gas. The results are summarized in Table 10. The variations in electricity price directly affect the OPEX. As these costs have a lower weight than CAPEX, the results in TAC are not as high as it could be expected in the first instance. On the one hand, the results using carbon dioxide show how a decrease of 20% in the COE implies a decrease in TAC of 1.5%, and an increase of 20% in the COE implies an increase in TAC of 1.5% as well. On the other hand, the results using hydrogen show how a decrease of 20% in the COE implies a decrease in TAC of 2.87%, and an increase of 20% in the COE implies an increase in TAC of 2.84%. Additionally, using hydrogen it must be noted that a decrease of 20% in COE implies a compressor ratio over than the maximum limit considered. In that case, the optimal configuration would be the one with four intercooling compression stages.

Table 10. Sensitivity analysis varying electricity price in comparison to optimized base case. (a) CO_2; (b) H_2.

	K	TAC (€/Year)	CAPEX (€)	a (€/Year)	OPEX (€/Year)	P (bar)	V (m^3)	Cr
(a)								
Optimization base	4-SC	60,068	847,505	56,966	3102	72.47	15.49	2.92
Decrease COE 20%	4-SC	59,164	847,505	56,966	2198	72.49	15.48	2.92
Increase COE 20%	4-SC	60,972	847,505	56,966	4006	72.46	15.51	2.92
(b)								
Optimization base	4-SC	83,734	1,121,000	75,380	8354	67.64	193.70	4.00
Decrease COE 20%	4-SC	81,329	1,121,000	75,318	6012	69.89	187.80	4.12
Increase COE 20%	4-SC	86,116	1,121,000	75,463	10,653	65.51	199.80	4.00

Secondly, we considered variations in the operational hours for the discrete values of 96 and 168 h/week (Table 11). This operation time was considered as the time when the compressors are actively compressing and storing the gas. The results of these variations in the operation time indicates that this parameter has more influence in TAC than fluctuations in the electricity price. On the one hand, duplicating operational hours using carbon dioxide implies an increase in TAC of 5.16%. Moreover, considering the compressors are fully working all week, the TAC increased by 12.91%. On the other hand, duplicating the hour of operation using hydrogen implies an increase in TAC of 9.84%. Finally, the increase in TAC is 24.12% considering the compressors working full-time.

Table 11. Sensitivity analysis varying the operational hours in comparison to the optimized base case: (a) CO_2; (b) H_2.

	K	TAC (€/Year)	CAPEX (€)	a (€/Year)	OPEX (€/Year)	P (bar)	V (m^3)	Cr
(a)								
Optimization Base	4-SC	60,068	847,505	56,966	3102	72.47	15.49	2.92
96 h/week (4 days/week)	4-SC	63,170	847,505	56,966	6204	72.46	15.51	2.92
168 h/week (7 days/week)	4-SC	67,824	847,505	56,966	10,858	72.44	15.53	2.92
(b)								
Optimization Base	4-SC	83,734	1,121,000	75,380	8354	67.64	193.70	4.00
96 h/week (4 days/week)	4-SC	91,974	1,121,000	75,318	16,258	61.18	213.40	3.94
168 h/week (7 days/week)	4-SC	103,935	1,121,000	75,463	27,388	53.31	243.80	3.76

It is concluded that the configuration and storage pressure that minimize the costs (under the assumption considered in this work) are four CO_2 compressor stages to a final pressure of 72.5 bar and three H_2 compressor stages to a final pressure of 67.6 bar. In both cases, for the different stages (three, four or five) the final storage pressure is relatively unchanged, but the cost clearly indicates the most feasible configuration. Adding an additional stage increases the TAC by 17.19% using CO_2 as the working gas, and by 11.87% using H_2.

These results could also be useful in other applications of temporary energy storage that make use of CO_2, as in the case of calcium looping for concentrated solar power applications [30,31] or H_2 in the form of gas. Evidently, in this last case, there are several options to storage H_2 [32,33]; we only consider a temporary gas storage and the results can vary from other sources. In any case, the possibility of H_2 pipe storage up to 100 bar is realistic and there are enough expertise when applied to natural gas [32].

4. Conclusions

The necessity of decarbonize the industrial and residential sectors is motivating a huge increment in renewable electricity production. In order to manage the mismatching between renewable production and consumption, it is essential to develop energy storage alternatives. Power to gas is a promising option to take advantage of renewable H_2 by converting it, together with the captured CO_2, into renewable gases, in particular renewable methane. It allows the temporal displacement (storage) in the use of renewable energy. Storage vessels for H_2 and CO_2 are necessary to smoothly run a methanation installation and then a new research line about the feasible operational variables that minimize the energy requirements in this storage is required.

The objective of this research was reached through a techno-economic analysis of the feasible layout and storage pressures that minimize the capital and operation cost of H_2 and CO_2 gas compression and storage vessels for power-to-gas applications. The main findings of the analysis are highlighted:

(i) Four compressor stages for CO_2 storage at a pressure of 72.5 bar minimize the annual storage cost. This value is just below the supercritical pressure. Increasing pressure above this value increases the compressor, installation, and operational cost, without reducing significantly the storage tank value and cost.
(ii) In the case of H_2, the minimum cost is found with a storage pressure of 67.6 bar, slightly lower than in the case of CO_2 and with one compressor stage less. This value is in agreement with the usual pressures to store and distribute natural gas.
(iii) In both cases the value of the pressure that minimize the cost remains practically unchanged despite the number of compressor stages. In any case, the effect of the number of stages on cost is evident and the economic differences are clear.
(iv) For the mass flow of H_2 and CO_2 was selected the production of a 1 MW electrolyzer and CO_2 to complete the conversion into CH_4. With this assumption, the H_2 storage cost are higher than the CO_2 cost, even with lower mass quantities; this is due to the lower H_2 density compared to CO_2.
(v) Finally, it is also concluded that the compressor costs are the most relevant cost for CO_2 compression but the storage tank cost are the most relevant in the case of H_2.

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Abbreviations

A	Annual costs (€/year)
CAPEX	Capital expenditure (€)
CCS	Carbon Capture and Storage
COE	Cost of electricity(€/kWh)
COG	Cost of natural gas (€/MWh)
$Cost_C$	Unitary compressor cost (€)
$Cost_{HE}$	Unitary heat exchanger cost (€)
$Cost_T$	Unitary tank cost (€)
Cr	Compression ratio
DAC	Direct Air Capture
Ei	Equipment cost (€)

GHG	Greenhouse gases
Hnu	Heat not used (kJ/kg)
Hu	Heat used (kJ/kg)
i	Annual interest (%)
k	Configuration
LHV	Low Heating Value (kJ/kg)
MF	Material factor
n	Service life (years)
OPEX	Operating expenditure (€/year)
PtG	Power to gas
PF	Pressure factor
SNG	Synthetic natural gas
TAC	Total annual costs (€/year)
To	Operation time (hours/year)
VF	Volume factor
Wnet	Net power (kJ/kg)

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