GRADO EN INGENIERÍA EN TECNOLOGÍAS INDUSTRIALES

FINAL DEGREE PROJECT

A THERMODYNAMIC APPROACH TO HYDROGEN STORAGE COST OPTIMIZATION

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Declaro, bajo mi responsabilidad, que el Proyecto presentado con el título

A thermodynamic approach to hydrogen storage cost optimization, en la ETS de Ingeniería - ICAI de la Universidad Pontificia Comillas en el

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"*The important thing is not to stop questioning*."
— *Albert Einstein*

To my family and friends, whose encouragement, patience, and unconditional support have been essential throughout these years.

I am especially grateful to my supervisors for their guidance and support, which have made a meaningful impact from the very beginning of this project.

UNA APROXIMACION TERMODNÁMICA A LA OPTIMIZACIÓN DE COSTES DE ALMACENEMIENTO DEL HIDROGENO

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RESUMEN DEL PROYECTO

El desarrollo de modelos de optimización para almacenamiento de hidrógeno es un paso esencial para el desarrollo de esta tecnología. Este proyecto plantea el modelado del coste variable de almacenamiento según el nivel de llenado, basado en un enfoque termodinámico. Se han representado varias tecnologías para almacenar hidrógeno y evaluando limitaciones, operación e impacto económico.

Palabras clave: Hidrógeno, Mercado Eléctrico, Almacenamiento de Energía, Compresión, Optimización.

1. Introducción

La transición energética hacia un modelo basado en renovables plantea una serie de desafíos técnicos, especialmente por la naturaleza incontrolable de estas tecnologías. Para garantizar la seguridad de suministro, el sistema eléctrico se ha visto obligado a sobredimensionar la potencia de generación instalada respecto a la demanda esperada, lo que implica mayores costes de inversión.

El almacenamiento de energía se ha posicionado como la solución clave, al permitir desplazar excedentes energéticos de fuentes de generación no despachables hacia periodos con déficit de generación. Entre las opciones de almacenamiento a gran escala, destacan tres tecnologías: las baterías, las centrales hidroeléctricas reversibles, y la generación de hidrógeno [1]. Este último ha demostrado aportar un buen equilibrio entre coste, escalabilidad y eficiencia, frente al resto de tecnologías.

El hidrógeno, puede almacenarse de múltiples formas, siendo la compresión y la licuefacción las más viables económicamente a gran escala. Sin embargo, los modelos de optimización para el almacenamiento de hidrógeno actuales simplifican el coste incurrido como constante, ignorando el impacto físico del nivel de llenado sobre el consumo energético de compresión.

Este proyecto aborda esa limitación desarrollando un modelo de optimización de los flujos de hidrogeno que representa el coste de almacenamiento de forma variable según la termodinámica del proceso, evaluando así su impacto técnico y económico.

2. Definición del proyecto

Esta aproximación termodinámica se fundamenta en la expresión no lineal de los procesos de compresión. La *Ecuación 1* muestra el trabajo necesario para comprimir un gas. Para nuestro problema todos los valores se pueden considerar constantes salvo la *r* que representa la relación entre la presión inicial y final. Considerando que la presión inicial es la presión ambiente y que el hidrogeno es un gas ideal que ofrece una relación lineal entre la cantidad de materia y la presión, se puede establecer una relación lineal entre la presión del tanque y su nivel de llenado. De ese modo, se puede demostrar que el incremento del nivel de llenado de los tanques provoca un crecimiento no lineal la energía especifica requerida para esa compresión.

$$w_{compresión} = \frac{n}{n-1} \cdot R \cdot T_{in} \cdot \left[r^{\frac{n-1}{n}} - 1 \right]$$

Ecuación 1 – Trabajo específico necesario para la compresión de un gas

Realizando un análisis preliminar sobre los costes de generación del hidrógeno y almacenamiento de hidrogeno, se ha cuantificado en alcance de esta aproximación termodinámica. Este cálculo se ha basado basados en parámetros económicos de este tipo de infraestructuras [2], además de datos del mercado eléctrico español.

El resultado, representado en la *Figura 1*, revela como la mayor parte del coste de almacenamiento se debe al consumo energético para la electrolisis. Añadiendo a este coste con los costes de generación se observó una diferencia del 9,4% del coste total entre el caso de operación con bajo nivel de llenado comparando con el caso de niveles altos.

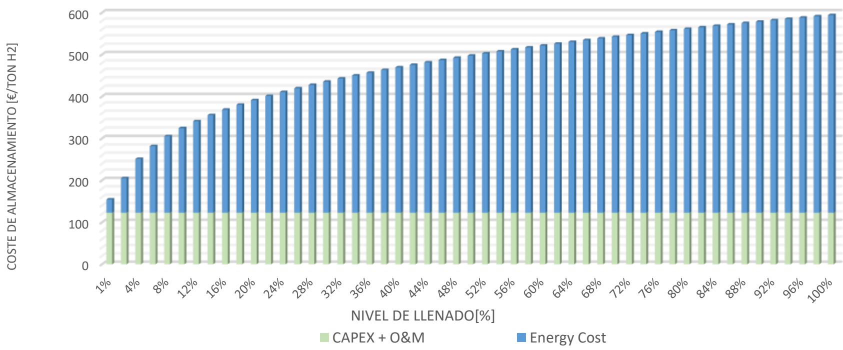

Figura 1 – Coste de almacenamiento de hidrogeno según nivel de llenado

3. Descripción del modelo

El modelo propuesto tiene como objetivo minimizar el coste total del sistema de hidrógeno, considerando generación, almacenamiento y consumo horario en un entorno centralizado. Para ello, se partió de un modelo de mercado eléctrico y de hidrógeno. Se eliminaron las zonas territoriales y los agentes. El objetivo del modelo era la representación de los costes de operación (al no contabilizar CAPEX). Se incluyeron dos tecnologías de producción (electrólisis y química) y tres tecnologías de almacenamiento (compresión, licuefacción y cavernas salinas), permitiendo que al modelo seleccionar dinámicamente la combinación más eficiente en cada momento.

La formulación tiene una resolución horaria y el horizonte de simulación considerado es de un año, e incluye balances de masa y energía, eficiencias por tecnología, límites de capacidad y pérdidas asociadas al almacenamiento. También se modela la posibilidad de usar el hidrógeno almacenado para generar electricidad a través de pilas de combustible.

Para modelar la interacción de esta infraestructura destinada a satisfacer una demanda inflexible de hidrogeno, se considera el precio de la electricidad como un parámetro exógeno al modelo. Éste se incorpora como una matriz de parámetros.

De cara a la resolución del modelo, la curva de los costes de compresión debe de ser representada (extraída de la *Ecuación 1*). Para ello se contemplaron cuatro estrategias de modelado, incluyendo una opción lineal. Sin embargo, el análisis realizado concluyó que el mejor compromiso entre tiempo de resolución y precisión en el modelado se consigue mediante la representación directa de la expresión de la *Ecuación 1*, pese a ser no lineal.

4. Resultados

En el modelo desarrollado se han contemplado distintos escenarios para evaluar el impacto de modelar los costes de almacenamiento de hidrógeno en función de la curva termodinámica, comparados con el enfoque tradicional de coste constante. Los resultados, construido sobre las proyecciones del PNIEC para España en 2030, demuestran que el almacenamiento en cavernas comprimidas destaca como la opción más eficaz para cubrir necesidades estacionales, representando más del 75% del volumen almacenado anual. Este tipo de almacenamiento ofrece bajos costes operativos (40–45 €/ton H_2) y mantiene perfiles de LoH (nivel de llenado de hidrógeno) estables, poco dependientes del modelo de costes simulado.

Por otro lado, los tanques comprimidos y el almacenamiento líquido actúan como tecnologías de corto plazo, dada su alta flexibilidad y baja capacidad, mostrando mayores diferencias operativas entre los enfoques de coste constante y curva. En particular, los tanques comprimidos presentan una diferencia relativa de hasta un 14,6% en sus perfiles de nivel de llenado, reflejando una mayor sensibilidad al método de modelado del consumo energético, demostrando que el efecto de la aproximación termodinámica se incrementa con la presión máxima del almacenamiento.

Además, la aplicación de la curva termodinámica reduce la necesidad de precios negativos de electricidad para lograr rentabilidad en el almacenamiento (del 57–70% al 8–13% del tiempo de operación), lo que evidencia una mayor versatilidad operativa. Esta diferencia operativa se puede observar en la *Figura 2*, donde se aprecia que el modelo de curva reduce más rápido su LoH para beneficiarse del menor coste de compresión correspondiente a esa zona, ya que la presión es menor.

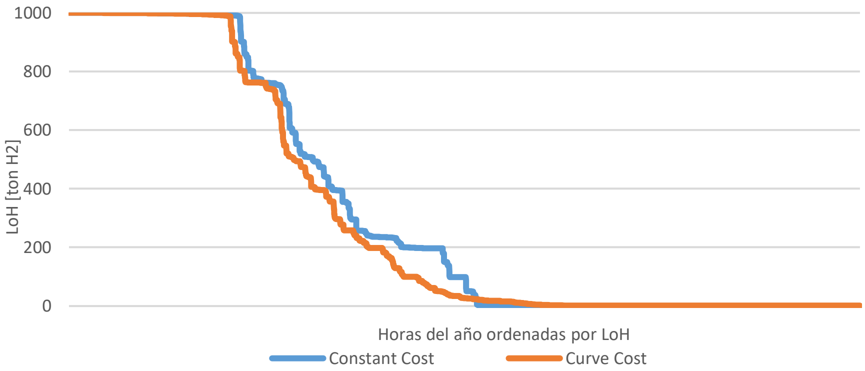

Figura 2 – Curva monótona de LoH del tanque de compresión

La precisión adicional del enfoque con curva implica un incremento significativo del tiempo de simulación (de ~1 min a ~30–45 min), lo que representa una relación coste-beneficio a considerar según el objetivo del modelo.

Finalmente, el estudio de escenarios con mayor capacidad de almacenamiento y de tecnologías de almacenamiento únicas permite concluir que los beneficios del enfoque detallado dependen en gran medida del tipo de tecnología y su presión de operación, proporcionando así criterios cuantificables para decidir entre precisión y eficiencia computacional.

5. Conclusiones

Los resultados obtenidos confirman que el modelo termodinámico del coste de compresión permite representar de forma más realista el comportamiento operativo de las tecnologías de almacenamiento de hidrógeno por compresión, especialmente aquellas con presiones de operación elevadas. Esta mejora en la precisión del modelo da lugar a patrones de operación más flexibles, una reducción significativa de la dependencia en los precios negativos, y un cálculo más realista del consumo energético, con diferencias de hasta un 10% en el coste.

El estudio concluye que el almacenamiento en cavernas comprimidas constituye la mejor alternativa para cubrir necesidades de almacenamiento estacional a gran escala, gracias a su elevada capacidad y bajo coste específico. A su vez, tecnologías como los tanques comprimidos o el almacenamiento líquido, aunque más costosas, ofrecen mayor agilidad operativa y podrían desempeñar un rol complementario en la gestión a corto plazo.

No obstante, el mayor tiempo de resolución por el uso de curvas no lineales plantea una disyuntiva entre precisión y eficiencia computacional. Mientras que agentes centrados en almacenamiento podrán justificar el uso del modelo detallado por su impacto directo en los costes operativos, otros agentes con foco en generación o trading podrían optar por modelos simplificados sin comprometer significativamente la calidad de los resultados.

Finalmente, el modelo desarrollado ha permitido cuantificar las diferencias operativas entre enfoques, representar múltiples tecnologías de almacenamiento de forma conjunta o individual, e incluir pérdidas por fugas, logrando así una mejor caracterización del almacenamiento de hidrógeno en un contexto de mercado nacional. Estas capacidades sientan las bases para futuros desarrollos que incluyan la formación de precios o nuevas tecnologías de almacenamiento emergentes.

6. Referencias

[1] Z. Abdin, A. Zafaranloo, A. Rafiee, W. Mérida, W. Lipiński, and K. R. Khalilpour, “Hydrogen as an energy vector,” *Renew. Sustain. Energy Rev.*, vol. 120, p. 109620, Mar. 2020, doi: 10.1016/j.rser.2019.109620.

[2] J. Michalski et al., “Hydrogen generation by electrolysis and storage in salt caverns: Potentials, economics and systems aspects with regard to the German energy transition,” Int. J. Hydrog. Energy, vol. 42, no. 19, pp. 13427–13443, May 2017, doi: 10.1016/j.ijhydene.2017.02.102.

A THERMODYNAMIC APPROACH TO HYDROGEN STORAGE COST OPTIMIZATION

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ABSTRACT

The development of optimization models for hydrogen storage is an essential step for the development of this technology. This project proposes the modeling of the variable storage cost according to the filling level, based on a thermodynamic approach. Several technologies for storing hydrogen have been represented, evaluating limitations, operation, and economic impact.

Keywords: Hydrogen, Electricity Market, Energy Storage, Compression, Optimization.

1. Introduction

The energy transition towards a model based on renewable energies poses a wide range of technical challenges, especially due to the uncontrollable nature of sources such as the sun, rain, or wind. To guarantee security of supply, the power system has been forced to oversize the installed generation capacity with respect to expected demand, which implies higher investment costs.
Energy storage has positioned itself as the key solution, as it allows shifting energy surpluses from non-dispatchable generation sources to periods with generation deficits. Among the large-scale storage options, three technologies stand out: batteries, reversible hydroelectric plants, and hydrogen generation [1]. The latter has proven to offer a good balance between cost, scalability, and efficiency compared to the other technologies.
Hydrogen can be stored in multiple ways, with compression and liquefaction being the most economically viable at large scale. However, current optimization models for hydrogen storage simplify the cost incurred as constant, ignoring the physical impact of the filling level on the energy consumption of compression.

This project addresses that limitation by developing an optimization model of hydrogen flows that represents the storage cost as a variable, according to the thermodynamics of the process, and evaluating its technical and economic impact.

2. Definition of the project

This thermodynamic approach is based on the nonlinear expression of compression processes. *Equation 1* shows the energy required to compress a gas. In this equation, for our problem all values can be considered constant except for r, which represents the ratio between the initial and final pressure. Considering that the initial pressure is atmospheric pressure, and that hydrogen is an ideal gas that offers a linear correlation between the amount of matter and pressure, a linear pattern can be established between the tank pressure and its filling level. In this way, it can be demonstrated that an increase in the filling level of the tanks causes a nonlinear growth in the specific energy required for that compression.

$$w_{compression} = \frac{n}{n-1} \cdot R \cdot T_{in} \cdot \left[r^{\frac{n-1}{n}} - 1 \right]$$

Equation 1 – Specific energy required to compress gas

By carrying out a preliminary analysis on hydrogen generation and hydrogen storage costs, the scope of this thermodynamic approach was quantified. This calculation has been based on economic parameters of this type of infrastructure [2], in addition to data from the Spanish electricity market.

The result, shown in *Figure 1*, reveals how most of the storage cost is due to the energy consumption for electrolysis. When adding this cost to the generation costs, a 9,4% difference in the total cost was observed between the cases of operation with a low filling level compared to the case with high levels.

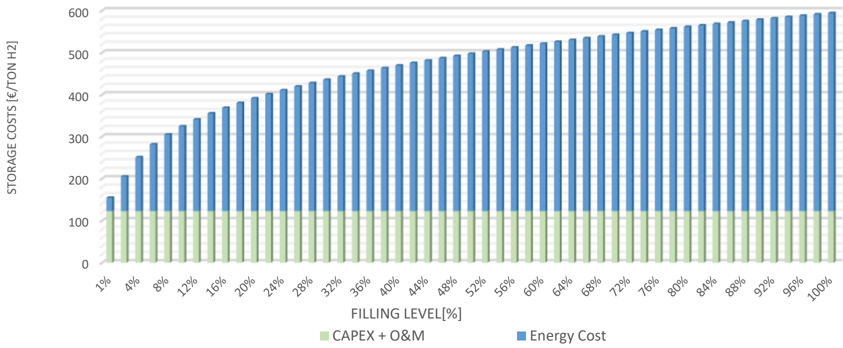

Figure 1 – Storage cost incurred by LoH level

3. Description of the model

The model proposed in this project aims to minimize the total cost of the hydrogen system, considering generation, storage, and hourly consumption in a centralized environment. For this purpose, the starting point was an electricity and hydrogen market model. Territorial divisions and different agents were removed. The objective of the model was the representation of operating costs (as investment costs were not considered). Two production technologies (electrolysis and grey production) and three storage technologies (compression, liquefaction, and salt caverns) were included, allowing the model to dynamically select the most efficient combination at each moment.

The formulation has an hourly resolution, and the simulation horizon considered is one year, and includes mass and energy balances, efficiencies by technology, capacity limits, and losses associated with storage. The possibility of using stored hydrogen to generate electricity through fuel cells is also modeled.

To model the interaction of this infrastructure intended to meet an inflexible hydrogen demand, the electricity price is considered as a parameter exogenous to the model. It is incorporated as a parameter matrix.

For the resolution of the model, the compression cost curve must be represented (extracted from *Equation 1*). For this purpose, four modeling strategies were considered, including a linear option. However, the analysis concluded that the best compromise between resolution time and modeling accuracy is achieved through the direct representation of the expression in Equation 1, despite being nonlinear.

4. Results

In the developed model, several different scenarios have been considered to evaluate the impact of modeling hydrogen storage costs based on the thermodynamic curve, compared to the traditional constant cost approach. The results, built on the PNIEC projections for Spain in 2030, show that compressed cavern storage stands out as the most effective option to cover seasonal needs, representing more than 75% of the annual stored volume. This type of storage offers low operating costs (40–45 €/ton H_2) and maintains stable LoH (level of hydrogen filling) profiles, with little dependence on the simulated cost model.

On the other hand, compressed tanks and liquid storage act as short-term technologies, given their high flexibility and low capacity, showing greater operational differences between the constant cost and curve-based approaches. Compressed tanks present a relative difference of up to 14,6% in their filling level profiles, reflecting a greater sensitivity to the modeling method of energy consumption, demonstrating that the effect of the thermodynamic approach increases with maximum storage pressure.

In addition, the application of the thermodynamic curve reduces the need for negative electricity prices to achieve profitability in storage (from 57–70% to 8–13% of operating time), which shows greater operational versatility. This operational difference can be observed in *Figure 2*, where it is seen that the curve model reduces its LoH more quickly to benefit from the lower compression cost corresponding to that zone, since the pressure is lower.

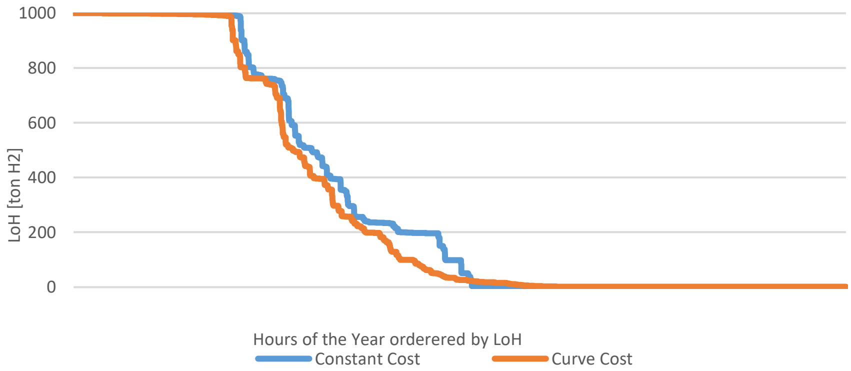

Figure 2 – Monotonic curve of compressed tank LoH

The additional accuracy of the curve-based approach implies a significant increase in simulation time (from ~1 min to ~30–45 min), which represents a cost-benefit trade-off to be considered depending on the model's objective.

Finally, the study of scenarios with greater storage capacity and single storage technologies allows us to conclude that the benefits of the detailed approach depend largely on the type of technology and its operating pressure and providing quantifiable criteria to decide between accuracy and computational efficiency.

5. Conclusions

The results obtained confirm that the thermodynamic model of compression cost allows for a more realistic representation of the operational behavior of hydrogen storage technologies by compression, especially those with high operating pressures. This improvement in model accuracy leads to more flexible operating patterns, a significant reduction in dependence on negative prices, and a more realistic calculation of energy consumption, with differences of up to 10% in cost.

The study concludes that compressed cavern storage is the best alternative to meet large-scale seasonal storage needs, thanks to its high capacity and low specific cost. At the same time, technologies such as compressed tanks or liquid storage, although more expensive, offer greater operational agility and could play a complementary role in short-term management.

However, the increased resolution time due to the use of nonlinear curves poses a trade-off between accuracy and computational efficiency. While agents focused on storage may justify the use of the detailed model due to its direct impact on operating costs, other agents focused on generation or trading could benefit from simplified models without significantly compromising the quality of the results.

Finally, the developed model has made it possible to quantify the operational differences between approaches, represent multiple storage technologies jointly or individually, and include leakage losses, while achieving a better characterization of hydrogen storage in a national market context. These capabilities lay the foundation for future developments that include price formation or emerging new storage technologies.

6. References

[1] Z. Abdin, A. Zafaranloo, A. Rafiee, W. Mérida, W. Lipiński, and K. R. Khalilpour, "Hydrogen as an energy vector," *Renew. Sustain. Energy Rev.*, vol. 120, p. 109620, Mar. 2020, doi: 10.1016/j.rser.2019.109620.

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Chapter 1. INTRODUCTION

1.1 THE NEED FOR ENERGY STORAGE SOLUTIONS

Renewable energy has been globally presented as one of the most important feasible solutions for energy supply in the future. This development has also been incentivized by governments, especially the European Union, with initiatives aiming to converge to a net cero emission economy by the year 2050 [1].

One of the key drivers is the electrification of energy consumption, combined with the development of renewable energy sources to satisfy the electrical demand. This new energy paradigm raises many technical challenges that need to be overcome before we can rely on renewable energy as the main source for electricity generation.

For the last 2 centuries, fossil fuels have been the main motor for the global economy. This technology had a lot of drawbacks, starting with CO_2 emissions, and dependance on fuel prices, with the corresponding geo-political challenges for the control of energy sources. On the other hand, these technologies offered great stability for the balance of electricity that is instantaneously needed between generation and demand as energy availability was only affected by the stock of fuel (coal, oil, gas, etc.) creating a predictable environment for this market.

These technologies are being progressively decommissioned, with Combined Cycle Power Plants (CCPP) been almost the only technology that is still in use for large scale electricity generation in Spain, with the closure of the last coal plants [2].

1.1.1 THE NEW RENEWABLE ENERGY MODEL

With the amortization and closure of fossil fuel thermal plants, the lack of generation has been compensated for using renewable energy sources, as shown in Figure 1. In this graph, it is clearly shown how renewable generation in Spain was stable before the year 2000. From that point, a new trend started, growing this energy source in both absolute and relative metrics. The last statistics [3], corresponding to the year 2024 (provided by Spanish TSO[1]: REE), show how renewable sources were up to 57% of the total energy generated corresponding to 149 TWh in that period.

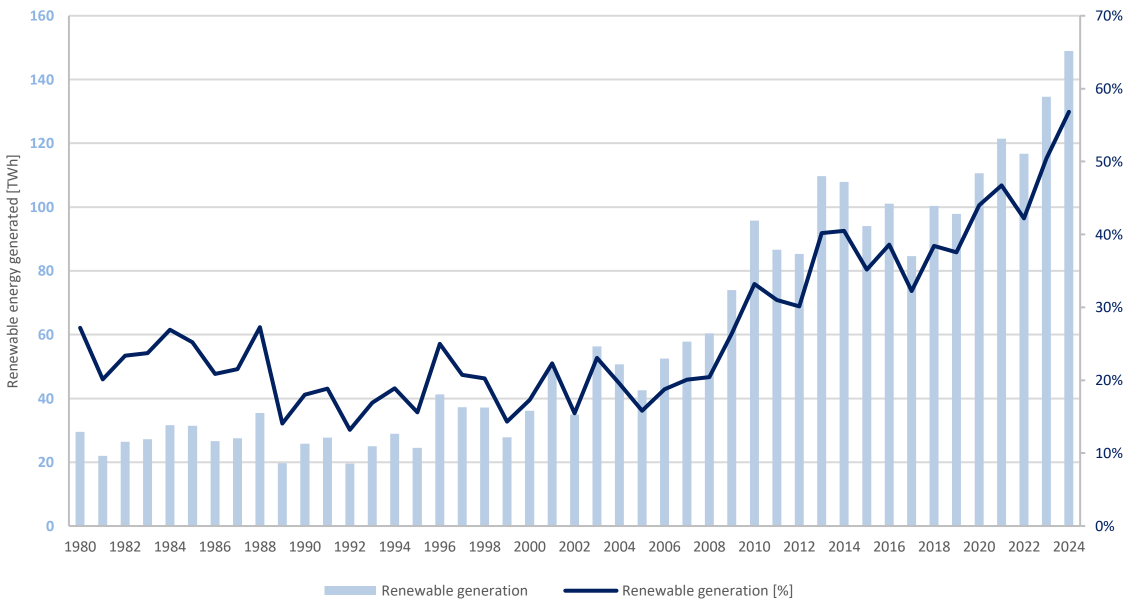


Figure 1 Renewable energy generation in Spain since 1980

These new renewable technologies offer important advantages starting with a negligible carbon footprint compared with fossil fuel energy. However, considering that they cannot be controlled (as they are based on rain, wind, sun, etc.) difficulties in the instant match of generation and demand rise. The main consequence of this uncontrollability can be observed

[1] TSO: Transport System Operator; REE: Red Electrica Española

by looking at renewable installed power and comparing it with the maximum demand of power of the Spanish system in that year, as shown in Figure 2 [4].

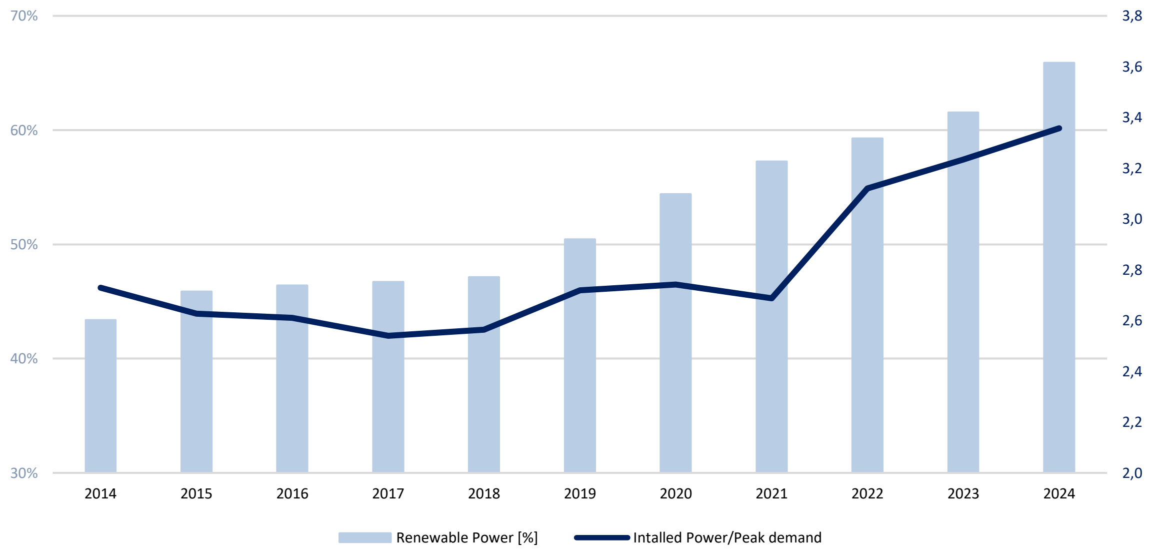


Figure 2 Renewable installed power and installed power to peak ratio in Spain

The trend to increase the weight of renewable energy, combined with the uncontrollable nature of this energy sources, causes the phenomenon shown in Figure 2, where it is clearly shown how this dilemma is solved by installing more power relative to the demand. That is the reason why a clear uptrend can be observed in the installed power to peak demand ratio that has grown continually since 2017 (except for 2021, because an especially cold summer that increased the peak demand of that year above expectations). This phenomenon may cause the energy infrastructure to be over dimensioned (relative to previous years) to ensure that on the worst-case scenario demand is met by generation.

By comparing the cost of investment (CAPEX) of renewable and non-renewable energy sources greener technologies tend to be more capital intensive with solar energy as the cheapest, with a cost of around 900 $/KW [5]. On the other hand, Combined Cycle Power Plants (CCPP) are the most capital efficient generation technology going as low as 500 $/KW [6] (for the simplest configurations although average specific CAPEX is around 730 €/KW [7] still representing the least capital intensive generation technology). Therefore, a renewable based energy system not only would require more installed power, but also at a higher capital cost [8]. On the other hand, these renewables technologies require a lower operating cost and manage to achieve a lower Levelized Cost of Energy (LCOE) compared to traditional generation sources [9].

The main renewable energy sources used are nature related (wind, sunlight and rain mainly), and therefore non-dispatchable in the short-term. However, in the long term, they tend to be seasonal.

This last aspect raises an interesting point; by using storage technology to absorb energy surplus and return it during energy deficit periods, this effect of renewable energy can be drastically reduced in the short-term. Therefore, installed to peak power ratios could go back to previous values, increasing total profitability of generation infrastructure and resource allocation.

1.2 MARKET SCALE STORAGE OPTIONS

1.2.1 BATTERY ENERGY STORAGE SYSTEMS (BESS)

Considering the explained need for energy storage solutions, several options have been explored for the electricity market. However, for large scale solutions, only 3 are feasible. Firstly, Battery Energy Storage Systems (BESS), that use redox chemical reactions to transform electrical into chemical energy. The main drawback of this technology is the CAPEX, projected to be around 189 $/KWh of capacity [10] (for Li-ion technology), as well as an important leakage factor [11]. These constraints mean that BESS are used mainly as a Flexible Alternating Current Transmission System (FACTS) for better regulation in power grids, but not as a long-term energy storage option.

1.2.2 PUMPING STATIONS

Hydroelectric pumping is a widely used technology on which hydroelectric generation is reversed by pumping water upwards to a higher reserve and transforming electricity into potential energy that can be extracted in the future. The main drawback of this technology is its scalability as several physical requirements must be met (water availability on the low point, combined with a naturally limited storage capacity, environmental impact). This type of technology is widely used. However, further expansion is limited and in the case of the Iberian Peninsula it is difficult due to the lack of feasible locations, making it insufficient for a market-scale storage solution.

1.2.3 HYDROGEN GENERATION

Hydrogen generation is the last of these options. This substance has interesting properties like a low weight and a Low Heating Value (LHV) of 120 MJ/Kg (4 times greater than coal, 2,86 greater than gasoline and 2,5 times greater than natural gas) this makes it an interesting option for energy storage [12]. Regarding generation, it can be synthesized chemically by refining fossil fuels (Grey Hydrogen), or it can be generated by electrolysis of water transforming electricity into chemical energy (as shown in Equation 1). If the electricity used for this purpose is mainly renewable, it would be considered green hydrogen.

$$2H_2O + energy \leftrightarrow 2H_2 + O_2$$

Equation 1 Hydrogen redox reaction

Once it is obtained, it can be used as fuel for a CCPP mixed with natural gas, or by itself (considering that when it burns, the only product of the combustion is water vapor, making it a carbon-free option). The other possibility is to reverse the electrochemical reaction in a fuel cell (FC), transforming hydrogen and oxygen into water and energy. All characteristics combined make hydrogen an option for large-scale energy storage solution. However, several technical challenges must be overcome to increase the profitability of this storage solution in the future, such as the low overall energy efficiency of the process. Specifically, current electrolyzers efficiencies are around 70% [13], compression storage requires energy intensities of (5-15% depending on storage pressure) and reverse energy generation efficiency can range between 50-60% for the best CCPP or FC technologies. Therefore, the total efficiency of the process of electrolysis, storage and generation of electricity are currently around 40% on the best-case scenario.

The three technologies mentioned are far from being the only options, despite that, other options like gravitational storage (moving large masses to generate and store energy) or thermo-solar (heating a fluid with sun to extract energy later with a thermodynamic cycle), however, regarding installed power, they are less extended that the mentioned technologies [14].

1.3 HYDROGEN GENERATION MODELS

Although hydrogen is currently an alternative for current global energy storage needs, it is far from being feasible as a solution for market scale operation. The main reason is the high CAPEX needs for this kind of power. An average alkaline electrolyzer costs nowadays 1400 $/KW [15] with an annual maintenance cost of 7% of its cost. However, this is projected to go as low as 607 $/KW by 2050 with annual costs going down as well to around 2%. On the other hand, nowadays, a conventional CCPP gas turbine has an average specific CAPEX of 730 €/KW with an operational cost of around 2% [7].

This important difference in CAPEX between conventional and new hydrogen energy-based infrastructure supports the use of optimization models to maximize profitability considering different hydrogen infrastructures configurations. These models are used to predict, in the medium and long term, the power and time to generate hydrogen considering different hydrogen storage options and the uncertainty inherent in the electricity market. In this regard, there is a lot of literature about hydrogen models to optimize generation and storage flows, but most of them focus on general market operation, and combination with generation sources, with poor representation of the storage infrastructure, its costs and constraints.

This project is centered precisely on market scale hydrogen storage modelling. The state of the art about this matter will be presented in the next section focusing on a thermodynamic approach to model compressed hydrogen storage. The lack of references about this matter, combined with some preliminary calculations that will be explained in the next sections, will define the specific objectives of this work, as well as the methodology for their completion.

Chapter 2. STATE OF THE ART

Hydrogen has been generated from chemical sources for decades. However, the need for electricity storage, combined with the improvements in this technology (especially the capacity and efficiency of electrolyzers and fuel cells) have caused an important increase in research and development, as well as infrastructure for this purpose. This increase has led to the appearance of several new storage technologies that improve the feasibility of hydrogen as a large-scale energy storage solution.

Many models exist nowadays to estimate future prices in the electricity and hydrogen markets. Most of the models published prior to this project focus on a specific technology or usage, evaluating the feasibility of hydrogen as a solution as well as the economic analysis to evaluate the return on the investment, as this kind of infrastructure is highly capital intensive.

2.1 STORAGE TECHNOLOGY OPTIONS

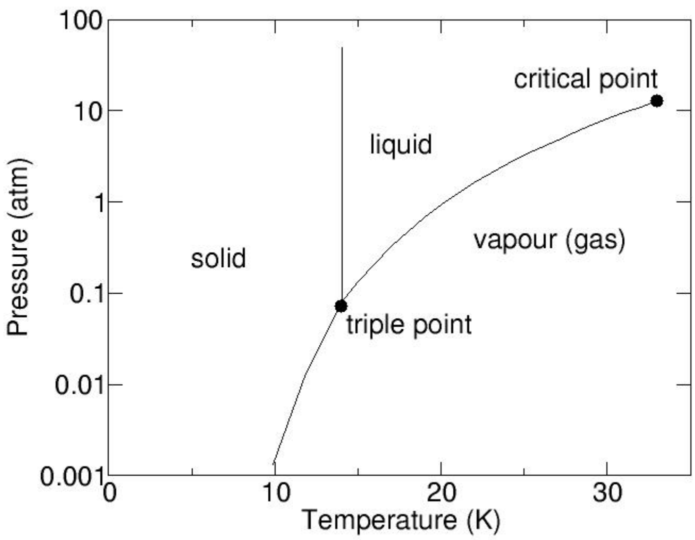
To formulate storage constraints in a hydrogen storage optimization model, the first step will be a technical analysis of all the options existing nowadays for hydrogen storage, from the newest concepts to fully stablished technologies. The study of their technical principles as well as their limitations will guide the development of hydrogen storage modeling.

Starting with a general review of the different technologies related to the storage of hydrogen, this section describes their main advantages and disadvantages, and their stage of development. The research conducted found several storage technologies for hydrogen, like compressed and liquified. However other option like metal hydride absorption [16] or compression in salt caves [17] are being developed to reduce storage cost, or increase energy density.

2.1.1 GENERAL CHARACTERISTICS OF HYDROGEN

From a chemical perspective, hydrogen is the smallest atom, composed only of a proton and an electron on its general form (other isotopes exist with one and two neutrons, called deuterium and tritium respectively). Being the simplest atom on the periodic table is also the most abundant element, making up around 75% of the total mass of matter in the universe.

As mentioned in the introduction section, hydrogen offers a much higher LHV, when compared to other conventional sources of energy (especially fossil fuels). However, on ambient conditions, hydrogen is found on gas state (with a liquification point close to absolute 0 K). Therefore, even though the LHV is high, it is calculated as the chemical energy per unit of mass, considering the gas nature of hydrogen, the volumetric energy density of 0.00962 MJ/L (calculated at 300K, 1 bar), resulting 3 orders of magnitude lower compared to liquid fuels like gas or LNG that go from 20-30 MJ/L. This is the reason why hydrogen is not stored in ambient conditions, as changing the physical properties of hydrogen can lead to densities of up to 8.5 MJ/L, closer to fossil fuel values.



[1]

Figure 3 Phase diagram of hydrogen

[1] Source: https://physics.uwo.ca/~jlandstr/planets/webfigs/matter/slide6.html

2.1.2 PHYSICAL BASED STORAGE TECHNOLOGIES

This technical limitation that rises from the nature of hydrogen can be solved by changing the physical properties of hydrogen to increase the value of its volumetric energy density up to reasonable values (by moving on the phase graph shown in Figure 3). The main storage technologies offer different approaches to address this challenge, from gas compression to liquification, as well as strategies to prevent losses while stored. The characteristics of these different technologies are shown in Table 1 [18], [19], [20].

Method	Compression range	Temperature	Energy intensity	Comments
Compressed	100-1000 bar	300K	3-15%	Losses by diffusion and safety concerns
Liquified	Ambient	20K	35%	Losses by boil-off and highest volume energy density
Cryo Compressed	250-350 bar	30K	>35%	High density without boil-off losses, most technically complex

Table 1 Physical based storage technologies

Looking at the table, there are 3 main technologies for hydrogen storage. Firstly, compression, working at the gas side of the phase diagram, whose main advantage is the temperature, as it can be stored at ambient temperature. This method raises some safety concerns, mainly because of the high operating pressures of this technology, but also, because compressed hydrogen diffuses through matter (escaping from the storage reservoirs and causing storage losses). It also causes accelerated embrittlement [21] in the tank, combining high mechanical stress due to high pressure with accelerated degradation in materials.

Secondly, liquified storage offers the best volumetric energy density, however, at the cost of maintaining hydrogen at cryogenic temperatures for a long period of time. It is a safer technology compared to compression, but at the cost of having a high energy intensity (energy used in the process of storage relative to the total energy stored). This technology also faces the challenges of losses due to boil-off [22]. This type of loss is caused by heat entering the tank and evaporating hydrogen, causing a rise in pressure. Consequently, hydrogen gas is released to prevent tank collapse due to overpressure.

Lastly, cryo-compressed hydrogen combines low temperature liquid hydrogen storage, on a pressurized tank. This technology is the most complex, as it combines both previously mentioned. It offers the high energy density of liquid hydrogen, preventing boil-off losses by using tanks rated for high pressure. These improvements are achieved at the cost of having the highest energy intensity, as well as technical complexity.

These different technologies are technically viable; however, the scale needed for a whole market model discarded most of the options based on the high capital investment requirements. These economic limitations make compression and liquification the only feasible alternatives for large-scale solutions. Regarding capital extensiveness and operating costs, the best option is salt cavern storage, which algo includes the benefit of thermal stability throughout the year as well as less diffusion losses [15].

This type of storage uses the same principle as compressed hydrogen, however, instead of tanks, hydrogen is stored in natural salt caverns, enabling the storage of a great amount of hydrogen with a fraction of the capital expenditure for infrastructure. Moreover, research performed by [17], estimates the CAPEX needs for salt cave storage, in 50 $/m^3. Using the ideal gas formula, with a pressure of 100 bar and a temperature of 300K, that volume could hold 962 MJ, equal to 0.267 MWh, obtaining a CAPEX of 0.187 $/KWh. Although this price does not include the infrastructure needed for compression, compared with current BESS prices of around 132 $/KWh [23], the difference is remarkable.

In contrast with most of models found in the literature, see for example [24], [25], [26], [27] which focus only on an specific option, in this project both of the viable options (compressed and liquified) will be considered, ;) even if compression has generally lower cost. The objective is that the model developed decides how much hydrogen to store with every technology, the unuse of a certain technology is a possibility whenever costs are too high.

2.1.3 OTHER STORAGE TECHNOLOGIES

From a purely technological standpoint, there are other options for hydrogen storage [28], apart from the previously explained physical-based methods. Two main technologies are used for this purpose. Firstly, chemical methods, also known as transformational methods [29], that use chemical bonds to create substances containing hydrogen that are easier for storage, for example ammonia (NH_3) or methanol. The characteristics of these technologies [30] are detailed in Table 2. These technologies offer interesting energy densities compared to physical based methods. However, they lack technical feasibility for short-term storage due to the high cost of the chemical processes involved.

Method	Compression range	Temperature	Energy density	Comments
NH_3 liquid pressurized	9 bar	300K	15,6 MJ/l	17,4% mass wight is H_2[1]
NH_3 atmospheric	Ambient	250K	11.5 MJ/l	NH_3 has also the advantage that has a demand for itself
Methanol	1 bar	300K	12 MJ/l	12.5% mass weight is H_2
Reference (compressed H_2)	750 bar	300K	7.21 MJ/L (or 8.5 for liquid H_2)	These methods also carry long-term losses, via diffusion or boil-off

Table 2 Transformative methods for hydrogen storage

Lastly, adsorption-based methods constitute another important technology used for hydrogen storage [16], [20], [28]. These methods use physical conditions (temperature and pressure) combined with porous materials, to store hydrogen inside these materials, and then reverse this process to obtain the hydrogen back. As a reference for their effectiveness for hydrogen storage, the concept of hydrogen mass percentage is introduced, meaning the maximum mass of hydrogen that can be stored per unit of adsorbent mass. These technologies offer the best volumetric density of energy, as can be seen in Table 3. However, the cost of complex adsorbents limits the scalability of the technology to the necessary

[1] H_2: Chemical notation of the hydrogen molecule

volumes, as well as the high energy intensity if the thermal processes are needed for storage.

Method	Hydrogen density	%Hydrogen mass	Energy density	Comments
Magnesium Hydride (MgH_2)	86 kg/m3	7.6%	10.32 MJ/L	Magnesium offers the best option for availability, high density and mass%, but the process requires temperatures of up to 573K
ABH type	90 kg/m3	2%	10.8 MJ/L	High energy activation procedure and equilibrium pressure
AB_5 H type	105 kg/m3	1.5%	12.6 MJ/L	One of the best, but the cost is high. Most common is $LaNi_5$
Lithium Bohrides	120 kg/m3	18%	14.4 MJ/L	Best performance, but poor stability and undesired side products

Table 3 Adsorption based methods for hydrogen storage

2.2 HYDROGEN STORAGE OPTIMIZATION MODELS

After the revision of the current technologies used for hydrogen storage, the second part of this state-of-the-art review is the study of the literature about hydrogen market operation models. This review focused specially on models that not only included hydrogen generation, but also the storage process. The most relevant models found are presented in Table 4.

The study of these references shows that the variable cost associated with hydrogen storage is considered as a fixed amount in all the references found. This is the gap this project tries to solve, as will be explained in the following sections. This characteristic for the different models can be found on the column of dynamic storage cost of Table 4, showing the innovative perspective of this project.

The rest of the columns of the table refer to specific characteristics of the models reviewed, not only from the storage part, but also from a model characteristics perspective. As this project aims to deepen the storage phase, the first column lists the different storage technologies modeled in each reference. Secondly, also from a storage perspective, the column about storage losses explains if this challenge of hydrogen diffusion (for compression storage) or boil-off (for liquid storage) is modeled.

The next columns of the table represent the general model characteristics of the references checked, starting with the method used to model the hydrogen market, (H_2 pricing mechanism column) meaning how the hydrogen price is computed in the model or if it is not calculated, as is the case of this project. Secondly, the energy economic deal for hydrogen generation (DA market[1], PPA[2], etc.).

Lastly, an important difference between the reviewed models is the final use of hydrogen as some of them assume a fixed and inelastic demand that must be satisfied to maximize profitability in a hydrogen market or to minimize production cost for hydrogen generation in a centralized system. Other mechanisms consider hydrogen as an energy vector [24] generating it with the objective of reversing this conversion during peak electricity demand moments. This last type of model would benefit the most from the dynamic storage pricing proposed for this project, as the storage represents a key variable, as it can be stored expecting a higher energy price in the future, or sold quickly, to minimize storage costs.

[1] DA Market: Day ahead Market
[2] PPA: Power Purchase Agreement

Reference	Technologies considered	Storage losses modeled	H_2 Pricing mechanism	Energy source	Final use (h2, e-, both)	Dynamic storage cost	Other remarkable constraints
[26]	Compressed tank	No	H_2 price inputted	DA market	H_2 demand	No	-
[24]	Compressed cave	No	No market participation	DA market	CCPP[1] Hydrogen to power	No	-
[25]	Compressed tank	No	H_2 price inputted	DA market and balancing market and contracts	H_2 demand	No	-
[31]	Compressed tank, pipelines, batteries	Fixed storage efficiency	H_2 price inputted	DA market	H_2 demand. Also, CCPP and FC[2], models decide if they used or not	No	CO_2 emission limits
[27]	Compressed tank	No	H_2 price inputted	DA market	H_2 demand	No	-
This project	Compressed tank, compressed cave and liquified	Modeled as storage efficiency	Inelastic H_2 demand	DA market	H_2 demand and Hydrogen to power	Thermodynamic compression curve	-

Table 4 Hydrogen storage modeling state-of-the-art references

[1] CCPP: Combined Cycle Power Plant
[2] FC: Fuel Cell (used for reversing electrolysis, converting H_2 back into electricity)

Chapter 3. DEFINITION OF THE PROJECT

3.1 JUSTIFICATION

The main objective of this project is to progress in the development of hydrogen storage optimization models to increase the feasibility of hydrogen infrastructure as a solution to current energy challenges.

During the research phase of the project, that concluded on the creation of Table 4, several hydrogen storage models have been reviewed. These models were very different from each other working on a specific challenge of hydrogen storage. However, a common characteristic has been found at the way that storage costs are calculated.

For all the models reviewed, the cost of storage for a unit of hydrogen was calculated directly as the flow of hydrogen of the time period, multiplied by a fixed amount. Therefore, the storage cost was modeled as constant regardless of the state of the storage infrastructure. This concept raises a lot of concerns, from a theoretical standpoint, as will be explained in the next section.

3.1.1 THERMODYNAMIC APPROACH

As shown in the reference table, the main storage technology used in the reviewed models is compression. This type of storage is composed of a tank with a fixed volume, on which hydrogen is compressed to be stored. The addition of new hydrogen (an ideal gas) in a fixed volume and temperature tank is calculated with Equation 2, where P represents the tank pressure, V the tank volume, n the total hydrogen in the tank, T the temperature and R being the ideal gas constant.

$$P \cdot V = n \cdot R \cdot T$$

Equation 2 Ideal gas equation

Considering the temperature as a constant (temperature may suffer short-term variations, but in the long term it can be computed as a constant), the tank pressure rises linearly with the total hydrogen stored in the tank. Therefore, the limit for storage will be the mechanical strength of the tank, resulting in a maximum gas pressure contained.

From this expression, the main conclusion that can be extracted is the linear relation between tank pressure and total hydrogen stored in the tank (From now on called LoH: Level of Hydrogen).

On the other hand, the relation between the final pressure and the energy needed for that compression is shown in Equation 3. On this expression, the Tin represents the inlet temperature, that is considered as constant as well as on the previous case, R represents again the ideal gas constant, n represents the polytropic index, that varies depending on the compression curve followed (varying between 1 and 1,4 for adiabatic processes), and lastly, r represents the pressure ratio (outlet pressure divided by inlet pressure), considering ambient inlet pressure, r is equal to final pressure.

$$w_{compression} = \frac{n}{n-1} \cdot R \cdot T_{in} \cdot \left[r^{\frac{n-1}{n}} - 1 \right]$$

Equation 3 Energy needed for gas compression

This expression leads to the graph shown in Figure 4, where it is clearly seen that the energy needed for hydrogen compression grows with tank pressure.

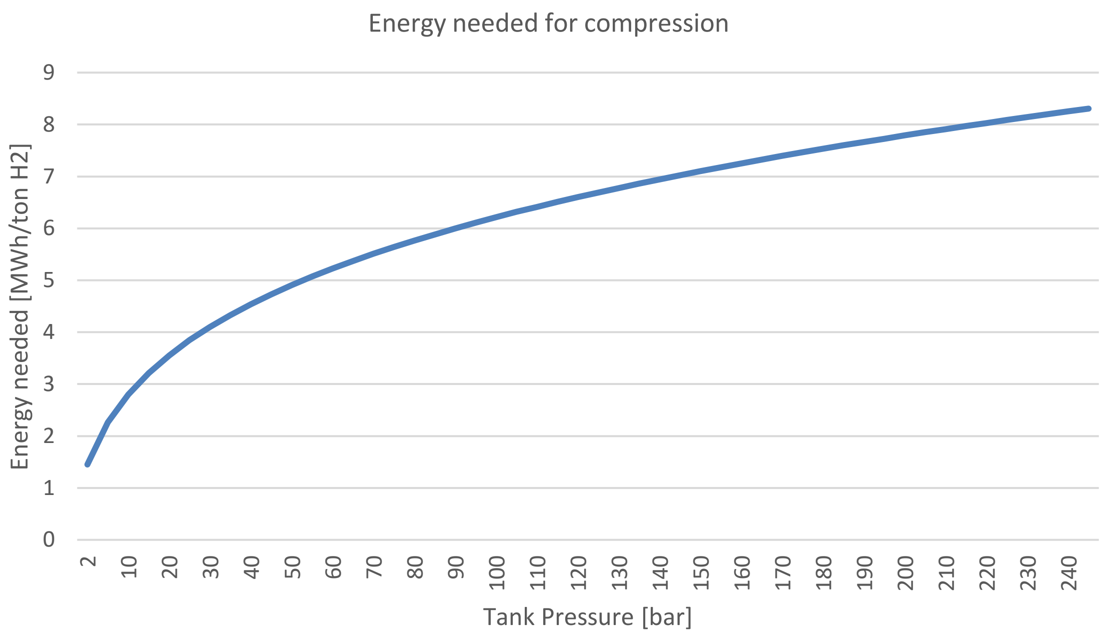


Figure 4 Specific energy needed for hydrogen compression

The linear relation between LoH and tank pressure combined with the specific compression energy growth with tank pressure, when combined, leads to the concept of marginal storage cost growth with LoH.

This concept breaks with the idea of constant storage costs, that are used by all references consulted. Indeed, when calculating the cost that is incurred when storing hydrogen by compression, the energy cost must be calculated considering the LoH of the tanks, meaning that storage cost will be lower when the LoH on the tanks is low, and will grow as the tank fills.

3.1.2 COST QUANTIFICATION

The next step is the estimation of the impact of this considering the dependency of the cost with the LoH, considering the other costs for developing and operating storage infrastructures.

For this purpose, an economic study of the cost of the storage infrastructure was conducted, including the investment cost of the compressor and the salt cave storage, the compressor needed for the tank, and the average energy cost of the year 2024.

The main inputs of this economic model were:

- 51000-ton H_2 produced per year (200 MW electrolyzer working continuously)
- 100 GWh Storage capacity (20 days' worth storage)
  - With a 250 bar cave results in 150000 m3 (Equation 2 with standard conditions)
  - 6,1 MWh/ton H_2 (Figure 4 average), resulting in a 36 MW compressor
- 46 €/m3 for cave and 1460 €/KW for compressor CAPEX, both with 2% yearly O&M costs [15]
- 63,04 €/MWh energy price (2024 average, REE [32], from 76,3 €/MWh excluding 21% VAT)
- 8,5% WACC [33] and 30 year investment period.

The results show that with a low LoH scenario (5%), the storage cost is 267,6 €/ton H_2, whereas a high LoH scenario (95%) results in 586,4 €/ton H_2. For reference, current prices of green hydrogen range between 3740-11700$ per ton [34]. The full view of the unit cost of storage for all LoH points is shown in Figure 5, where the cost is broken down between CAPEX and O&M costs, resulting in a fixed 122,8 €/ton H_2, combined with the energy cost, that ranges from 0 (ideally when tanks are empty) to 471,3€ that would cost to fit the last ton inside the cave. Therefore, storage costs can range between 122,8-594,1€, meaning a potential price difference of 9,43% (considering a 5000 €/ton

H_2 price), if hydrogen is stored with low tank LoH compared to high. (from 5122,8 to 5594,1€).

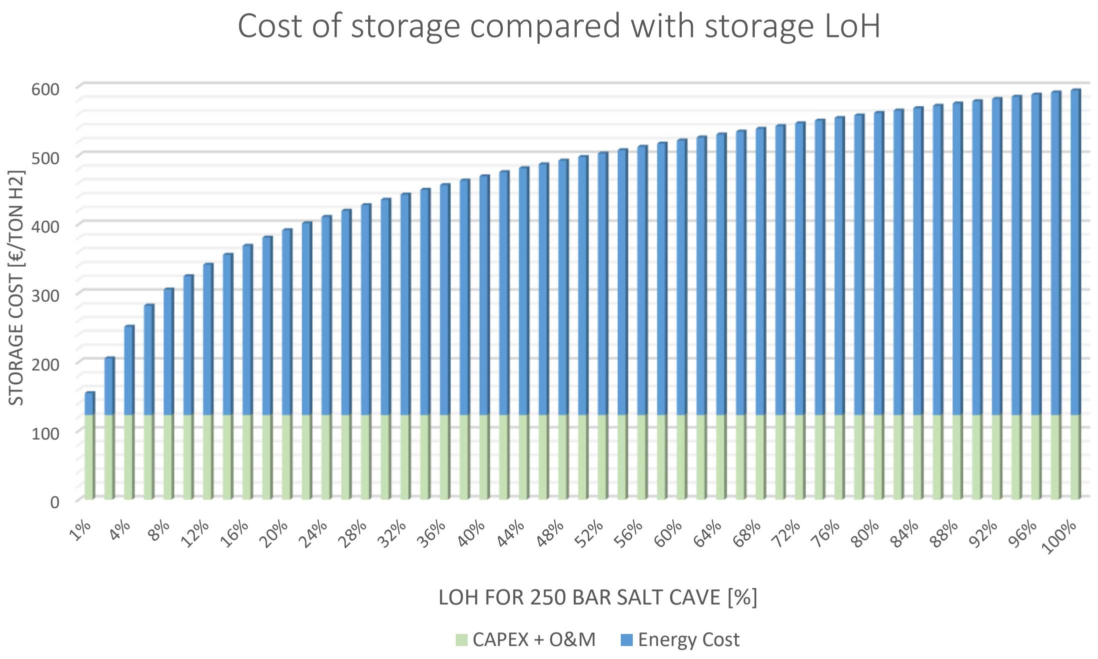


Figure 5 Total storage cost by LoH level

The base thermodynamical hypothesis, combined with this 9,4% potential saving, justifies the development of a storage model that computes storage price as a variable with LoH, to estimate the market impact of this thermodynamic approach, which is the aim of this project.

3.2 OBJECTIVES

After analyzing the state of hydrogen infrastructure in general, and storage technologies in particular, as well as the previously mentioned calculations and thermodynamic approach, the objectives proposed for this project are the following.

1. Development of an optimization model that computes storage costs following the thermodynamic compression curve.
2. Quantify operating differences of using this approach.

Considering the hypothesis and calculations mentioned, a full optimization model will be developed to quantify the effect of this finer representation of the thermodynamics of compression storage. This quantification is necessary as the new, and more complex model will require greater computational power to be solved. The overall improvement in representation must be compared with the extra effort made to accomplish it, to justify the implementation of this new storage cost modeling technique.

3. Development of a model centered on the storage phase.
4. Modeling of several different storage technologies.

The baseline of this project was hydrogen storage modeling, which led to the state-of-the-art review that concluded on the thermodynamic approach presented. However, that state of the art review showed how other models only considered one storage technology. This is why this project will develop a model that represents more than one technology. The model developed will decide on which technology to store hydrogen (between compressed tank, compressed cave and liquified storage), considering the technical constraints and costs. The selection of the different technologies on the different scenarios proposed will be analyzed to show the main advantages and drawbacks of each storage technology.

3.3 METHODOLOGY

As mentioned previously, the aim of this project is the development of an optimization model for the hydrogen market. This model will be based on a mid-term optimization model [35], that will be modified to properly satisfy the presented objectives.

The model was programed in GAMS, and several study cases were performed to analyze the impact of the thermodynamic approach presented, as well as all the other objectives.

3.3.1 PHASES AND CHRONOLOGY

The phases to accomplish this project objectives are presented in Table 5.

Name	Description
State of the art review	Review of current technologies in the hydrogen sector as well as optimization model proposed prior to this project. Design of Table 4
Preliminary calculations	Estimating the cost of hydrogen storage to quantify the possible impact of the project.
Creation and refinement of the model	Developing the constraints and writing the GAMS code to develop and refine a functional model
Parameter selection and results	Using technical research, deciding the parameters values and obtaining results, and extracting conclusions based on the objectives if the project explained.
Project memory writing	Writing the final report of the project explaining the final model and concluding based on results. Design of the final presentation for the final phase of the project.

Table 5 Proposed phases for the project

This project started around July 2024, with several months of state-of-the-art review, after the final definition of the project and phases and based on estimation of the time needed for each phase, the following chronogram is presented for the project in Figure 6. The timeline is based on the faces concluded prior to the writing of this document, as well as the projected duration for the phases remaining.

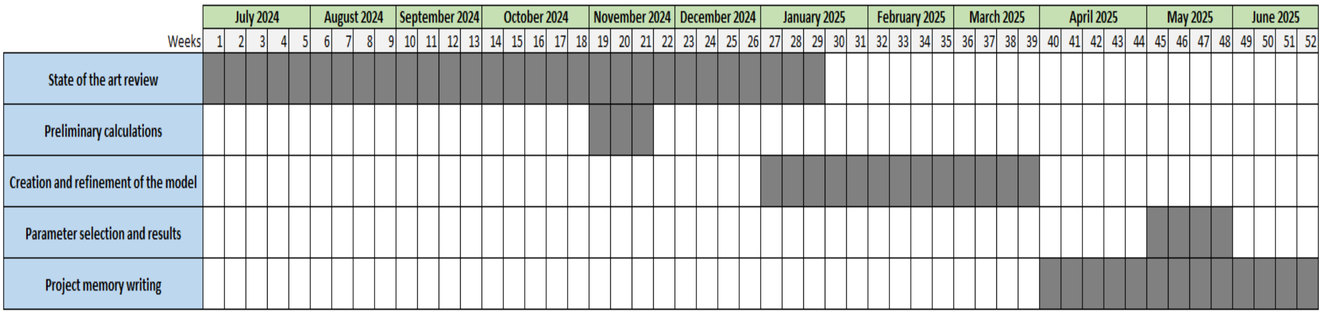


Figure 6 Proposed chronogram for the different project phases

3.4 SDGs ALIGNMENT

The United Nations Sustainable Development Goals (SDGs) are part of a worldwide strategy aiming to address the world's most pressing challenges by 2030. In the context of the energy transition, several SDGs provide a roadmap for aligning technological innovation with sustainable development. This project contributes directly to the development towards the completion of several of these objectives.

- SDG 7 – Affordable and clean energy

Firstly, the project advances SDG 7 by promoting the efficient and flexible integration of hydrogen into renewable energy systems, increasing the potential of these technologies to work independently from fossil-fuel based generation. Hydrogen is widely recognized as a key enabler for decarbonizing sectors where direct electrification is not feasible and for balancing electricity systems dominated by uncontrollable sources such as wind and solar. By improving the modeling of storage costs, particularly through a thermodynamic approach that reflects operational behavior, the project enhances the realism and performance of hydrogen system simulations. This contributes to the development of more robust, cost-effective solutions for clean energy storage and distribution.

- SDG 9 – Industry innovation and infrastructure

Secondly, the project aligns with SDG 9, which emphasizes the importance of building reliable infrastructure, promoting inclusive and sustainable industrialization, and promoting innovation. The optimization model developed in this project incorporates advanced mathematical formulations, considers multiple hydrogen production and storage technologies, and integrates real-world electricity market data. This approach not only supports the design of more efficient energy infrastructures but also promotes technological innovation in energy system planning, a key factor in enabling the large-scale deployment of hydrogen technologies.

- SDG 13 – Climate action

Finally, the project supports SDG 13 by promoting climate action through a detailed understanding of the energy and cost implications of different hydrogen storage strategies. The improved precision in estimating compression energy consumption helps identify the most suitable storage technologies and operation patterns to reduce energy consumption, and therefore emissions. This enables more effective strategies for integrating hydrogen into decarbonization pathways, by working in two directions: reduction of energy consumption and reduction on the dependance on polluting energy sources.

Chapter 4. PROPOSED MODEL

Following the objectives and methodology explained in Chapter 3, this chapter describes the optimization model developed in this thesis. Aiming to evaluate the effect of modeling the variable cost associated with storage as a curve obtained by thermodynamic equations, a base model will be described firstly.

4.1 CHARACTERISTICS AND ASSUMPTIONS

The base model is considered a medium-term model. From an economic perspective, the difference with a long-term model is the consideration of the CAPEX for the hydrogen infrastructure of the model. Therefore, just operational expenses (OPEX) have been considered. Moreover, the model considers only the supply part. Therefore, hydrogen demand is represented as a fixed and inelastic demand that must be fulfilled. The model objective is the minimization of the total cost for hydrogen generation. The possibility of selling energy back to the grid is considered as a negative expense in the objective cost function.

Another important aspect of this model is the consideration of multiple sources of hydrogen generation. Particularly, in this case, the two sources modelled are grey hydrogen (from chemical origin, normally obtained from natural gas) and electrolytic hydrogen. This last production method, depending on the origin of the electricity used, can result in various types of hydrogen: pink (nuclear energy), green (renewable) or yellow (just solar energy) [36].

4.2 FLOW DIAGRAM

With all the considerations explained previously, the base model follows the flow diagram shown in Figure 7. On this diagram the different energy transformations are shown. Starting with the power consumed from the grid by electrolyzers to produce hydrogen, this flow, combined with the chemically generated hydrogen (Grey H_2), can be used for shipment for demand or storage. Lastly, on the storage phase, a small amount of the stored hydrogen is lost due to the leakage of the tank. Once stored, hydrogen can either be used to satisfy hydrogen demand if the generation is insufficient, or to generate electricity on fuel cells if necessary for the grid.

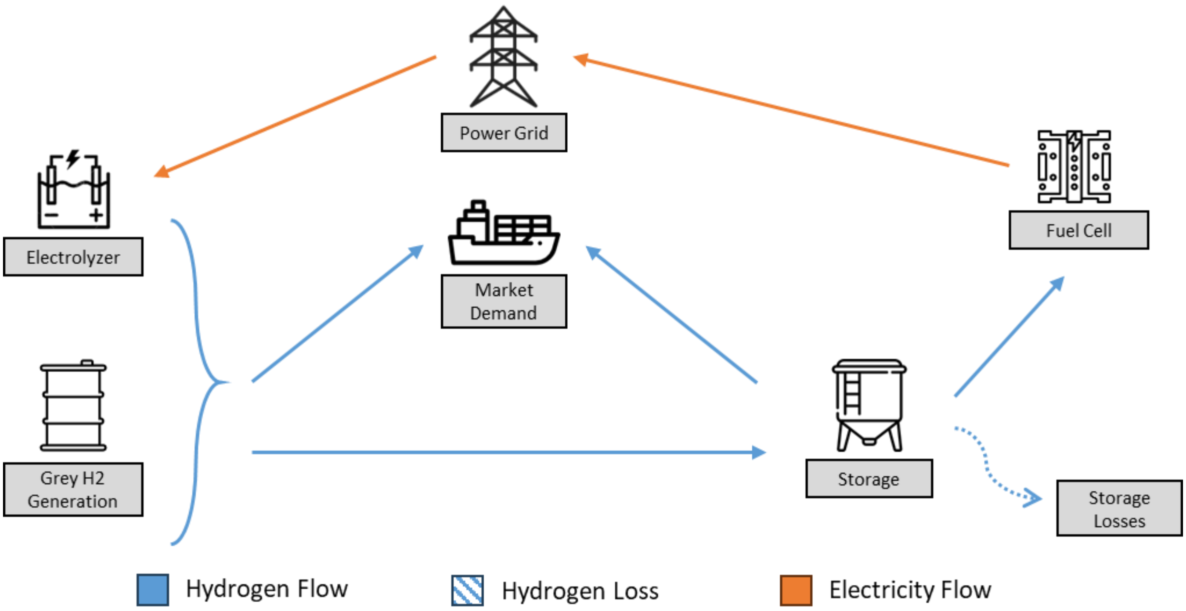


Figure 7 Base Model Flow Diagram

This base model seeks to minimize the cost to satisfy market demand by generating hydrogen during periods of low system marginal cost and selling electricity back to the grid using FCs if the generation, storage, and FC costs incurred in the process are reduced.

4.3 BASE MODEL MATHEMATICAL FORMULATION

The base model that was used as base [35], aimed to provide a full representation of the hydrogen market, as well as the relation with the electricity market. As a close representation of electricity market behavior is not part of the proposed objectives for this project, only variables and parameters related to the hydrogen sector will be used to simplify the formulation as much as possible, while keeping the details of the complexity of the hydrogen storage variable cost.

4.3.1 SETS

The original model uses the following sets, presented in Table 6.

Set	Name	Description
z	Zone	Identifies the different zones for generation and storage infrastructure. Hydrogen demand is satisfied for all zones.
h	Hour	The 24 hours associated with every day of the model
d	Day	The 365 days associated with every year of the model
y	Year	Defines the years that will be simulated
s	Agent	The different agents taking part in the hydrogen market

Table 6 Sets presented in the original model

As the sets show, the original model aims to provide a close representation of the hydrogen market, especially the geographical distribution of the hydrogen generation and storage infrastructure (with the use of the zone set) as well as the relations inside the market (using the agent set). It also aims to provide a precise and broken-down view of all the local activities, breaking down demand by location, and considering that it must be fulfilled with the capacity of that region.

4.3.2 PARAMETERS

Parameter	Description	Unit
$\boldsymbol{H2^{DEM}_{z,s,d,y}}$	H_2 demand	[ton H_2]
$\boldsymbol{CAP^{ELE}_{z,s}}$	Electrolysis installed capacity	[MW]
$\boldsymbol{CAP^{GREY}_{z,s}}$	Grey hydrogen production available capacity	[ton H_2]
$\boldsymbol{CAP^{STO}_{z,s}}$	H_2 storage installed capacity	[ton H_2]
$\boldsymbol{E^{ELE}_{z,y}}$	Electrolyzer efficiency	[%]
$\boldsymbol{E^{STO}_{z,y}}$	H_2 storing efficiency	[%]
$\boldsymbol{E^{UN}_{z,y}}$	H_2 unstoring efficiency	[%]
$\boldsymbol{LF^{STO}_{z,y}}$	Leakage factor of the H_2 storage system	[%]
$\boldsymbol{CGH_{z,y}}$	Electricity to H_2 conversion rate	[ton H_2/MWh]
$\boldsymbol{CHG_{z,y}}$	H_2 to electricity conversion rate	[MWh/ton H_2]
$\boldsymbol{CH^{ELE}_{z,y}}$	Variable costs associated to electrolyzers	[€/MWh]
$\boldsymbol{CH^{GREY}_{z,y}}$	Variable costs associated with grey hydrogen production facilities	[€/ton H_2]
$\boldsymbol{CH^{STO}_{z,y}}$	Variable costs associated with H_2 storage	[€/ton H_2]
$\boldsymbol{OC^{ELE}_{z,y}}$	Annual fixed operating costs for electrolyzers	[€/MW]
$\boldsymbol{OC^{GREY}_{z,y}}$	Annual fixed operating costs for grey hydrogen production facilities	[€/ton H_2]
$\boldsymbol{OC^{STO}_{z,y}}$	Annual fixed operating costs for H_2 storage	[€/ton H_2]

Table 7 Parameters of the original model

As shown in Table 7, the different parameters are used to quantify all the characteristics of the model, starting with the H_2 demand. This demand must be met by the agents, in every zone, and at a time. Additionally, several parameters define the generation capacity, infrastructure efficiencies and conversion rates. Lastly, the variable and fixed cost are determined by the installed units for the fixed ones and generation/storage for the variable ones.

4.3.3 VARIABLES

Variable	Description	Unit
$h2^{ELE}_{z,s,h,y}$	H_2 production from electrolyzers	[ton H_2]
$h2^{GREY}_{z,s,d,y}$	Grey H_2 production	[ton H_2]
$h2^{STO}_{z,s,d,y}$	H_2 produced that is stored	[ton H_2]
$h2^{UN}_{z,s,d,y}$	H_2 stored that is released to cover the demand	[ton H_2]
$sh2_{z,s,d,y}$	H_2 stored level	[ton H_2]
$h2c^{ELE}_{z,s,h,y}$	H_2 stored that is consumed to produce electricity in fuel cells	[ton H_2]
$pc^{ELE}_{z,h,y}$	Power consumption for the electrolyzers	[MWh]
$pp^{ELE}_{z,h,y}$	Power production from the fuel cells	[MWh]

Table 8 Variables of the original model

Table 8 show the variables presented in the original model, representing the different flows of hydrogen and power, as represented in Figure 7. These differences in energy flows are calculated for all the zones and agents present in the model.

4.3.4 OBJECTIVE FUNCTION

The following objective function is proposed to minimize the hydrogen system costs.

$$\sum_z \sum_s (\sum_y [\sum_d (CH^{ELE}_{z,y}.CHG_{z,y}.\sum_{h€d}[h2^{ELE}_{z,s,h,y} + h2c^{ELE}_{z,s,h,y}] + h2^{GREY}_{z,s,d,y}.CH^{GREY}_{z,y} + sh2_{z,s,d,y}.CH^{STO}_{z,y}) + CAP^{ELE}_{z,s}.OC^{ELE}_{z,y} + CAP^{GREY}_{z,s}.OC^{GREY}_{z,y} + CAP^{STO}_{z,s}.OC^{STO}_{z,y}])$$

Equation 4 Objective function of the original model

Equation 4 represents the sum of all the cost associated with the hydrogen demand to be fulfilled. The first part of the expression (corresponding to the top line of the equation) represents the total variable costs incurred during the timespan of the simulation, which is calculated by adding the total production, on every zone, agent, and time, and multiplying by the unit variable cost. The second part, corresponding to the bottom part of the expression, represents the fixed costs, which are defined by the capacity selected, therefore independent from the variables. The reason why these constants have been included (knowing they do not affect the optimal solution) is to compute the total cost considering also the size of the generation/storage used, allowing them to compare results among the simulations performed, considering the same demand (on any a unitary cost per ton of H_2 if the demand parameter is changed across simulations).

As can be seen, considering the flowchart presented in previous sections (see Figure 7), the hydrogen that is unstored to generate power back to the grid is considered as an expense, alongside the stored hydrogen, but with no economic benefit (regarding the objective function value, composed only of the addition of positive terms, see Equation 4). Therefore, the model will have no incentive to generate electricity back to the grid. From a purely economic perspective, reselling energy back to the grid will result in revenue (which will be computed as a negative cost) that is not considered in this base model, therefore, on the presented model, this aspect will be revised.

Lastly, for a solution approach, as the objective function represents the addition of all the costs incurred during the generation of H_2, the aim would be to reduce the total cost as much as possible.

4.3.5 CONSTRAINTS

On this section the main constraints of the model will be presented.

Equation 5 shows the main hydrogen balance constraint of the model. The left side of the equation adds all the different inflows of the model on every zone and period: the sum of all the electrically generated (that is calculated on an hourly basis) as well as the grey hydrogen produced in the day and the total amount that is unstored. On the right side the total outflows are presented: the stored hydrogen on that day, as well as the hydrogen shipped for demand.

$$\sum_{h€d} h2^{ELE}_{z,s,h,y} + h2^{GREY}_{z,s,d,y} + h2^{UN}_{z,s,d,y} = H2^{DEM}_{z,s,d,y} + h2^{STO}_{z,s,d,y}$$

Equation 5 Hydrogen generation balance of the original model

Equation 6 shows the balance used of hydrogen storage and ensures that the storage level is between the admissible values for every zone. In particular, the storage level (Left side) is calculated starting from the storage level on the previous time and applying the total inflows (from generation) and outflows of storage (to demand and energy generation) with their respective efficiencies (that result in the loss of a fraction of the total hydrogen moved).

$$sh2_{z,s,d,y} = LF^{STO}_{z,y} . sh2_{z,s,d-1,y} + h2^{STO}_{z,s,d,y} . E^{STO}_{z,y} - \frac{h2^{UN}_{z,s,d,y}}{E^{UN}_{z,y}} - \sum_{h€d} h2c^{ELE}_{z,s,h,y}$$

Equation 6 Storage balance equation of the original model

Other constraints that use upper bounds from Table 7 are omitted by simplicity. However, they are considered when coding the model.

4.4 MATHEMATICAL FORMULATION OF THE PROPOSED MODEL

The formulation of the proposed model is based on the one detailed in the previous section, with several modifications to shift the focus to a finer representation of hydrogen storage. This section will detail all these differences. As it will be seen, the mathematical formulation of the model results in several non-linearities that will be dealt with in the next section.

4.4.1 SETS

Starting with the sets, the proposed model is designed as a mid-term model. Considering that the aim is the representation of storage, the hydrogen-electricity market interactions are irrelevant. Therefore, both agent and zone sets will be eliminated. This perspective considers all of each zone's generation and storage as a centralized structure, regardless of the physical location of the infrastructure or the agent responsible for the generation/consumption of the hydrogen. Lastly, to include several storage technologies, another set will be included, to separate the different types of storage explained in the state of the art. The new list of sets for the proposed model is presented in Table 9.

Set	Name	Description
h	Hour	The 24 hours associated with every day of the model
d	Day	The 365 days associated with every year of the model
t	Technology	The different technologies modeled for storage

Table 9 Sets for the proposed model

4.4.2 PARAMETERS

The parameters used in the proposed model start with the ones explained in the original model including the total demand, as well as the different installed capacities (for H_2 generation and storage). The efficiencies have also been reused, except for the storing and unstoring efficiencies that now also depend on the set *t*, as the process efficiency depends on what technology is used for storage. To clarify the sets used in the parameters of the proposed model, the full set list has been included in Table 10.

Parameter	Description	Unit
$\boldsymbol{H2_d^{DEM}}$	H_2 demand	[ton H_2]
$\boldsymbol{CAP^{ELE}}$	Electrolysis installed capacity	[MW]
$\boldsymbol{CAP^{GREY}}$	Grey hydrogen production available capacity	[ton H_2/day]
$\boldsymbol{CAP_t^{STO}}$	H_2 storage installed capacity	[ton H_2]
$\boldsymbol{STO_t^{FLOW}}$	Upper boundary to the flow of hydrogen into storage for every tech.	[ton H_2]
$\boldsymbol{E^{ELE}}$	Electrolyzer efficiency	[%]
$\boldsymbol{E^{FC}}$	Fuel cell efficiency	[%]
$\boldsymbol{E_t^{STO}}$	H_2 storing efficiency	[%]
$\boldsymbol{E_t^{UN}}$	H_2 unstoring efficiency	[%]
$\boldsymbol{LF_t^{STO}}$	Leakage factor of the H_2 storage system	[%]
$\boldsymbol{EH2}$	Electricity to H_2 conversion rate	[ton H_2/MWh]
$\boldsymbol{CH^{ELE}}$	Variable costs associated to electrolysis	[€/ton H_2]
$\boldsymbol{CH^{GREY}}$	Variable costs associated with grey hydrogen production facilities	[€/ton H_2]
$\boldsymbol{CH_t^{STO}}$	Variable costs associated with H_2 storage (excluded power)	[€/ton H_2]
$\boldsymbol{EPRI_h^{BUY}}$	Prices for electricity to buy on each hour	[€/MWh]
$\boldsymbol{EPRI_h^{SELL}}$	Prices for electricity to sell on each hour	[€/MWh]

Table 10 Updated list of parameters for the proposed model

One of the key changes made to the model is the elimination of the fixed cost parameters. The reason for this change is that the installed capacity is a parameter, therefore, these fixed cost would not affect the objective function of the model, rendering them irrelevant for this approach.

With the aim of representing opportunity costs from different sources of energy, two prices have been considered as exogenous parameters, one used to buy ($\boldsymbol{EPRI_h^{BUY}}$) and another to sell ($\boldsymbol{EPRI_h^{SELL}}$) energy to and from the grid. The difference between them will be used as an incentive for the model to increase hydrogen storage, when buy prices are low, and to reduce it when sell prices are high enough to offer profitability in selling energy back to the grid (profitability is represented in the proposed model to a higher negative cost of selling compared with the cost of generation and storage, resulting in lower total net cost for the objective function). This representation takes also into account the effect of the inclusion of the variable cost for storage, derived from the thermodynamic expressions, as explained in the objectives of the project.

4.4.3 VARIABLES

For the variables of the final model, several changes have been made to the original model. The main change in the variable list is the inclusion of a variable that represents the total electric power used for the compression of hydrogen for storage. On the parameter list the variable cost has been changed to exclude the costs for electricity, which are now represented in this new variable: $cons^{STO}$. The value of this variable will change every hour, depending on the level of hydrogen of that hour of that storage, following the expression of Equation 3. The adaptation of this variable to something manageable for the model will be discussed in the next section: Resolution Approach.

With this change, as well as all the necessary adaptations, Table 11 shows all the variables of this project's model.

Variable	Description	Unit
$\mathbf{h2_h^{ELE}}$	H_2 production from electrolyzers	[ton H_2]
$\mathbf{h2_h^{GREY}}$	Grey H_2 production	[ton H_2]
$\mathbf{h2_{h,t}^{STO}}$	H_2 produced that is stored	[ton H_2]
$\boldsymbol{h2_{h,t}^{UNSTO}}$	H_2 is produced that is unstored to generate electricity	[ton H_2]
$\boldsymbol{loh_{h,t}}$	H_2 stored level	[ton H_2]
$\boldsymbol{dh2s_h^{GEN}}$	H_2 that is shipped for consumption directly from generation	[ton H_2]
$\boldsymbol{dh2s_{h,t}^{STO}}$	H_2 that is shipped for consumption from storage	[ton H_2]
$\boldsymbol{lh2_{h,t}^{STO}}$	H_2 that is lost while stored	[ton H_2]
$\boldsymbol{cons_{h,t}^{STO}}$	Power consumption associated with H_2 storage	[MWh/ton H_2]
$\boldsymbol{pow_h^{ELE}}$	Total electric power consumed by electrolysis on a determined hour	[MWh]
$\boldsymbol{pow_h^{GEN}}$	Total electric power generated back to grid on a determined hour	[MWh]
$\boldsymbol{pow_h^{STO}}$	Total electric power consumed by storage on a determined hour	[MWh]
$\boldsymbol{pres_{h,t}^{STO}}$	Storage pressure for every technology on a determined hour	[bar]

Table 11 Updated list of variables for proposed model

Power consumed from the grid and sold back to the grid are calculated every hour and computed at the objective function. Another change made from the original model is the inclusion of variable $lh2^{STO}$ to calculate how much hydrogen is lost in storage every hour, so that it can later be processed as an output of the model.

4.4.4 OBJECTIVE FUNCTION

Starting with the objective function of the original model, the first change is the creation of variables to record the total costs for every hour, which will be used to analyze later the different cases of study.

$$pow_h^{ELE} = (h2_h^{ELE}/EH2 \ \ )/E^{ELE}$$

Equation 7 Total hourly power consumption of electrolysis of the proposed model

$$pow_h^{STO} = \sum_t (h2_{h,t}^{STO} \cdot cons_{h,t}^{STO})/EP_t^{ELE}$$

Equation 8 Total hourly power consumption of storage of the proposed model

$$pow_h^{GEN} = (\frac{\sum_t h2_{h,t}^{UNSTO}}{\mathrm{EH2}}) \cdot E^{FC}$$

Equation 9 Total hourly power generation of the proposed model

$$VarCost_h = CH^{ELE} \cdot h2_h^{ELE} + CH^{GREY} \cdot h2_h^{GREY} + \sum_t CH_t^{STO} \cdot h2_{h,t}^{STO} + EPRI_h^{BUY} \cdot (pow_h^{ELE} + pow_h^{STO})$$

Equation 10 Hourly variable cost of the proposed model

These equations simplify the expression of the final objective function, with the added benefit of keeping the record of all the cost on a detailed scale for deep analysis and conclusions. Equation 7 represents the total hourly power consumption of the system's electrolyzers. Equation 8 calculates the total power used by the storage infrastructure. The same logic used for power consumption is applied to Equation 9 to calculate the total power generated and sold back to the grid, used later to calculate the revenue from fuel cells. Lastly, combining the power consumed with all the hydrogen flows calculated by the model, Equation 10 calculate the total variable cost of the system.

This last expression of the variable cost is the most important among all the calculated expressions, as a lower value in the variable cost for the main simulation (using the power consumption shown in Figure 4) compared to a fixed value for variable cost will mean that the thermodynamic approach can bring operational advantages.

$$\sum_{h} VarCost_h - pow_h^{GEN} \cdot EPRI_h^{SELL}$$

Equation 11 Proposed model objective function

Combining all the expressions explained, the calculation of the objective function becomes a trivial matter. The final expression of the objective function is the sum of the hourly cost. That value represents the total cost for generating all the hydrogen of the simulation. The additional revenue from selling energy back to the grid is subtracted to the total cost to reduce its magnitude.

For the solution of this objective function, just like on the original model, considering that it computes the total cost associated with the generation, the aim will be to minimize the value of the expression.

4.4.5 CONSTRAINTS

Combining all the variables and parameters explained in previous parts of this section. For the proposed model, several modifications have been made to the original equations for a better understanding of the results, and better adaptation to the new set structure.

$$H2_d^{DEM} = \sum_{h \in d} ((\sum_{t} dh2s_{h,t}^{STO}) + dh2s_h^{GEN})$$

Equation 12 Demand balance for the proposed model

Starting with the demand balance, Equation 12 represents a single constraint per day, instead of being part of a general production constraint. On the left side of the equation, the daily demand is represented, on the right side we find the sum of the generation shipped to cover demand from generation and from every storage technology in all the hours of that day.

$$h2_{h}^{ELE} + h2_{h}^{GREY} = \sum_{t} h2_{h,t}^{STO} + dh2s_{h}^{GEN}$$

Equation 13 Generation Balance of the original model

As shown on Equation 13, the generation balance of the proposed model is simpler as the terms related to unstoring hydrogen disappear from the expression. Therefore, the generation balance has a left side with the hourly sum of hydrogen generated (electrolytic and grey). On the other side of the expression, the hydrogen generated can either be shipped directly for demand coverage or go to storage.

From the storage side, two constraints are considered.

$$lh2_{h,t}^{STO} = \frac{loh_{h-1,t} + loh_{h,t}}{2} \cdot LF_{t}^{STO}$$

Equation 14 Storage losses for the proposed model

$$loh_{h,t} = loh_{h-1,t} + h2_{h,t}^{STO} \cdot E_{t}^{STO} - \frac{dh2s_{h,t}^{STO} + h2_{h,t}^{UNSTO}}{E_{t}^{UN}} - lh2_{h,t}^{STO}$$

Equation 15 Storage balance for the proposed model

Firstly, Equation 14 is used to calculate the storage losses on every hour and technology by multiplying the average LoH of the storage on that hour by a leakage factor that is different for every technology. Lastly, Equation 15, represents the general storage balance, starting with the LoH of the previous hour, and computing the inflows (from generation) with their respective efficiency, as well as the outflows. For the outflows we find two types, the desired outflows (composed of the flows dispatched towards demand satisfaction and the flow for fuel cells to sell energy back to the grid) with their respective efficiency. The second type of outflow is the storage losses, which are calculated in Equation 14 and added to the total. The use of a direct variable for the losses will be useful at the result face to quantify the total hydrogen lost in the duration of the simulation.

4.5 RESOLUTION APPROACH

As shown in Equation 8, the proposed model presents a non-linearity when calculating the total power consumed by the storage infrastructure. On that expression, the total hydrogen flow towards storage is multiplied by the variable representing the specific energy required for that compression (that is dependent on LoH level of the storage facility).

To address this situation, four approaches were considered to represent the variable energy for compression curve shown in Figure 4.

4.5.1 STEP LINEAR APPROXIMATION

Considering the non-linear character of the compression curve, the first approach considered to model this curve aimed to result in a linear model. The proposed strategy to achieve this linearization of the compression energy requirement is the representation of the curve with a stepwise curve, as shown in Figure 8.

To measure the quality of the representation of the resolution approaches, the coefficient R squared will be used, considering that a value of 1 means a perfect representation and values lower that 0 means a representation worse than the average value of the curve. In the case of the proposed step model, the R squared value is 0.946.

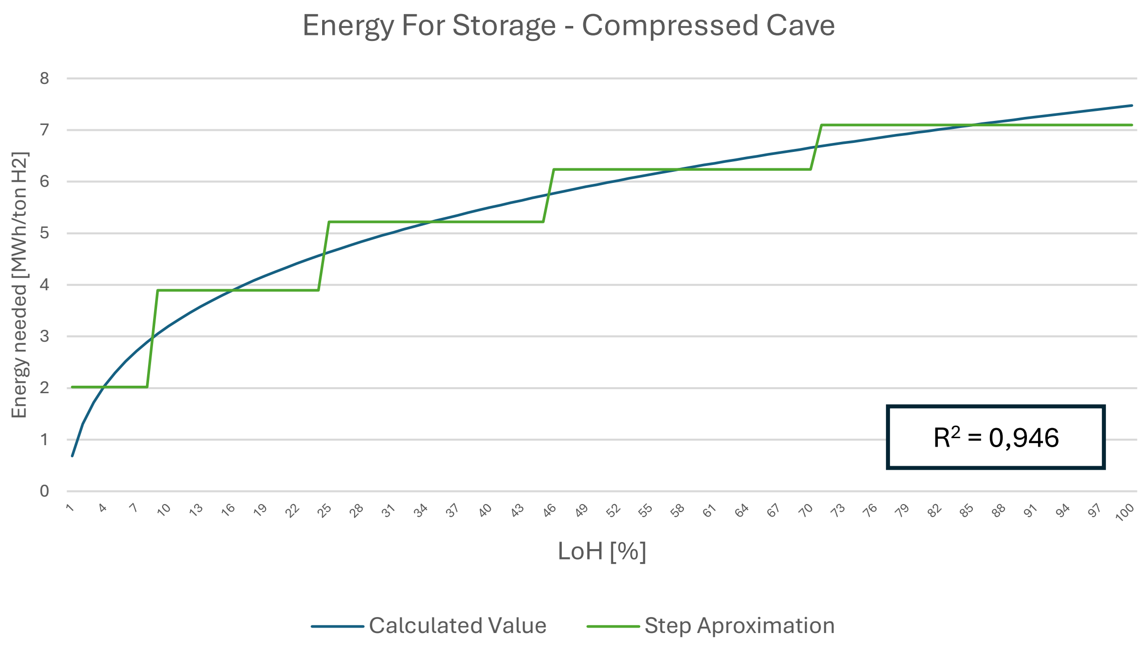


Figure 8 Step approximation to energy for compression curve

This approximation introduced a new set that represented the different steps on which the cost curve is broken down. Then for every hour and technology, a binary variable indicates on which zone of the curve is the current LoH found. With this binary guideline, a new variable can be created, representing 0 on all storage zones and 1 where the LoH is located, on which the value will be the total storage inflow in that technology and time. Considering that all values but one are 0, the product of this variable and a vector of parameters representing the height of every step will result in the total power consumption of storage in that hour.

Even though the linear approach would seem to be the best option to solve the model, the inclusion of the new set resulted in that for every step level that is introduced, 26.352 binary variables are introduced in the model, complicating the resolution.

This model was tested and simulated. However, resolution times were as high as 1 day (compared to 1 minute to solve the constant storage cost model) reaching mediocre convergence criteria (relative tolerance >1%). Moreover, the creation of storage zones resulted in the discretization of storage costs. Therefore, from an optimization standpoint, the model created virtual barriers at the end of every level, and the solver kept LoH most of the time below this virtual barrier. This pattern was unrealistic, as these barriers were virtual, and nothing prevents real storage infrastructure from going above those levels.

4.5.2 TANGENT LINES APPROXIMATION

Aiming to maximize representation, the tangent lines approach was presented, achieving an R squared of 0.995, meaning a practically perfect representation of the cost curve, as shown in Figure 9.

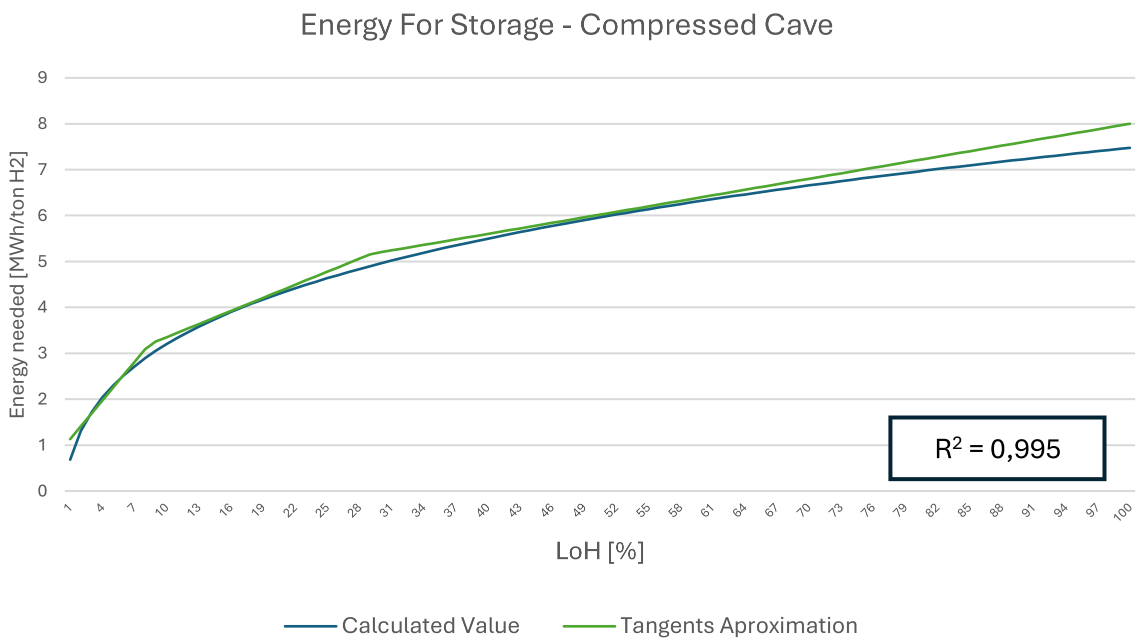


Figure 9 Tangent Lines approximation to energy for compression curve

This approach, from a modeling standpoint, required the use of binary variables to identify what tangent line is activated in every moment, depending on that time LoH. Additionally, after calculating the storage consumption of that period and technology, it is multiplied by the storage inflow, resulting in non-linearities.

The combination of tens of thousands of binary variables (as happened on the step representation) with non-linearities, rendered this approach even harder to solve. Therefore, this approximation will not be used in this project.

4.5.3 SINGLE LINE APPROACH

Following the non-linear options, a single line approach was assessed, as shown in Figure 10. By eliminating the multiple lines approach, and using only one-line, binary variables were eliminated from the model. The simplification of the model, eliminating several lines came with the cost of an overall worse representation of the curve, with an R squared value of 0.897. Even though this value is lower, it still represents a great adjustment to the curve, which could be enough for many situations.

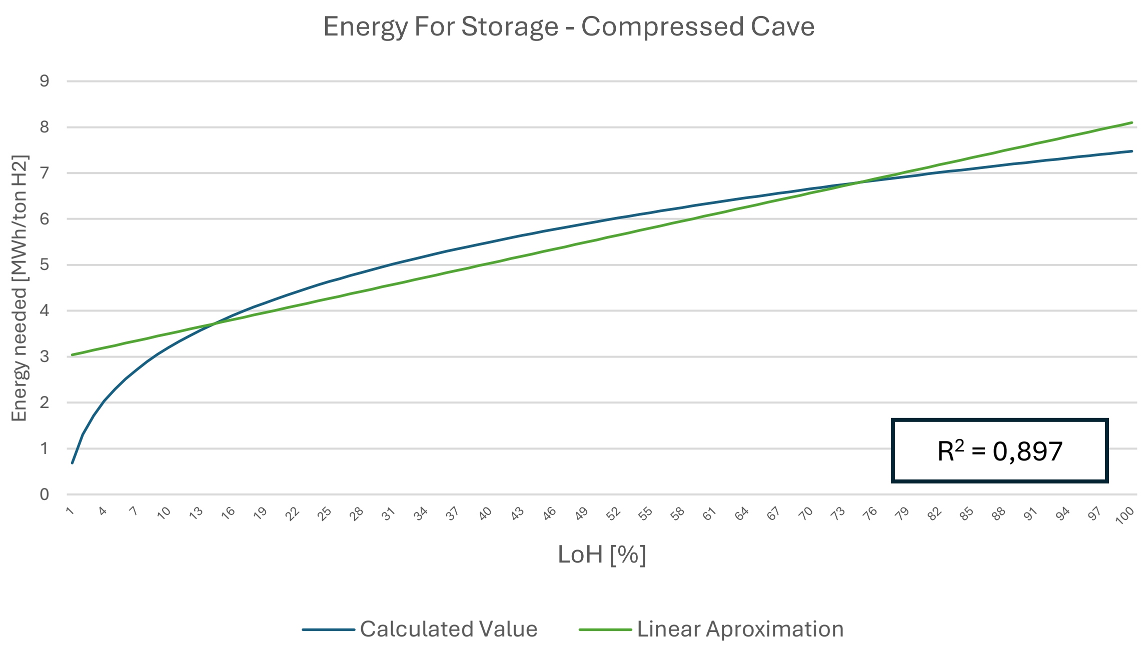


Figure 10 Single Line approximation to energy for compression curve

The new non-linear model resulted in solving times of around 20 minutes, two orders of magnitude lower than the step-wise approach.

4.5.4 DIRECT REPRESENTATION

After assessing the non-linear model's resolution times, considered as acceptable, and aiming to increase the R squared as much as possible, the idea of direct representation of the real cost curve in the model was investigated. This approach meant double non-linearity. Firstly, and same as single line approach, the product of storage consumption and storage inflow. Secondly, when calculating the storage consumption, a constant power is applied to the tank pressure (see Equation 3). This added non-linearity increased solve times to the range of 30 minutes.

Considering that only single line and direct representation approach were feasible options for this model, the decision of what representation technique had to be made. However, considering the time difference of 10 minutes in solve time resulted in a perfect representation of the cost curve, the decision was easy to make, and the direct representation was selected as the best option.

Chapter 5. RESULTS ANALYSIS

Considering the presented model and the resolution approach shown in the previous sections, the results obtained after simulating several case studies of the model will be presented in this section.

5.1 BASE CASE

Considering the aim of this project is the development of a model to promote hydrogen usage with an accurate representation of hydrogen storage technologies, the base case study simulated will be based on the Spanish energy market on 2030. This year sets the deadline for the *Plan Nacional Integrado de Energía y Clima* [37] (from now on PNIEC) that presents a roadmap for the development of the Energy Sector in Spain. Some of goals related to national infrastructure will be extracted from this document, presented by Spanish Ecological Transition ministry.

5.1.1 PARAMETER SELECTION

Considering the predictive nature of the presented base case, a deep research exercise for model inputs will be performed in this section. The aim is to accurately represent the hydrogen market big numbers for this 5 year into the future time horizon.

5.1.1.1 Hydrogen Market Inputs

As explained on the model definition, the presented model takes market characteristics as exogenous parameters, therefore, hydrogen market demand as well as the projected generation infrastructure must be estimated.

For market demand of hydrogen, a public document that can be uses as reference is *Hoja de Ruta del Hidrógeno: Una Apuesta por el Hidrógeno Verde Renovable* [38] (from now on HRH), where the Spanish strategy to address hydrogen development is presented. This document states that the current Spanish hydrogen demand is 500000 tons per year, and according to the market trends and the expected rise on hydrogen mobility, hydrogen demand is expected to double by 2030 [39]. For the simulation, market demand is calculated daily, and therefore, it will be computed for 2030 as a daily demand of 3000 tons (1095000 tons per year).

For the generation side, two sources of hydrogen are considered: electrolyzer (yellow hydrogen, or green if electricity is mostly renewable) and chemically generated (grey hydrogen or blue if carbon capture processes are used).

Regarding electrolyzers, PNIEC projects an installed electrolysis capacity of 12 GW for 2030.

Regarding chemical hydrogen capacity, HRH serves as a reference. Considering current demand of hydrogen is mostly satisfied using chemical hydrogen, current capacity can be estimated in the range of the 500000 tons of demand per year. The references consulted state that by the end of the decade, green hydrogen will overcome chemical from a profitability standpoint [40]. Considering this decline in profitability, the model will consider a daily limit of 1000 tons of chemical hydrogen (365000 tons per year).

5.1.1.2 Hydrogen Storage Inputs

From the analysis of the state of the art of hydrogen technology, the main storage technologies used at market scale operation are Compressed Tank Storage, Compressed Cave Storage and Cryogenic Tank Storage. All these technologies but cryogenic are affected by the thermodynamic approach, as the energy required for compression varies with the tank LoH.

Regarding the aggregate capacity of each technology, all projects carried out by private agents (utility companies mainly), must be added to achieve a proper representation. Regarding compressed hydrogen, HRH presents the objective of building 150 hydrogen stations (that store hydrogen on compressed tanks), as well as several industrial electrolyzers that include storage facilities [41]. Considering the average size of a hydrogen station combined with these projects, the total computed compressed tank capacity will be set to 1000 tons.

For liquid storage, a similar approach has been followed, considering that most of the liquid capacity is found in industrial tanks in coastal areas [42]. These tanks account for 1000 tons of hydrogen storage, which will be used as the input for the model.

Lastly, for cave storage, large projects promoted by big energy companies [43], [44], [45] (as they are the only companies that can profit for an storge of that scale) bring an aggregate of 31000 tons. This capacity is much greater than other technologies as the specific CAPEX needed for this storage is the lowest among all technologies and is projected to cover stational storage needs. However, from an operational standpoint, this technology is concentrated regarding maximum inflow/outflow, as for geological reasons, the maximum daily pressure difference can't exceed 1MPa [24] (10 bar). Considering the maximum storage pressure of 250 bar [15], and the total capacity of 31000 tons, the maximum hourly inflow/outflow won't exceed 51,7 tons.

Regarding storage leakage, compressed tanks leak at a daily average rate of 0,2% [46] (for a 750 bar tank), via hydrogen diffusion through the atoms of the tank. For liquid storage, losses are produce due to boil-off (hydrogen released due to pressure increase as hydrogen condenses, that must be released to prevent the tank from collapsing), that leaks at an average daily rate of 1% [47]. Lastly, cave storage offers close to 0 losses, although some studies calculate losses due to biological activity of bacteria, to be around 0,0005% [48].

	Leakage [%/day]	Capacity [tons]	Maximum Flow [tons/hour]
Compressed tank	0,2	1000	No Limit
Compressed cave	0,0005	31000	51,7
Liquified	1	1000	No Limit

Table 12 Base Case Storage Parameters Summary

5.1.1.3 Electricity Market Modeling

For this baseline, the SPOT market prices will be inputted into the model, both as buy and sell prices for energy. Even though this model represents the market of 2030, real recent data were used as inputs for the model. At the time of this project, Spain's market operator OMIE, offers the full hourly prices for the year 2024 [49], with an average value of 63,04 €/MWh.

The 8784 data points extracted from [49] were formatted in excel and imported into GAMS for these simulations.

5.1.1.4 Operational parameters

Lastly, to complete the parameter selection, the different efficiencies, as well as the operational costs, must be calculated.

Regarding operational efficiencies, for the electrolyzer, current technology offer around 70% [13]. Another key element of the hydrogen system are fuel cells (operating as reversed electrolysis) that typically have an efficiency of 60% [50].

Regarding operational costs, fuel cells and electrolyzers offer similar values (although for the model they are expressed as €/ton H_2 for electrolyzers and €/MWh for fuel cells). The references consulted express the values as 2-4% of the CAPEX [51] for O&M costs. After accounting for the average load factor of this infrastructure and excluding the cost of energy (as they are computed separately on the model), the cost calculated is 50 €/ton H_2 for electrolyzers, that equals 1,5 €/MWh for fuel cell (applying a conversion rate of 0,03 ton H_2/MWh, calculated by expressing the LHV of H_2 of 120 GJ/ton H_2 into MWh/ton H_2). Lastly, for calculating the total cost of chemically generated H_2, the consulted references state an average cost of 2,13€/Kg H_2 (2130 €/ton H_2) [40], that will be used as model input.

For the calculation of storage cost (excluding the cost of energy), the main expense is compressor O&M cost. For this calculation, the baseline was extracted from the business case presented in *Cost quantification*, and excluding the cost of energy by using the cost breakdown presented in [52], the cost is estimated is 19,4 €/ton H_2 for compression storage. In the case of liquid storage, consulted references [53] calculate that liquid storage costs an average of 0,25 $/Kg H_2, that using and exchange rate of 1,15 $/€, the model will use a total cost of 215 €/ton H_2.

The main contribution of this project compared with the consulted literature is the modelling of the cost of storage following the thermodynamic curve (see Figure 4). For this purpose, Equation 3 is included in the model. Considering that adiabatic coefficient, R, and Temperature are constant values across the process, the expression can be simplified:

$$cons_{h,t}^{STO} = K_{STO} * \left((pres_{h,t}^{STO})^{EXP_{STO}} - 1 \right)$$

Equation 16 Adapted energy for compression equation expression

Considering hydrogen's R coefficient, an adiabatic coefficient of 1,3 and a temperature of 290K (and applying the necessary conversions to express the energy W in MWh/ton H_2 when pressure in bar is entered), K_{STO} equals 2,901 and EXP_{STO} equals 0,231. These will be the values used in the model, considering a maximum storage pressure of 250 bar for cave storage and 750 bar for compressed tank storage. For the compressor efficiency that applies to these processes, consulted references state a 90% power efficiency.

Lastly, regarding liquid storage, this technology isn't affected by the curve as the pressure is constant at 1 bar. The consulted references [54] find that energy extraction needed for liquification is 1,3 MWh/ton H_2, and the process efficiency for the cryogenic infrastructure is 22%, totaling 5,9 MWh/ton H_2.

5.1.2 SIMULATION RESULTS

Considering that the model includes a constraint that ensures that the initial LoH inside the tanks must equal the end value at the end of the simulation, the initial LoH conditions the pressure ranges of the tank operation through the simulated year (mostly for the cave storage, as it has the highest capacity combined with inflow/outflow limitations, resulting in LoH profiles been greatly influenced by the initial LoH level). Considering this, the simulations are performed starting at a 5% LoH and a 95% LoH, to force the modification of the compressed cave LoH profiles through the year and analyzing the consequences of this patterns.

To evaluate the impact of using the curve-based approach to represent the energy intensity of storage, as compared to assuming a constant energy requirement for compression, both cases will be simulated. The base case will consist of four simulations, resulting from the combination of two cost calculation methods (constant or curve) and two initial LoHs (5 or 95%).

5.1.2.1 Differences across models

Base Case		Constant Cost LoH 5%	Curve Cost LoH 5%	Constant Cost LoH 95%	Curve Cost LoH 95%
Storage Costs [€/ton H_2]	Compressed tank	45,09	45,26	47,53	67,61
	Compressed cave	45,20	39,84	47,83	45,52
	Liquified	254,16	261,19	272,11	277,19
Number of hours of Storage	Compressed tank	831	2425	835	2403
	Compressed cave	867	986	872	938
	Liquified	466	612	479	536
Number of hours of Storage with 0 or negative price	Compressed tank	480	332	475	330
	Compressed cave	448	451	448	450
	Liquified	223	281	224	264
Negative price hour to total hours ratio [%]	Compressed tank	57,76%	13,69%	56,89%	13,73%
	Compressed cave	51,67%	45,74%	51,38%	47,97%
	Liquified	47,85%	45,92%	46,76%	49,25%
Average Storage LoH [%]	Compressed tank	33,04%	30,89%	34,15%	32,40%
	Compressed cave	55,18%	55,32%	65,39%	65,71%
	Liquified	15,39%	15,85%	18,67%	19,47%
Hydrogen amount Stored [tons H_2]	Compressed tank	46358	46230	47169	48487
	Compressed cave	204041	206346	201822	200627
	Liquified	18730	18893	19115	19190

Table 13 Base Case Simulation Result Summary

To compare the results obtained in the different simulations, several metrics of storage cost have been selected to properly analyze the difference between cases, that have been represented in Table 13.

Firstly, the main metric is storage cost, calculated as the total operational expense incurred by a determined storage technology, divided by the total amount of hydrogen stored on that technology. Secondly, the number of hours of storage, representing the total amount of the 8784 hours (since the selected year is a leap year) of the year on which hydrogen is stored on each technology. Then, to reference the market conditions necessary for storage, the count of those storage hours that occur at times of 0 or negative energy price are counted, and their relative weight is also calculated.

Considering the metrics mentioned, the main differences observed across models are:

- Compressed cave storage offers the lowest storage cost, and the curve cost model manages to reduce cost even further (from 45,2 to 39,84 and from 47,83 to 45,52 depending on the starting LoH). It is also the reason why it covers most of the total storage (~75% of total storage). Similarly, compressed tank storage also results in lower storage cost when using the curve approach.

- The use of the curve approach increases the total hours of storage of all technologies, not only to the ones that are affected by compression processes (cave and tank storage). This difference is maximum in tank storage (from ~800 to ~2400), as the curve approach finds more cost-efficient opportunities than the constant cost model.

- Curve model reduces dependence on negative prices on almost all cases. This effect is maximum on Compressed Tank Storage (going from ~57% to ~13%), as it operates on the highest pressure. Therefore, it is affected the most by the curve approach that causes exponential growth of the energy required with the storage pressure.

- Average LoH remains similar in cave storage and falls ~2% from when using the curve approach in the compressed tank storage. Lower LoH means lower power consumption and therefore lower cost, so compressed tank storage benefits the most as it operates on higher pressures.

Even though the differences across models have shown to be maximum in compressed tank storage, an objective metric was developed to properly quantify the differences.

The Root Mean Square Error (from now on RMSE, calculated following Equation 17) has been selected as the primary metric to quantify this difference across modeling strategies. It offers sensitivity to both the magnitude and frequency of deviations across time. RMSE captures the accumulated discrepancy between two profiles by penalizing larger deviations more heavily, which is particularly relevant in energy storage systems where significant operational mismatches may occur.

$$RMSE = \sqrt{\frac{\sum_{d=0}^{d=366}(\sum_{h=0}^{h=24}(LoH_{Curve}{}^{2} - LoH_{Constant}{}^{2}))}{366 * 24}}$$

Equation 17 RMSE formula applied to tanks LoH

To ensure comparability across simulations with different storage capacities, the RMSE will be normalized with respect to a fixed reference scale: the maximum storage capacity of that technology. This Normalized RMSE (from now on NRMSE) allows for dimensionless (expressed in %) interpretation of operating differences, enabling equal evaluation across cases.

This metric has been applied to the LoH profiles of the different storage technologies and starting LoH, calculating their difference. The results of this calculation are shown in Table 14.

NRMSE	LoH 5%	LoH 95%
Compressed tank	11,68%	14,62%
Compressed cave	1,08%	0,85%
Liquified	3,55%	4,67%

Table 14 Base Model LoH NRMSE by technology and starting LoH

This table supports the theory that the higher the operating pressure, the higher the difference between the curve and constant model is across storages technologies. In addition, the compressed tank storage shows a difference of ~11-15% when the rest of storage options remain below the 5% mark.

Lastly, aiming to assess the differences in power consumption across models, the average power consumed by the different storage technologies has been calculated in Table 15.

[MWh/ton H_2]	Constant Cost LoH 5%	Curve Cost LoH 5%	Constant Cost LoH 95%	Curve Cost LoH 95%
Compressed tank	8,905	9,287	8,905	9,330
Compressed cave	6,188	6,196	6,188	6,746
Liquified	5,909	5,909	5,909	5,909

Table 15 Base Model average storage power consumption

This table shown how, in all cases, the constant approach underestimates the power consumption of the storage technologies that are affected by compression. Aligned with expectations, the cases with the highest yearly average LoH (see Table 13) offer the highest difference (~9%) in power consumption between models (in this case, compressed cave 95% starting LoH, that showed the highest average LoH across all simulations ~65%).

Considering that compression tank offers the highest operational differences across models, the LoH values obtained from the simulations have been ordered to create the monotonic curve of Figure 11. On this graph it is clearly represented how the differences between the models are accumulated through the year. The constant cost model shows a tendency to hold higher LoH, as it is not penalized by the higher compression cost that the curve model represents more properly. On the other hand, when LoH falls below the 50%-mark, curve approach slows the decrease, following an asymptotic trend, as it benefits from the reduced power consumption compared to constant model.

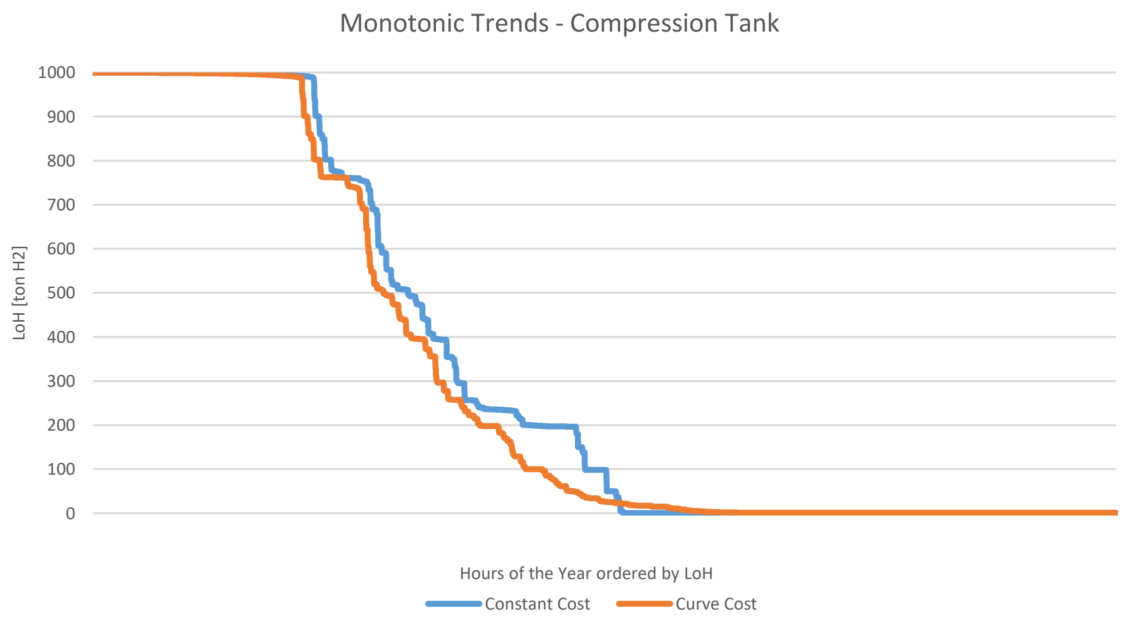


Figure 11 Monotonic LoH curve of compression tank in the Base Case

5.1.2.2 Differences between technologies

From a quick analysis of the results obtained in the simulations, a key takeaway is the use of compressed cave storage. This technology presents low operational costs (44,6 €/ton vs 51,34 €/ton for the tank and 266,16 €/ton for liquified on average across simulations), and its high capacity can be used to cover market seasonal's storage needs (covering at least 75% of total hydrogen stored).

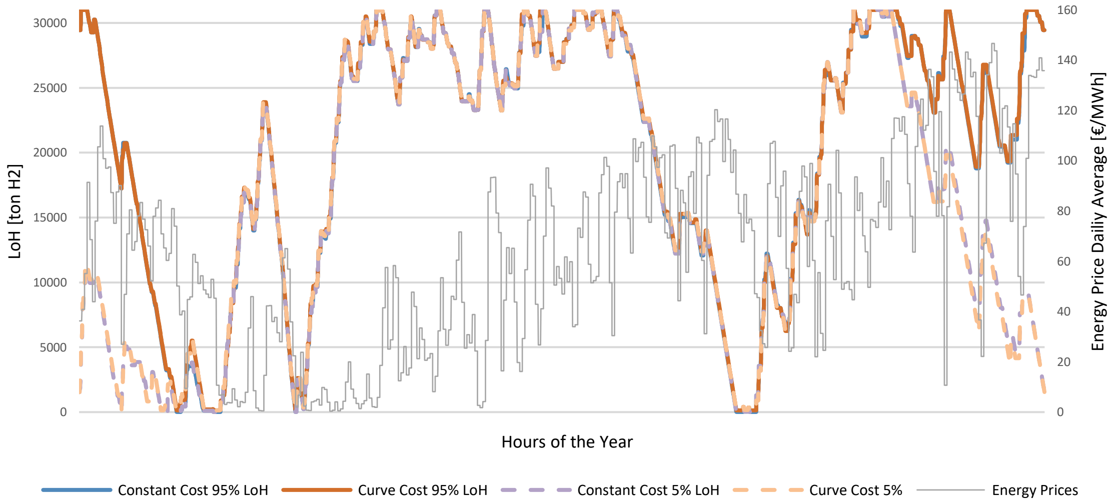


Figure 12 Base Model Cave Storage LoH

The main argument to support this compressed cave as the main seasonal storage technology is the LoH profile difference between the simulations, as shown in Figure 12. This graph shows how the constant model and the curve model operate equally throughout the year for this storage technology, not only when starting from the same LoH point, but also when starting from different points, except for the start and end days, as the curves must start and end on different points. Indeed, they soon converge to the same behavior. This pattern supports the theory of the seasonal storage, as different models and staring LoH points produce similar LoH yearly profiles, as the energy price distribution es equal across all cases.

To further support this theory, when examined on a closer timeframe, and comparing with energy prices, LoH increases when they are low and waits until energy prices rise to release its hydrogen. This pattern is clearly observed on Figure 13, which represents a detailed view of Figure 12 for the hours 2500-3000 of the selected year, and it operates the same, regardless of the model used.

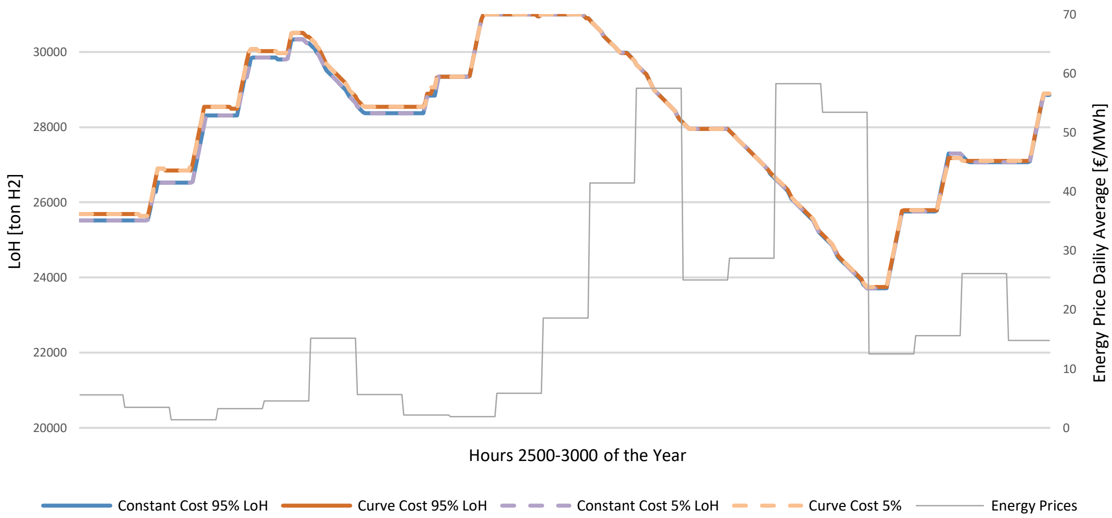


Figure 13 Detail of Base Model Cave Storage LoH

On the other hand, compression tank and liquid storage, are used as short-term storage, with pronounced load cycles (going from full to empty) in a matter of days at most. The two main reasons that cause this phenomenon are the smaller capacity of these storages (1000 tons compared with 31000 tons of cave storage) as well as the fact that storage inflows and outflows are not limited in these technologies (unlike cave storage).

The operation of these two technologies is similar. However, costs for compressed storage are lower, therefore, the model finds more short-term storage opportunities for compressed tank storage (storing around 47000 tons yearly compared to liquid's 19000, see Table 13). This pattern is clearly seen in Figure 14 and Figure 15, where it is shown that compressed storage performs more cycles. Precisely, liquid storage offers the lowest difference between curve and constant approaches (as shown on its NRMSE, that is around a third of the NRMSE of compressed tank storage, see Table 14), as its cost is not affected by the thermodynamic curve, considering that the storage process does not require compression.

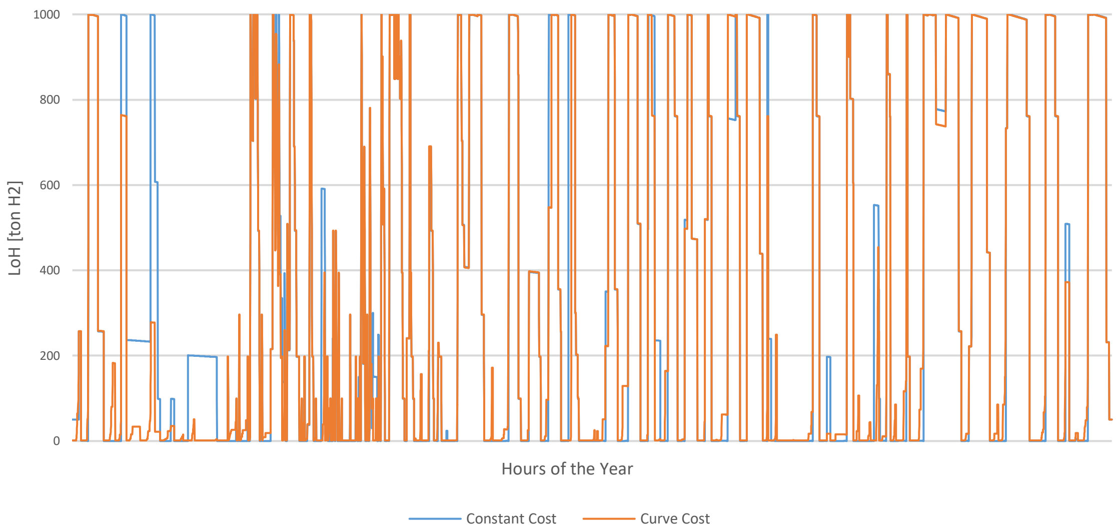


Figure 14 Base Case Compressed Tank LoH (5% starting level)

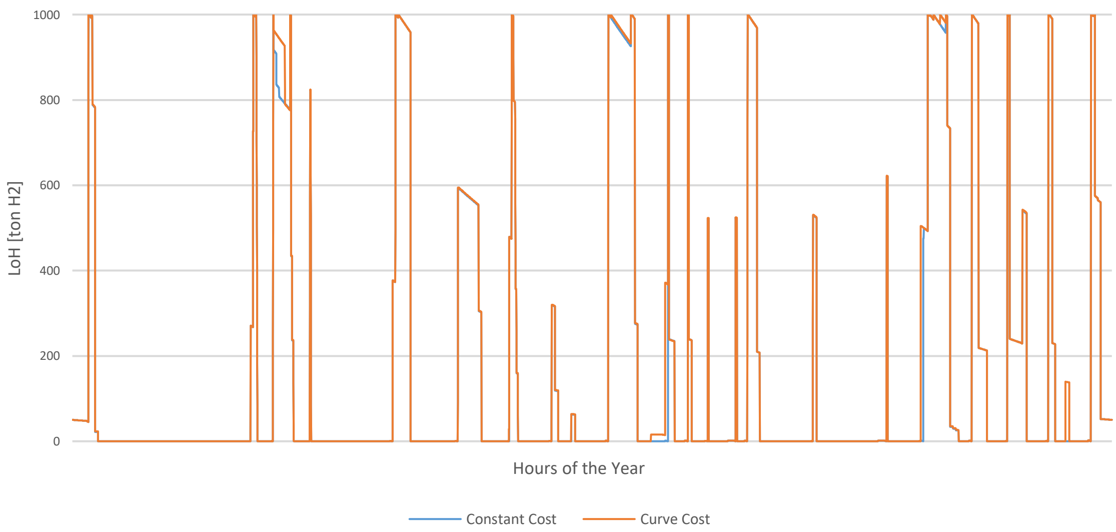


Figure 15 Base Case Liquid Storage LoH (5% starting level)

5.1.3 SIMULATION TIMES

As explained in the objective section, this project aims to assess the potential implementation of the thermodynamic equations on a hydrogen market model. Considering that in reality compression follows the curve expression, this implementation results in an objective improvement in model's rigor. However, considering that the inclusion of the cost curve results in non-linearity, the overall computational power required to solve the different cases must be included in the analysis.

Regarding the hardware used for the times presented, the simulations were performed on a laptop, using an intel 12700H processor that offers 14 cores (6 performance and 8 for efficiency) and 20 threads, operating at a maximum frequency of 4,7 GHz.

Simulation times to solve the base case were ~1 minute for constant cost simulations and ~30 minutes for cost curve simulations.

5.2 DOUBLE CAPACITY CASE

Base case showed that storage operates near full capacity, and that stational storage (considering stational as compressed cave storage) would only cover 10 days of the projected 2030 hydrogen demand. Considering this, another case study has been evaluated, doubling the storage capacity of all the technologies. Therefore, compressed cave storage is computed with a 62000 tons capacity, 2000 for compressed tank and 2000 for liquified.

5.2.1 SIMULATION RESULTS

5.2.1.1 Differences across models

Following the result structure presented in base case scenario, the main results when the storage capacity for each technology is doubled are shown in Table 16

Double capacity Scenario		Constant Cost LoH 5%	Curve Cost LoH 5%	Constant Cost LoH 95%	Curve Cost LoH 95%
Storage Costs [€/ton H_2]	Compressed tank	19,70	44,23	24,92	53,65
	Compressed cave	44,18	36,69	45,89	41,64
	Liquified	254,08	264,09	311,66	325,44
Number of hours of Storage	Compressed tank	529	2809	570	2752
	Compressed cave	1052	1114	1043	1061
	Liquified	135	186	181	263
Number of hours of Storage with 0 or negative price	Compressed tank	386	239	381	233
	Compressed cave	529	524	529	529
	Liquified	78	93	78	101
Negative price hour to total hours ratio [%]	Compressed tank	72,97%	8,51%	66,84%	8,47%
	Compressed cave	50,29%	47,04%	50,72%	49,86%
	Liquified	57,78%	50,00%	43,09%	38,40%
Average Storage LoH [%]	Compressed tank	13,15%	13,81%	20,98%	19,40%
	Compressed cave	59,25%	59,41%	70,60%	70,92%
	Liquified	4,54%	5,13%	8,51%	9,11%
Hydrogen amount Stored [tons H_2]	Compressed tank	26963	33780	33353	42895
	Compressed cave	260780	256872	246579	239166
	Liquified	9689	9939	14173	14211

Table 16 Double Capacity Case Simulation Result Summary

- Compressed cave storage remains as the lowest storage cost option, by doubling total capacity, the maximum inflow/outflow also doubles. This difference enables this double capacity to reduce costs even further compared to base case. The differences in cost between models also increase on this double capacity scenario, going from ~13% to ~20% for 5% staring LoH and from ~5% to ~10% for 95% starting level.

- Aligned with the base case, but in a higher scale, the number of hours of storage rises when using the curve approach compared to the constant cost model (going as high as ~2800 compared to base case's ~2400).

- Curve models reduce dependence on negative prices on all cases. This effect is maximum on Compressed Tank Storage (going from ~70% to ~8% compared to base case's from ~57% to ~13%).

- Unlike the base case, this double capacity scenario shown practically no difference in yearly LoH average. This could be explained by the relative increase in total storage covered by compressed cave (that showed the least average LoH difference in the base case scenario).

Following the same pattern as in the base case scenario, the LoH difference across models has been calculated using the NRMSE, shown in Table 17.

NRMSE	LoH 5%	LoH 95%
Compressed tank	10,05%	15,04%
Compressed cave	0,46%	0,67%
Liquified	3,37%	3,48%

Table 17 Double Capacity Case LoH NRMSE by technology and starting LoH

The results obtained from this table are similar to the ones obtained in the base case, supporting again that the short-term storage (compressed tank and liquid) shows the highest difference between both modelling approaches, specially the compressed tank, considering the higher storage pressure of this technology.

Some key observations can be extracted from the analysis of the average power consumption of this double capacity simulation, shown in Table 18. Aligned with base case results, the compressed cave storage underestimates power consumption of the storage.

On the other hand, the total storage falls in compressed tank and rises in compressed cave storage. This pattern means that compressed tank requires lower costs to start operation, and therefore it operates on lower LoH levels, achieving a power consumption below the constant cost of 8,905 MWh/ton H_2. This statement is also sustained by the fact that on the base simulation, there was practically no difference across models in total storage for the compressed tank (between 46K and 48K tons/year in all simulations). On this double capacity simulation total storage in compressed tank rises from 26963 to 33780 and from 33353 to 42895 tons/year. This means that the curve model manages to find more lower cost opportunities that the constant model.

[MWh/ton H_2]	Constant Cost LoH 5%	Curve Cost LoH 5%	Constant Cost LoH 95%	Curve Cost LoH 95%
Compressed tank	8,905	8,459	8,905	8,215
Compressed cave	6,188	6,195	6,188	6,737
Liquified	5,909	5,909	5,909	5,909

Table 18 Double Capacity Case average storage power consumption

As this results showed the most variability in the compressed tank storage, the monotonic curve of this storage has been represented in Figure 16.

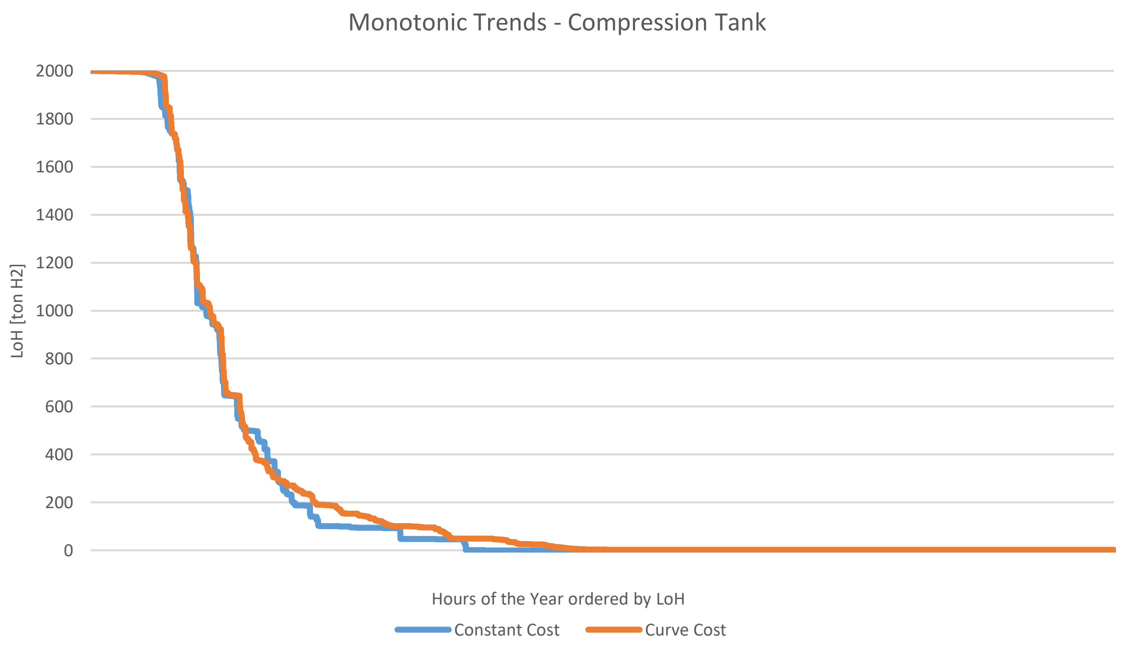


Figure 16 Monotonic LoH curve of compression tank in the Double Capacity Case

Aligned with results shown in the base case, both models have a similar pattern on the top 50% LoH level. However, on the bottom 50% level, the curve approach separates, spending more hours in this zone that the constant model. The same asymptotic pattern in shown in this graph. The additional hours spent in this zone for the curve approach explain why the curve model is able to offer a lower average storage consumption, as this region offers close to 0 power consumption in the curve model, unlike the constant approach.

5.2.1.2 Differences between technologies

For stational storage, that showed to increase its yearly volume, the LoH profile is shown in Figure 17. The resulted profile is practically identical to the base case results, showing a correlation index of 0,95 (correlation index is used instead of NRMSE aiming to measure shape deviation, while NRMSE measures magnitude deviation). Therefore, on a double capacity scenario, cave storage still serves as a seasonal long-term storage. This observation also sustains the correlation of the cave LoH profile and the energy price yearly profile, as doubling storage capacity does not change practically the LoH profile of this technology, as energy prices are kept the same.

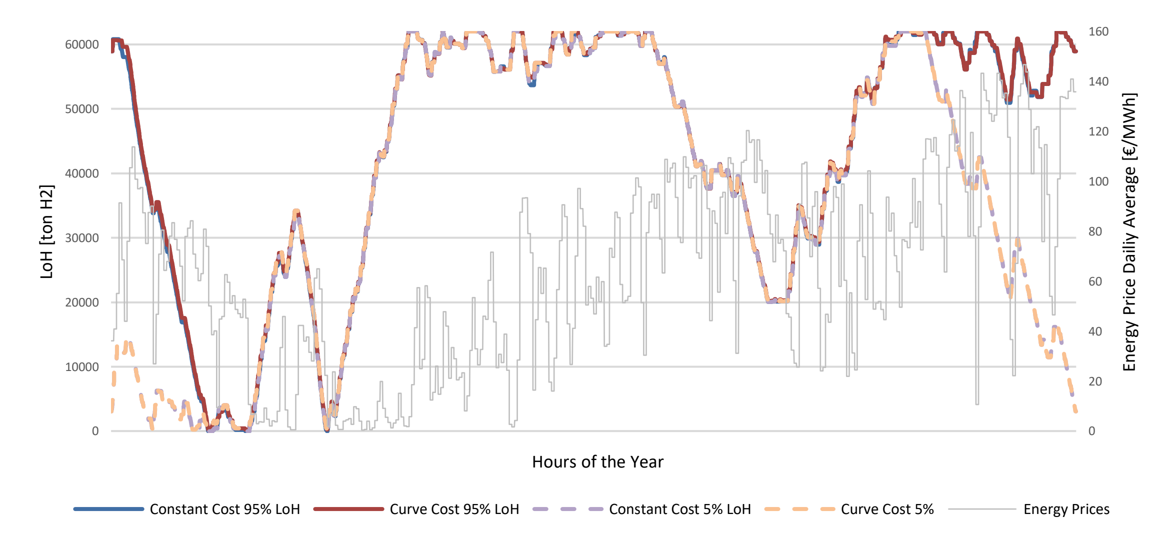


Figure 17 Double Capacity Case Cave Storage LoH

For the rest of the technologies analyzed, considering that total storage amount decreases in this double capacity scenario, and that now a single storage cycle covers 2000 tons, a clear reduction in the number of cycles is observed (see Figure 18 and Figure 19). Particularly, in liquid storage, it is shown how only 5 full cycles are concluded through the year and 11 for compressed tank technology. Even though the price of this technologies is higher than compressed cave storage, the solver manages to find cost-efficient storage opportunities due to their increased flexibility, been capable of filling from empty in a matter of hours, compared to compressed cave, that takes weeks.

It is clear how increasing compressed cave storage can bring some benefits to operation, however, the projected storage capacity for compressed tank and liquified storage is sufficient for the projected demand of 2030. On the other hand, compressed caves are limited in potential capacity as it requires natural caves, and the total inflows/outflows are limited unlike the other technologies. This shows that even though the costs are cheaper for compressed cave, the 3 technologies may coexist to maximize market flexibility. With this in mind, deeper analysis could be carried out in future projects to determine the ideal capacity of each technology.

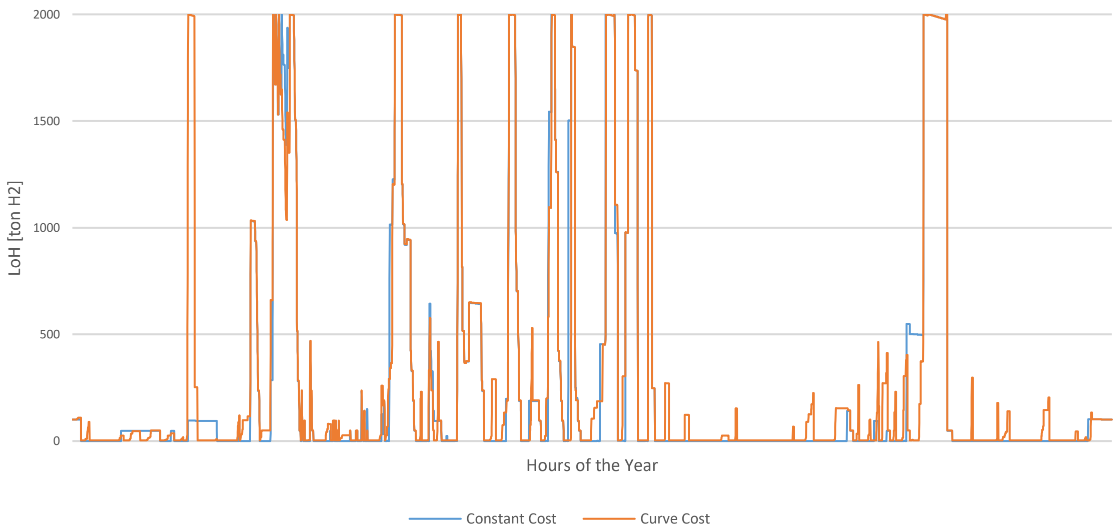


Figure 18 Double Capacity Case Compressed Tank LoH (5% starting level)

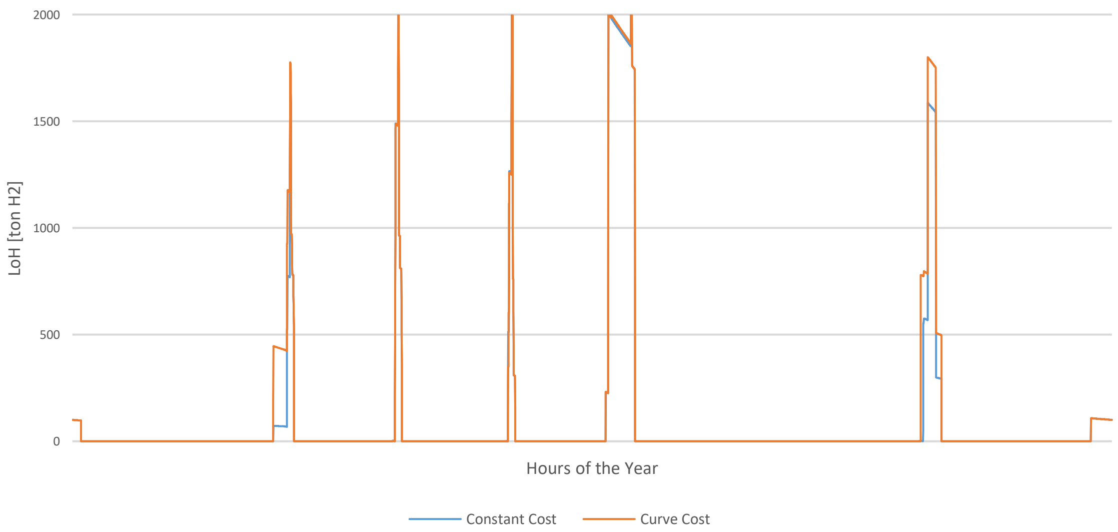


Figure 19 Double Capacity Case Liquid Storage LoH (5% starting level)

5.2.2 SIMULATION TIMES

For this double capacity case, the hardware used was the same as explained in section 5.1.3. Simulation times to solve the base case were ~1 minute for constant cost simulations and ~45 minutes for cost curve simulations. Therefore, constant cost was aligned with base case times, and curve approach required an additional 15 minutes to find an optimal solution to the model.

5.3 SINGLE TECHNOLOGY SIMULATIONS

Aiming to calculate a reference price for each technology, a new case study was analyzed, computing all the market parameters explained previously, but modelling storage technologies separately. Therefore, this case study was broken down into 3 sub-cases, simulating that only one technology is used throughout the year.

The 3 sub-cases input the operational parameters of every technology (explained in 5.1.1.4) and considered a total storage capacity of 33000 tons (the total storage computed across technologies on the base case: 31000 cave storage, 1000 compressed tank and 1000 liquified).

Then for every sub-case, the 4-simulation presented in the base case were performed, (constant and curve approaches, combined with 5% and 95% starting LoH).

5.3.1 SIMULATION RESULTS

5.3.1.1 Differences across models

After computing the 3 sub-cases, the reference storage cost values are presented in Table 19. In the case of liquid storage, the reference values of constant cost and curve cost are equal for the same LoH level because this technology is not affected by the compression curve.

Storage Cost [€/ton H_2]	Constant Cost LoH 5%	Curve Cost LoH 5%	Constant Cost LoH 95%	Curve Cost LoH 95%
Compressed tank	58,08 €	59,50 €	58,70 €	65,95 €
Compressed cave	42,22 €	39,03 €	44,01 €	47,50 €
Liquified	245,90 €	245,90 €	262,39 €	262,39 €

Table 19 Single Technology Cases Storage Cost

Comparing the results obtained in this single case simulation with the previous cases, similar patterns can be observed in results. Firstly, in the case of compressed tank storage, the constant approach always underestimates total storage cost, that difference becomes especially significant for the 95% LoH scenario, by starting the tank near its maximum capacity, the yearly average LoH increases, and therefore, the difference between constant cost and curve approach increases. On the other hand, the cases where average LoH of the curve approach are like the value used to calculate the constant cost (50% LoH in these simulations) show closer values between the constant and curve approach. This pattern is represented in Table 16 for the compressed cave storage, where an average LoH of ~47% results in a price difference of ~20% across models(5% start LoH) compared to an average LoH of ~50% that results in a price difference of ~10% (95% start LoH).

From this observation, it can be extracted that if the operating pressures of a determined storage are relatively stable on a determined level, the constant cost calculated around that pressure range could provide finer results at a fraction of the computation cost.

Although the results for cave storage differ between the LoH scenarios, this is explained by the technical limitation of a maximum 10-bar daily pressure variation. This constraint prevents cave storage from making rapid changes in LoH, unlike compressed tank storage. As a result, cave storage shows a greater average LoH difference between simulations. This effect can be seen in Figure 20, where the overall profiles are nearly identical, but compressed tank storage consistently exhibits sharper LoH variations, storing more during low-price periods and releasing more during high-price ones. Due to its limitation, when starting at 5% LoH, the cave storage remains longer in low LoH zones (where compression costs are lower), and when starting at 95%, it stays longer in high-price situations. This pattern helps explain the particular behavior of cave storage when applying the cost curve model.

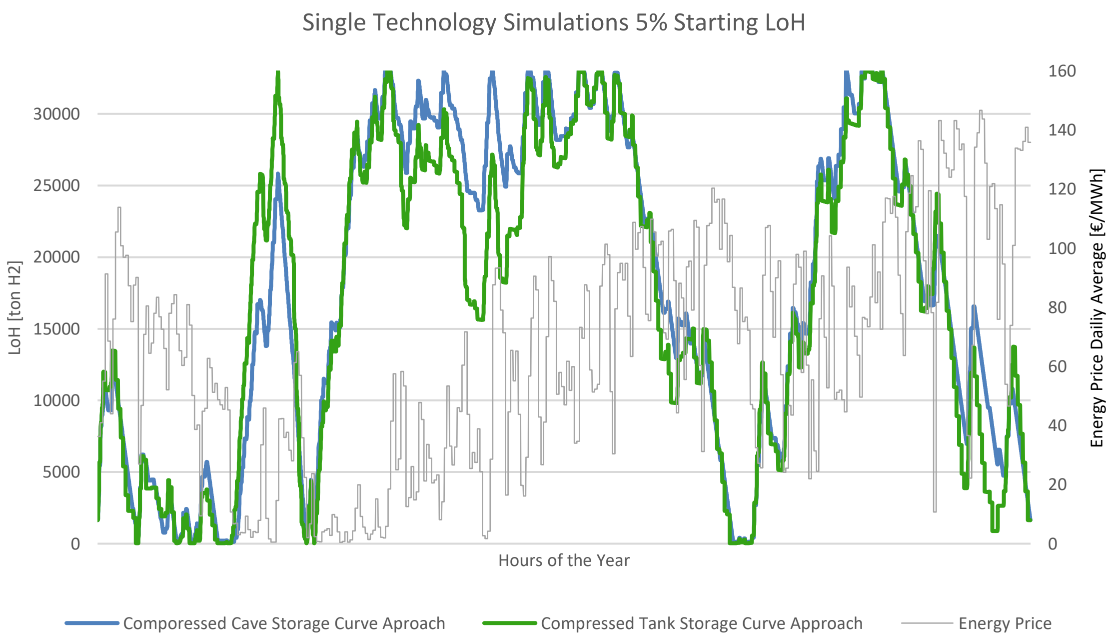


Figure 20 Single Technology LoH Profiles of Compressed Cave and Compressed Tank

5.3.2 Storage Cost Comparison

Considering the single technology storage costs obtained (showed in Table 19), and comparing them with the rest of case studies, shown in Table 13 and Table 16, the following cost comparison is performed, shown in Table 20. This table represents the cost difference (in percentage) of the base case and the double capacity simulations. The table has been formatted to show in green when base/double capacity storage cost obtained is higher that single technology, and red whenever multiple technology simulations have resulted in lower storage costs.

Compared to single Technology Results	Base Case				Double capacity Case			
	5% Base LoH		95% Base LoH		5% Base LoH		95% Base LoH	
	Constant	Curve	Constant	Curve	Constant	Curve	Constant	Curve
Compressed tank	-22,37%	-23,94%	-19,04%	2,53%	-66,09%	-25,66%	-57,56%	-18,65%
Compressed cave	7,05%	2,08%	8,67%	-4,15%	4,63%	-5,99%	4,26%	-12,32%
Liquified	3,36%	6,22%	3,70%	5,64%	3,32%	7,40%	18,77%	24,03%

Table 20 Storage Cost Comparison Between Models

Several key conclusions can be drawn from the storage cost comparison table. Firstly, compressed tank storage does not appear suitable for large-scale seasonal storage, since in almost all cases, the resulting storage costs are lower when it is combined with other technologies than when it is used alone. In contrast, the opposite applies to liquid storage, which is the least competitive option. When operating alongside other technologies, the most profitable opportunities are captured by the other systems, resulting in higher costs for the liquid storage component. As a result, the single-technology scenario for liquid storage consistently shows lower average costs across all simulations.

Lastly, compression cave storage changes the least between combined and single technology simulations (as the only difference is passing from 31000 tons to 33000 capacity). The tendency in cost difference is not clear in this case, considering that the use of other technologies, even though they operate at higher storage costs, bring flexibility to the system, making that the elimination of them can benefit average storage cost in some cases and penalize it in other scenarios.

Chapter 6. CONCLUSION AND FUTURE DEVELOPMENTS

6.1 MAIN CONCLUSIONS

After performing this deep analysis in hydrogen storage technologies, and market outlook for Spain by 2030, some general conclusions have been extracted that will be presented in this section.

1. The use of the thermodynamic approach presents a finer representation of the compression cost incurred during storage.
2. The effect of applying this approach increases with the difference in pressure of the real storage, compared with the value used in the constant approach.
3. The use of the thermodynamic approach reduces greatly the dependance on negative energy prices to find profitability in hydrogen storage and increases versatility of storage infrastructure.
4. Compressed Cave Storage has proven to be the best option for a market scale seasonal storage
5. Computational requirements for reaching an optimal solution increase greatly due to the non-linearities introduced in the model. A trade-off analysis must be carried out between precision and solving times.
6. The storage cost for technologies that involve compression is influenced by the nominal operating pressures of the storage facilities, rather than the maximum/minimum operation boundaries.

6.1.1 THERMODYNAMIC MODELING OF COMPRESSION

As shown in the project definitions section and based on the real mathematical expression of the thermodynamics of hydrogen compression, the use of the curve approach goes a step further in the process of creating a realistic cost optimization model for hydrogen storage.

On the other hand, even though the increase in modeling precision is objective, the added computation cost will not always cover the gains in precision. This dilemma will be addressed further in this section as it is one of the key takeaways of this project.

6.1.2 COST CURVE APPROACH IMPACT ON RESULTS

As has been shown across the different study cases, the exponential character of the compression curve equation causes that the impact of its implementation increases with the absolute difference between the real tank pressure and the value used to calculate the constant cost of that technology. Current compression curve infrastructure ranges greatly in operating pressures, from around (see Table 1) from a around 100 bar, up to 1000 for state-of-the-art technology (for this project compression tank storage was calculated at a maximum pressure of 750 bar).

Considering this difference in operating pressure, and that increasing character of impact in operation for the curve approach, some case studies using that operate on lower pressures may not require the implementation of the curve to achieve acceptable precision in results, as the expression es exponential.

To assess the need of this approach in other models, an early analysis can be performed prior to the main simulation. The use of the constant cost and curve approaches to evaluate the potential precision lost due to the simplification of the compression curve may be an essential step in future projects, aiming to justify the simplification made by the constant cost approach.

6.1.3 OPERATING DIFFERENCES ACROSS MODELS

The results obtained, especially in the base case simulation, sustain the fact that curve approach increases operating versatility. For example, a high energy price can become profitable for the curve approach if LoH is low, as power consumption would be minimal in that instant, however, constant curve approach would not operate on that time as its power consumption is decoupled from LoH levels.

The implications of this difference between models are obvious (as shown in results section) as constant cost models rely on negative prices to store hydrogen (~55% for base case and ~70% for double capacity) in contrast to curve storage (~13% for base case and ~8% for double capacity).

When creating an optimization model that uses energy price fluctuation to generate profit, via storage, this approach must be used. In compression storage technologies, as constant storage cost models pass on most opportunities due to oversimplification. On this situation, model precision increases justify the added computer effort required for reaching optimal solutions.

6.1.4 MARKET SCALE STORAGE OPTIONS

Following the presented objectives, current literature regarding hydrogen storage optimization model focused on single technology storage. This project aimed to represent more than one technology and evaluate their potential and combination at a national market scale.

The results obtained across the different simulations performed show that compressed cave storage represents the best option for storing large amounts (the order of tens of thousands of tons) for long periods of time. This method of storing energy could bring increased stability to the electricity market, increasing potential consumption during excess energy hours (especially during daytime due to the increase in solar installed power of the last decade) and reverse that electrolysis to generate energy (via fuel cell or hydrogen CCPP), creating a new source of stable power, and therefore reducing dependance on gas-powered CCPP.

Even though long-term storage need would be covered by this technology, compressed tank storage will also play an important role in short term market regulation, offering no limitation in potential inflows/outflows. The increased versatility of this technology would enable it as a secondary source of storage to work alongside cave storage, but on a smaller scale.

6.1.5 ACCURACY RELATIVE TO COMPUTATIONAL COST

The simulations performed showed that the curve approach increases around 30 times the total simulation time required to reach optimality to the GAMS non-linear solver. The increase on precision of the curve approach has proven to be important and changing results obtained and operating patterns.

Regarding operating differences, constant models have shown a tendency to underestimate storage power consumption, showing a difference of around 10% of extra cost when modeling using the compression curve. From the perspective of a market agent, the total storage cost of a kilo of hydrogen obtained in this project can range as much as ~0,04 € to ~0,3 € depending on storage technology and model used. Considering the current hydrogen price of 5 €/Kg, this difference becomes less important.

This type of agent may prefer a finer representation of the electricity and hydrogen market, rendering less important the storage cost, as it represents a relatively small amount in the total cost incurred on hydrogen production.

On the other hand, an agent that dedicates exclusively to hydrogen storage will find that difference of ~0,04 € to ~0,3 € to justify the extra computational cost of a fine representation. For this agent, the use of a realistic model can mean to multiply the total cost incurred by 7,5 times, regardless of the generation cost or the market price of hydrogen.

This differentiation shows that different agents can profit or not from the use of this model, therefore, this approach represents an extra tool than must be considered. However, storage cost has a limited impact on total cost, so the benefit will not always cover the added cost.

6.1.6 OPERATING PATTERNS BENEFITS

The results of the simulations show that when storage average LoH is closer to the 50% mark, the difference between the constant cost and curve approaches is reduced. From this observation a key conclusion can be extracted: if operating pressures of a storage facility range in a known and relatively narrow region, the use of a cost curve approach renders inefficient. For example, in the case of a compressed tank that shows patters of operating most of the time in the range of 500-600 bar, the use of a constant cost approach of 550 bar may bring accurate enough results at a fraction of the computational cost of modelling the full 0-1000 bar curve.

The curve approach offers a generalist view that will bring accurate results in all cases. However, identifying patterns in storage, if possible, can bring important simplifications to the model resolution without compromising precision in results.

6.2 OBJECTIVES COMPLETION

The objectives presented in the definition of the project section have guided the development of this project. On this section the proposed objectives will be presented and explained their degree of completion.

6.2.1 MODEL DEVELOPMENT

Regarding the first objective, it stated: "*Development of a hydrogen optimization model that computes storage costs following the thermodynamic compression curve*". The representation of the compression curve directly and as precise as possible has always been the aim of this project. Even though during the resolution approach some potential simplifications were considered, the curve itself proven to be the best cost-reward option for this model. The full mathematical expression of the compression curve was computed on the final model, so this objective has been completed entirely.

6.2.2 OPERATING DIFFERENCES QUANTIFICATION

The second of the proposed objectives stated: "*Quantify operating differences of using this approach*." Not only have the operative characteristics of this model been quantified, but also for the constant approach. This method enabled a comparison between the constant cost and cost curve approaches and performed a cost-reward analysis to justify the use (or not) of this thermodynamic approach to compression costs modeling. Considering these results, this objective is believed to be fulfilled.

6.2.3 STORAGE CENTERED MODEL

The third objective proposed for this project stated: "*Development of a model centered on the storage phase*." For this aim, the variable structure of the base model was modified to compute the storage costs on an independent way, maximizing result traceability. Following this objective, and considering the state-of-the-art review, technical studies showed the importance of leakage in hydrogen storage, however most of modeling references did not consider these losses on the hydrogen flows proposed. This project included this aspect of hydrogen storage aiming to maximize the precision of the model. The inclusion of storage leakage showed to have no relevant impact in overall model complexity, therefore further projects of this aim may include this characteristic on their models.

Considering this new contribution from this project, this objective would be completed entirely.

6.2.4 MULTIPLE TECHNOLOGY MODELED

The last of the proposed objectives stated: "*Modeling of several different storage technologies*." For this aim, following the current storage technologies that were identified on the state-of-the-art review, all the methods that had reached a level of maturity for operating on a market scale were considered. Not only were they simulated independently, but also collectively, analyzing how they operate and coordinate. This analysis showed how cave storage will be the best option for long term storage, aligning with the current investment trends that project this technology to be the majority storage method by 2030. It

The presented contribution of this project covers entirely the reach of this last objective; therefore, it is completed.

6.3 FUTURE DEVELOPMENTS

Even though the objectives presented in this project have been covered, during the execution phase, several potential future developments have been identified.

6.3.1 MARKET INTERACTIONS MODELING

The definition of this project, following the trends of the rest of modeling references consulted, considered the energy prices as an exogenous parameter, and hydrogen cost was not considered as the aim of the model was cost minimization.

However, the scale of the power consumptions of hydrogen by 2030, of 12 GW, considering that the average peak demand of Spain's peninsular system is around 38 GW [55], the power consumption of the electrolysis infrastructure would influence energy price, rather than taking it as an input. The same logic applies to the hydrogen market, as a high hydrogen price can justify incurring higher costs for generation.

Considering these aspects, the inclusion of this thermodynamic approach in a more complex model that computes price in a profit maximization model will constitute an interesting continuation to the conclusions presented in this project.

6.3.2 NEW STORAGE TECHNOLOGIES

Even though this project considered the three hydrogen storage technologies that would be feasible on a market scale, state of the art review showed how there are other storage technologies that offer interesting characteristics: specially transformative methods like ammonia (see Table 2) or adsorption based methods (see Table 3) that offer interesting operating characteristics.

As development advances rapidly, as big investments are being made in hydrogen technologies, many of these technologies may be more competitive in a couple years, and they may be considered as well as feasible storage options in projects of this nature.

Furthermore, shifting away from hydrogen-based models like this, other energy storage technologies may be represented like hydroelectric pumping or BESS could be modeled in combination with storage technologies to create a full market model.

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ANNEX I – FULL GAMS CODE

```
**FINAL DEGREE PROJECT - A THERMODYNAMIC APPROACH TO HYDROGEN STORAGE COST
OPTIMIZATION
**BY ALEJANDRO MONTERO DIAZ


* SETS DECLARATION
Sets
    d   'days of the year' /D1*D366/
    h   'hours of the day' /H1*H24/
    t   'storage technologies' /COMPT,COMPC,LIQ/;
   alias(d,pd)
   alias(h,ph)
;
*SCALARS DECLARARTION

Parameter
    CAP_ELE 'Electrolysis installed power [MW]'
    EH2 'Conversion MWh->ton h2 [ton h2/MWh]'
    E_ELE 'Electrolyzer efficiencies'
    E_FC 'Fuel Cell efficiency'
    CH_ELE 'Variable Cost of storage [€/ton h2]'
    CH_GREY 'Variable cost of grey hydrogen [€/ton h2]'
    CAP_GREY 'Daily generation capacity of grey hydrogen [ton h2/day]'
    CAP_FC 'Installed Fuel cell power [MW]'
    CH_FC 'Variable cost of fuel cells [€/MWh]'
    K_STO 'Constant of compression curve'
    EXP_STO 'Power of compression curve'
;

$call gdxxrw Parametros.xlsx output=Scalars.gdx par=CAP_ELE rng=Escalares!C2
rdim=0 cdim=0 par=EH2 rng=Escalares!C3 rdim=0 cdim=0 par=E_ELE
rng=Escalares!C4 rdim=0 cdim=0 par=E_FC rng=Escalares!C5 rdim=0 cdim=0
par=CH_ELE rng=Escalares!C6 rdim=0 cdim=0 par=CH_GREY rng=Escalares!C7
rdim=0 cdim=0 par=CAP_GREY rng=Escalares!C8 rdim=0 cdim=0 par=CAP_FC
rng=Escalares!C9 rdim=0 cdim=0 par=CH_FC rng=Escalares!C10 rdim=0 cdim=0
par=K_STO rng=Escalares!C11 rdim=0 cdim=0 par=EXP_STO rng=Escalares!C12
rdim=0 cdim=0
$gdxIn Scalars.gdx
$load CAP_ELE
```

```
$load EH2
$load E_ELE
$load E_FC
$load CH_ELE
$load CH_GREY
$load CAP_GREY
$load CAP_FC
$load CH_FC
$load K_STO
$load EXP_STO
$gdxIn

*PARAMETERS DECLARATION

Parameter

    H2_DEM(d) 'Daily hydrogen demand'
    H2_CAP(t)  'Storage capacities [ton h2]'
    EP_ELE_STO(t)'Storage power efficiency'
    LEAK_STO(t)'Daily rate of hydrogen leakage'
    CH_STO(t)'Variable cost of storage, excluded energy'
    START_CAP(t) 'Initial storage LoH'
    STO_FLOW(t) 'Storage flow limit [ton h2/hour]'
;

$call gdxxrw Parametros.xlsx output=Parametros.gdx par=H2_DEM
rng=Inputs!B4:C369 rdim=1 cdim=0 par=H2_CAP rng=Inputs!E4:F6 rdim=1 cdim=0
par=EP_ELE_STO rng=Inputs!H4:I6 rdim=1 cdim=0 par=LEAK_STO
rng=Inputs!H11:I13 rdim=1 cdim=0 par=CH_STO rng=Inputs!K11:L13 rdim=1 cdim=0
par=OC_STO rng=Inputs!E18:F20 rdim=1 cdim=0 par=START_CAP rng=Inputs!E25:F27
rdim=1 cdim=0 par=STO_FLOW rng=Inputs!N11:O13 rdim=1 cdim=0

$gdxIn Parametros.gdx
$load H2_DEM
$load H2_CAP
$load EP_ELE_STO
$load LEAK_STO
$load CH_STO
$load OC_STO
$load START_CAP
$load STO_FLOW
$gdxin
```

```
*TABLES DECLARATION

Parameter

   PRICE_BUY(d,h) 'Energy buy prices'
   PRICE_SELL(d,h) 'Energy sell prices'

;
$call gdxxrw Parametros.xlsx output=BUY.gdx par=PRICE_BUY
rng=Precios_BUY!B2:Z368 rdim=1 cdim=1
$gdxin BUY.gdx
$load PRICE_BUY
$gdxIn

$call gdxxrw Parametros.xlsx output=SELL.gdx par=PRICE_SELL
rng=Precios_SELL!B2:Z368 rdim=1 cdim=1
$gdxin SELL.gdx
$load PRICE_SELL
$gdxIn


Variable
    z
;
Positive Variable

    h2_ele(d,h) 'h2 generated by electrolysis'
    h2_grey(d,h) 'h2 generated chemically'
    h2_sto(d,h,t) 'h2 stored in every tech'
    h2_unsto(d,h,t) 'h2 unstored to generate power'
    loh(d,h,t) 'loh of every storage'
    dh2s_gen(d,h) 'h2 generated shiped directly to demand'
    dh2s_sto(d,h,t) 'h2 unstored to cover demand'
    lh2_sto(d,t) 'deily leakage if hydrogen'
    pow_ele(d,h) 'power consumption of electrolyzers'
    pow_fc(d,h) 'power generation of fuel cells'
    pow_sto(d,h,t) 'power consumption of storage'
    var_cost(d,h) 'total hourly variable cost'
    cons_sto(d,h,t) 'power consumption of every storage following curve
apprach'
    sto_pres(d,h,t) 'storage pressure of every technology'
    sto_cost(d,h,t) 'total cost of storage'
    gen_cost(d,h) 'total cost of generation'
```

```
;

***VARIABLE BOUNDARIES
pow_ele.up(d,h) = CAP_ELE;
pow_fc.up(d,h) = CAP_FC;
loh.up(d,h,t)=H2_CAP(t);
h2_unsto.up(d,h,t)=STO_FLOW(t);
dh2s_sto.up(d,h,t)=STO_FLOW(t);

**FINAL LOH IS EQUAL TO BALANCE
loh.fx('D366','H24',t)=START_CAP(t);
**FIXED LIQUID STORAGE CONSUMPTION
cons_sto.fx(d,h,'LIQ')=1.3;

Equation
*GENERATION AND DEMAND BALANCES
    Grey_Limit(d) 'Daily limit of grey hydrogen'
    Demand_Balance(d) 'Daily demand balance'
    Generation_Balance(d,h) 'Hourly balance of generation'

*STORAGE
    Storage_Balance_0(t) 'First period of the storage balance'
    Storage_Balance_1(d,t,pd) 'First hour of the day storage balance'
    Storage_Balance_2(d,h,t,ph) 'Hourly balance of storage'
    Leakage(d,t) 'Hydrogen lost by leackage'
*COST CALCULATION
    Tank_pressure(d,h) 'Calculates tank pressure'
    Cave_pressure(d,h) 'Calculates cave pressure'
    Consumpltion_Calculation(d,h,t) 'Power consumption of storages'
*OBJECTIVE FUNCTION
    Generation_Cost(d,h) 'Total cost of generation'
    Storage_Cost(d,h,t) 'Total cost of storage'
    Variable_Costs(d,h) 'Total variable costs'
    Energy_Electrolyzer(d,h) 'Power cosumption of electrolyzers'
    Energy_Storage(d,h,t) 'Power consumption of storage'
    Energy_Generated(h,d) 'Energy sent back to grid'
    OF
;
***CONSTRAINTS

*GENERATION AND DEMAND BALANCES
Grey_Limit(d)..
sum(h,h2_grey(d,h))
```

```
=L=
CAP_GREY;

Demand_Balance(d)..
H2_DEM(d)
=E=
sum(h,dh2s_gen(d,h)+(sum(t,dh2s_sto(d,h,t))));

Generation_Balance(d,h)..
h2_ele(d,h)+h2_grey(d,h)
=E=
sum(t,h2_sto(d,h,t))+dh2s_gen(d,h);

*STORAGE
Storage_Balance_0(t)..
loh('D1','H1',t)
=E=
START_CAP(t)+h2_sto('D1','H1',t)-
(dh2s_sto('D1','H1',t)+h2_unsto('D1','H1',t))-lh2_sto('D1',t)/24;

Storage_Balance_1(d,t,pd)$(ord(pd)=ord(d)-1)..
loh(d,'H1',t)
=E=
loh(pd,'H24',t)+h2_sto(d,'H1',t)-(dh2s_sto(d,'H1',t)+h2_unsto(d,'H1',t))-
lh2_sto(d,t)/24;

Storage_Balance_2(d,h,t,ph)$(ord(ph) = ord(h) - 1)..
loh(d,h,t)
=E=
loh(d,ph,t)+h2_sto(d,h,t)-(dh2s_sto(d,h,t)+h2_unsto(d,h,t))-lh2_sto(d,t)/24;

Leakage(d,t)..
lh2_sto(d,t)
=E=
(sum(h,loh(d,h,t))/24)*LEAK_STO(t);

*COST CALCULATION
Tank_pressure(d,h)..
sto_pres(d,h,'COMPT')
=E=
(loh(d,h,'COMPT')/H2_CAP('COMPT'))*750;

Cave_pressure(d,h)..
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```
sto_pres(d,h,'COMPC')
=E=
(loh(d,h,'COMPC')/H2_CAP('COMPC'))*250;

Consumpltion_Calculation(d,h,t)..

cons_sto(d,h,t)
=E=
K_STO*(sto_pres(d,h,t)**EXP_STO-1);

*OBJECTIVE FUNCTION
Variable_Costs(d,h)..
var_cost(d,h)
=E=
gen_cost(d,h)+sum(t,sto_cost(d,h,t));

Energy_Electrolyzer(d,h)..
pow_ele(d,h)
=E=
(h2_ele(d,h)/EH2)/E_ELE;

Energy_Storage(d,h,t)..
pow_sto(d,h,t)
=E=
h2_sto(d,h,t)*cons_sto(d,h,t)/EP_ELE_STO(t);

Energy_Generated(h,d)..
pow_fc(d,h)
=E=
(sum(t,h2_unsto(d,h,t))/EH2)*E_FC;

Generation_Cost(d,h)..
gen_cost(d,h)
=E=
CH_ELE*h2_ele(d,h)+CH_GREY*h2_grey(d,h)+pow_ele(d,h)*PRICE_BUY(d,h);

Storage_Cost(d,h,t)..
sto_cost(d,h,t)
=E=
h2_sto(d,h,t)*CH_STO(t)+pow_sto(d,h,t)*PRICE_BUY(d,h);

OF..
z
```

```
=E=
sum((d,h), var_cost(d,h) - pow_fc(d,h)*PRICE_SELL(d,h)+pow_fc(d,h)*CH_FC);

Model HydrogenStorage /all/;
Solve HydrogenStorage using NLP  Minimizing z;
```