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*Master Thesis*

# Techno-economic model for Power-to-X hybrid plants

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## SUMMARY

The current shift towards decarbonization have fostered the study and implementation of hydrogen as a clean energy carrier. In a scenario of high renewable penetration in the electricity mix, electrolysis can take advantage of curtailments and produce low carbon hydrogen, which can then be used in other intensive carbon sectors where renewable electricity implementation is not feasible, i.e. chemicals production, high-heat industrial processes or transportation.

Hydrogen projects promoters face huge risks due to high Capital Expenditures (CAPEX) intensity, volatility of electricity prices and low maturity of electrolyzers. Risks can be reduced by performing pre-feasibility studies with the appropriate tools. In this work an algorithm capable of calculating the optimal hourly dispatch of Power-to-X and hydrogen plants has been developed. The model can be easily adapted to switch between configurations -in this work, a green ammonia synthesis plant and a green hydrogen production plant for direct injection into the European Hydrogen Backbone (EHB) are simulated to showcase this feature.

The algorithm takes into account the owned renewable production and the grid prices to find the minimum cost solution to produce the required quantity of derivative product or hydrogen set by the user. Furthermore, a cutting-edge method for implementing both the electrolysis non-linear efficiency curve and the different states of the electrolyzer has been included, diverging from the state-of-the-art solutions. Additionally, Battery Energy Storage Systems (BESS) degradation has been modelled as well.

The algorithm implementation onto Pyomo and Gurobi showcases that an optimal solution can be found in polynomial time, allowing for real time operations thus enabling its use in Power-to-X and electrolysis plants Energy Management Systems (EMS).

The studied cases highlight the harsh scenario of hydrogen projects, finding it difficult to reach profitability while maintaining low levels of risk. Hence, financial and regulatory aids must be implemented to promote hydrogen implementation as green energy carrier.

**Keywords: Hydrogen Economy, Mathematical Optimization, Energy Transition, Feasibility Study**

## RESUMEN

El actual giro hacia la descarbonización ha impulsado el estudio y la implementación del hidrógeno como vector de energía limpia. En un escenario futuro de alta penetración renovable en el mix eléctrico, la electrólisis puede aprovechar los vertidos para producir hidrógeno, que puede ser usado más tarde en sectores con una alta huella de carbono donde la implementación de electricidad renovable no es posible, como la industria petroquímica, procesos industriales con grandes requerimientos de calor o el sector del transporte.

Los promotores de proyectos de hidrógeno se enfrentan a grandes riesgos debido a la naturaleza altamente intensiva en CAPEX de dichos proyectos, a la alta volatilidad de los precios de la electricidad y a la poca madurez tecnológica de los electrolizadores. Estos riesgos pueden ser mitigados mediante estudios de viabilidad que utilicen las herramientas adecuadas. En este trabajo se desarrolla un algoritmo capaz de calcular el despacho horario óptimo de plantas Power-to-X y de producción de hidrógeno. El modelo puede ser fácilmente adaptado para simular la configuración deseada; por ejemplo, en este trabajo se analiza una planta de producción de amoníaco verde y otra planta de producción de hidrógeno para su inyección en el European Hydrogen Backbone.

El algoritmo tiene en cuenta la producción de las plantas renovables y los precios de electricidad en la red para buscar la solución de mínimo coste, produciendo la cantidad anual de producto derivado o de hidrógeno que el usuario desee. Se implementa un método innovador para poder modelar correctamente la naturaleza no lineal de la curva de eficiencia de los electrolizadores, así como los diferentes estados en los que puede encontrarse, difiriendo así de las soluciones propuestas en la literatura. Adicionalmente, se ha modelado la degradación de las baterías electroquímicas.

La implementación del algoritmo en Pyomo y Gurobi muestra que la solución óptima puede alcanzarse en tiempo polinómico, permitiendo así el uso de la herramienta en operaciones en tiempo real, como en EMS de plantas Power-to-X o de producción de hidrógeno.

Los casos de estudios analizados en el trabajo demuestran la dificultad de encontrar proyectos rentables de hidrógeno manteniendo unos niveles de riesgo bajos. Como consecuencia, tanto ayudas financieras como un mejor marco regulatorio se vuelven necesarios para promover la implementación del hidrógeno como vector energético.

**Keywords: Economía del Hidrógeno, Optimización Matemática, Transición Energética, Estudio de Viabilidad**

*Man betrays themselves if they fail to realize that their destiny is to know*

**Antonio Escobedo**

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# 1. INTRODUCTION

## 1.1. Historical context

In recent years, the global energy landscape has undergone a transformative shift towards sustainability and decarbonization. This transition is driven by the urgent need to combat climate change, as underscored by international agreements such as the *Paris Agreement*, adopted in 2015 [1]. The *Paris Agreement* aims to limit global warming to well below 2 degrees Celsius above pre-industrial levels, necessitating a significant reduction in greenhouse gas emissions. As a result, nations worldwide have committed to increasing their share of renewable energy in the overall energy mix, fostering innovations in green energy technologies and implementation strategies.

Further efforts have been made specifically in the European Union for the last 5 years. The first of them is the *Fit for 55* package, a comprehensive set of legislative proposals aimed at ensuring the EU meets its target of reducing net greenhouse gas emissions by at least 55% by 2030 [2]. On the other hand, the *REPowerEU* plan, introduced in response to the urgent need to reduce dependency on fossil fuels, particularly in light of geopolitical tensions, aims to diversify energy supplies and increase the use of renewable energy [3]. It emphasizes the expansion of renewable energy capacity, energy efficiency measures, and the acceleration of hydrogen production and infrastructure development.

As a consequence of these events, hydrogen has emerged as a pivotal element in this green energy transition. Historically, Europe has been heavily dependent on fossil fuel imports, particularly natural gas from politically volatile regions. The transition to hydrogen, especially green hydrogen produced via electrolysis using renewable energy sources, reduces this dependency. By developing domestic hydrogen production capabilities, Europe can decrease its reliance on imported fossil fuels, thus mitigating the geopolitical risks associated with energy supply disruptions. This shift also allows Europe to exert greater control over its energy future, reducing vulnerability to external political and economic pressures.

Particularly, Spain aims to become one of the main hubs of Europe in the production of green hydrogen after the release of the *National Energy and Climate Plan of 2023*. In this document, the importance of hydrogen is highlighted in sectors such as industry, refineries, transportation or electricity generation, although the main bet for Spain is the great demand response electrolysis provides [4].

## 1.2. Hydrogen production and its uses

Throughout the 20th century, the industrial production of hydrogen with Steam Methane Reforming (SMR) became the dominant method due to its cost-effectiveness and scalability. However, SMR relies on natural gas and emits significant amounts of carbon dioxide, prompting the search for cleaner alternatives. The late 20th and early 21st centuries saw renewed interest in electrolysis, particularly with the development of advanced electrolyzer technologies such as Anion Exchange Membrane (AEM) and Proton Exchange Membrane (PEM) systems. These innovations have significantly improved the efficiency and feasibility of producing green hydrogen, positioning it as a key player in the global energy transition aimed at reducing carbon emissions and achieving sustainability.

AEM electrolysis, a well-established technology in the chemical industry, uses an aqueous solution of potassium hydroxide as the electrolyte, which enhances conductivity and minimizes energy loss at the anode. This method is notable for its simplicity and capability for large-scale hydrogen production [5]. Alkaline electrolyzers have been demonstrated to produce hydrogen efficiently over the last century.

On the other hand, PEM electrolysis operates on the principle inverse to that of PEM fuel cells, using a solid polymer membrane as the electrolyte. This technology is distinguished by its low operational temperature, reduced maintenance requirements due to the absence of a liquid electrolyte, and high efficiency. PEM systems can operate at high current densities for extended periods, and they are capable of rapid start-up and part-load operations, making them highly adaptable to the dynamic energy supply renewable sources provide.

Despite these promising applications, current electrolysis systems face challenges related to efficiency, cost, and operational durability. Improving the lifetime of electrolyzer stacks, enhancing energy efficiency, and reducing both capital and operational expenditures are critical areas for ongoing research and development.

Hydrogen produced through electrolysis has a variety of strategic uses. In the mobility sector, hydrogen can supply Fuel Cell Electric Vehicles (FCEVs), providing a clean alternative to conventional internal combustion engines. Additionally, hydrogen can be utilized for re-electrification through fuel cells, offering a viable solution for energy storage and power generation in remote locations, military applications, and as a support mechanism for weak electrical grids. Furthermore, hydrogen can be injected into the natural gas network, providing a greener alternative to natural gas and leveraging existing infrastructure for energy storage.

### 1.2.1. Power-to-X

The concept of Power-to-X (PtX) encompasses a range of processes that convert electrical power into other forms of energy carriers, such as hydrogen (Power-to-Hydrogen),

synthetic fuels (Power-to-Fuels), or chemicals (Power-to-Chemicals). These processes enable the integration of renewable electricity into sectors that are challenging to electrify directly, such as transport, industry, and heating.

The importance of Power-to-X lies in its potential to enhance energy system flexibility and stability while contributing to the decarbonization of various sectors. Europe, in particular, has recognized the strategic value of PtX technologies in achieving its ambitious climate goals. The European Union's Green Deal, for instance, sets forth a comprehensive plan to make Europe the first climate-neutral continent by 2050. Within this framework, hydrogen and PtX technologies are highlighted as critical components for reducing emissions, improving energy security, and fostering economic growth.

By converting surplus renewable electricity into storable and transportable energy carriers, PtX not only mitigates the intermittency challenges associated with renewable energy sources but also supports the decarbonization of hard-to-abate sectors:

1. In the chemical industry hydrogen has been used for decades, so the current main efforts focus on changing the origin of this hydrogen i.e. from steam reforming to water electrolysis. The main pioneer example in Spain is Fertiberia's facility based in Puertollano, dedicated to the production of fertilizers. Fertiberia has been using hydrogen from steam reforming -known as grey hydrogen, since the sixties to obtain fertilizers. On 2022, they began to obtain green hydrogen thanks to the construction of a 20 MW electrolyzer, one of the biggest in the world at that time.
2. In petroleum refineries, progress has also been made to use green hydrogen as input. In the region of Castellón, British Petroleum is investing huge amounts of capital in achieving this goal. The application of this new method in refineries means cleaner fossil fuels.
3. In industrial processes that require high temperatures, the current solution is to burn gas or coal to produce heat. For instance, the world's largest steel manufacturer, ArcelorMittal, is investing in reducing its carbon footprint by introducing green hydrogen in its processes in a joint-venture known as HyDeal.
4. Sustainable fuels production, although not mainstream, is one promising application of hydrogen, with many luxury car manufacturers such as Porsche and Lamborghini pushing forward as a way to fit internal combustion engines in the net-zero future. In Spain, the chemical valley of Huelva will gain importance thanks to green methanol, which is planned to be introduced as container ships fuels, substituting diesel.

Power-to-X represents a versatile and promising approach to advancing the green energy transition. By harnessing renewable energy to produce green hydrogen and other sustainable fuels, PtX can play a crucial role in achieving Europe's climate objectives, fostering innovation, and promoting a sustainable energy future.

### 1.3. Motivation and objectives

Introducing green hydrogen consumption in industry processes is highly intensive in CAPEX, requiring great amount of initial investment in technologies that are not mature yet. To protect themselves -and investors from the risks of entering the green hydrogen market, companies usually perform what is called pre-feasibility studies. This consists on a preliminary assessment of the plant operation, and how it may behave under dynamic conditions.

The current challenge lies on the electrolysis process, which has varying efficiencies and degradation depending on the load-factor and the conditions it runs in. These two metrics will impact, on one side, the time before a replacement of the electrolyzer must happen, and the output product. With such high prices on electrolyzers -specially PEMs, and in green hydrogen and its derivatives, these become pivotal parameters to account for in any pre-feasibility study, as these will greatly impact the profitability of the project.

As more elements are added, such as batteries, variable renewable supply, hydrogen storage, the assessment becomes more difficult, requiring big models. Not only these models must be capable of doing the proper energy balances, but also they must be intelligent enough to fully use any elements in the system to search profitability -for example, use the battery to perform arbitrage if possible.

At this date, these intelligent solutions for Power-to-X processes are scarce in the industry and in academics. This works pretend to fill this gap by developing a mathematical framework which is then implemented in Python.

Additionally, with the introduction of Power-to-X processes in the several industry sectors explained before, the industry will not only depend on the highly volatile wholesale price of electricity, as it has been for the last few years - they will also suffer from fluctuations in the availability of its feedstock i.e. hydrogen. As a consequence, they will both need to forecast electricity prices and hydrogen availability, which will greatly depend on renewable production and also wholesale grid prices.

Companies will need to update their EMS to account for all these phenomena and interactions. The developed algorithm may also fill this gap by performing continuous calculations, taking as input the latest electricity price and renewable production forecasts and providing to the EMS the optimal dispatch solution.



## 2. MODEL FORMULATION

In this chapter an insight on the mathematical formulation of the model will be provided. To do so, a brief introduction to *mathematical programming* and *microeconomics* is given in section 2.1 to provide necessary background. Then, on section 2.2 each of the elements of the plant will be explained along how they are included in the model via constraints in the optimization problem. The objective function is shown on section 2.3, and the implementation method on section 2.4.

### 2.1. Introduction. The cost minimization problem

To understand the reasoning and motivation behind the modelling of our hybrid PtX plant firstly it will be needed to break down the hybrid plant. As it stands, the system consists of a set of generators and energy storage systems connected to an electrolyzer which will supply hydrogen to the demand point or store it for later use -in other words, a transformation facility which purchases a commodity, transforms it, and supplies the product to some demand.

Let  $x$  be the amount resources consumed,  $y$  the quantity produced, and  $a$  and  $b$  prices associated with those products. Obviously, the producer will look to maximize its revenue, giving the following linear optimization problem:

$$\max_{x,y} \quad b \cdot y - a \cdot x \quad (2.1a)$$

The electrolyzer plant will be coupled to an inelastic demand denoted as  $D$  such as an ammonia production plant depending on hydrogen to produce fertilizers, or a hydrogen fuelled container ship. Thus, the quantity produced  $y$  will be constant and can be removed from the objective function (2.1a). Therefore, the operation of the facility will amount to maximize the negative of the costs, i.e. to minimize the costs, so the optimization problem becomes:

$$\min_x \quad a \cdot x \quad (2.1b)$$

$$\text{subject to} \quad y(x) = D \quad (2.1c)$$

This formulation allows the modeler to work without a priori knowledge of the hydrogen price, differing from the models in the state of the art [6] [7] [8] [9], which usually require information about the prices of the commodities being traded.

Additionally, this formulation provides an elegant way of obtaining the hydrogen production price taking advantage of *Duality Theory* by the so-called *dual variables* or *Lagrangian multipliers*.

Duality theory establishes a relationship between the primal optimization problem  $\mathcal{P}$  and its corresponding dual problem  $\mathcal{D}$ . For a given primal problem, the dual problem provides a lower (upper) bound on the optimal value of the primal minimization (maximization) problem. The difference between the solutions of both problems is known as duality gap. This gap is zero for *Linear Problems* (LP), so solving one problem also gives the solution of the other problem, as seen on Fig. 2.1. For *Mixed-Integer Linear Problems* (MILP), this difference is non-zero.

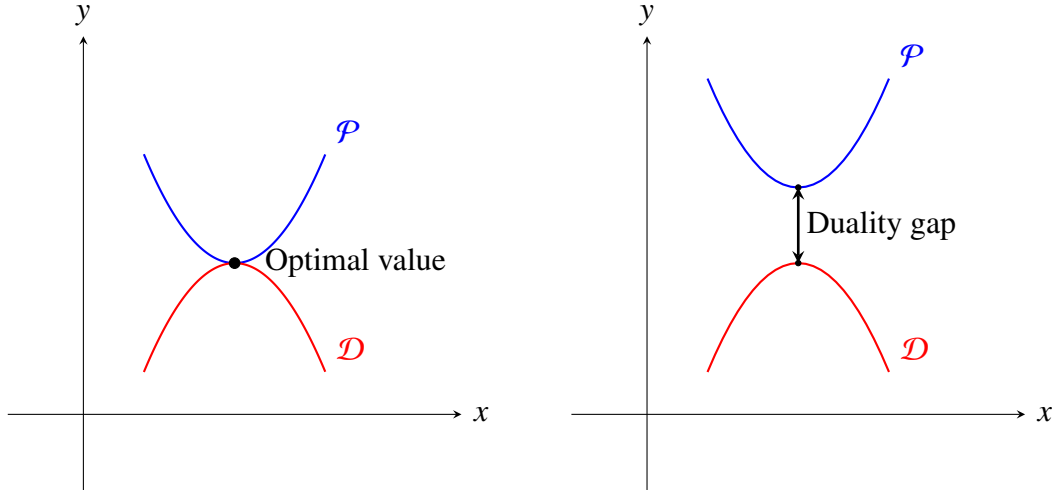


Fig. 2.1. Primal and dual problems in LP (left) and MILP (right)

More importantly for this work, the variables of the dual problem, called dual variables, are associated with a constraint of the primal problem, describing how a marginal change in that constraint affects the primal problem's objective function.

For this case, the dual variable associated with the hydrogen demand constraint (2.1c) indicates how much costs will change when the hydrogen demand grows by one unit, this is, the marginal cost of the additional unit of hydrogen. By the *Complementary Slackness Theorem*, it is known that this dual variable will be non-negative, as it is associated with an equal-to constraint. This seems reasonable, as one should expect the costs to increase when the demand increases.

As one may think, the company producing hydrogen will not engage in producing that additional unit unless the consumer pays for that unit, at least, the increase in total cost, i.e. the value of the dual variable associated with the demand constraint. However, if the consumer paid more than this amount, the producer would obtain benefits, which cannot happen in perfectly competitive markets. Thus, the value given by the dual variable -the marginal cost, equals the marginal price in a perfectly competitive market.

Unfortunately, this convenient economic interpretation of Dual Theory only holds always true for LPs [10]. As the reader will see on Section 2.2, to enhance the modelling of electrolyzer by including states, ramps or a piece wise function for the efficiency curve, binary variables will be needed. This makes the problem become a MILP, for which the

duality gap is no longer zero, as seen on 2.1. This gap can be somewhat interpreted as the accuracy of the economic interpretation made in the MILP [11].

A smart workaround to this hurdle is to fix the binary variables to the optimal value obtained after solving. This way, an LP is obtained which can then be solved again to obtain a more accurate description of the marginal cost.

However, as binary variables become parameters in the objective function, the terms associated to those binary variables will no longer be optimized. Thus, the marginal costs obtained may not account for costs associated with these binary variables and cost recovery cannot be guaranteed. In our problem, these costs are BESS and electrolyzer degradation and electrolyzer start-up costs.

To sum up, the formulation provided is able to give a price for hydrogen in perfect competitive markets through the usage of dual variables or Lagrangian multipliers. If the formulation is upgraded to a mixed integer linear formulation, an additional solve fixing binary variables is needed to accurately obtain marginal prices.

## 2.2. Constraints

In this section it will be explained how each component's behavior will be modelled using constraints. For better understanding of the equations, variables, parameters and indices, the reader is encouraged to have a glance at the appendices.

For better understanding on the system to be modeled, a flow chart of a typical Power-to-X system is shown below. Usually, Power-to-X plants need grid connection to supply all the elements in the system. The on-site generators and Energy Storage Systems (ESS), if any, are able also to provide power to the electrolysis system, the H<sub>2</sub> compression and storage and the derivatives reactor. The hydrogen output from the electrolyzer can go directly towards the reactor, or if there is an excess of production, pass through the compressor and be stored in hydrogen tanks for future use.

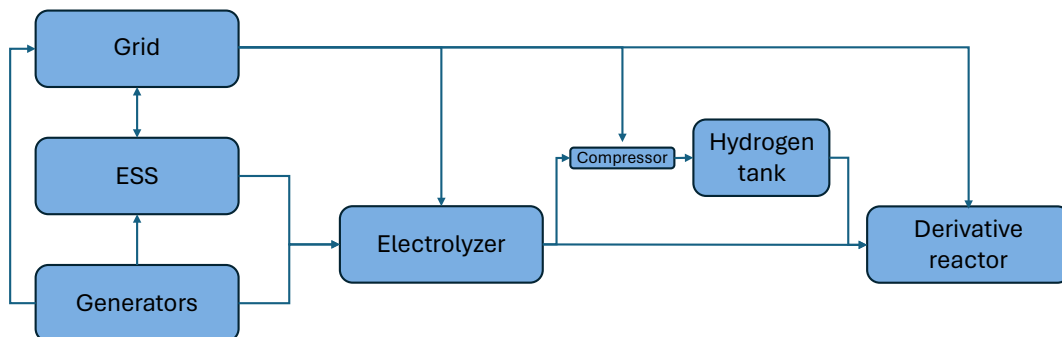


Fig. 2.2. Power-to-X system flow chart

### 2.2.1. Electrolyzer

The electrolyzer is the main component of Power-to-X systems. Although hydrogen has been used for decades now, electrolysis process fed with renewable energy is a really modern technology, so not many optimization algorithms that account for the synergies between variable electricity supply and electrolysis have been developed yet. As explained in the introduction, the most promising technologies are AEM and PEM, both of which have great flexibility and are able to adapt to the variability of sun and wind. For this reason, the model will focus on these types of electrolyzers. However, if other high-temperature electrolyzers with low flexibility wish to be included, one can easily adapt the model to include ramp ups and downs. The main points of this section are the modeling of 3 states to account for the degradation of the membrane and the non-linear model of the efficiency curve, which is quite scarce in the literature.

#### Electrolyzer states

As in Battery Energy Storage Systems projects, degradation is one key factor to account for, since it will greatly impact the revenues of the plant. In Power-to-X systems, the degradation of the membrane in the electrolyzer is also important, due to the high CAPEX of the stacks -specially on PEM technology. For this reason, it is clear that any optimization algorithm of Power-to-X plants should, one way or another, minimize the degradation of the membrane.

Degradation in low-temperature electrolyzers such as AEM or PEM occurs when start-stop operations are performed, or when the voltage falls below a certain limit [12]. To be able to model this, three states are defined:

1. On state: the electrolyzer produces hydrogen at a given load factor, which can go from a minimum set value to full nominal power. At this stage, the electrolyzer can perform ramp-ups and downs with no restrictions, allowing for great flexibility. When the electrolyzer  $h$  is at on state during time  $h$ , the variable  $z_{on}^{t,h}$  will be set to 1.
2. Stand-by state: when the power falls below the minimum limit for on state operation, the electrolyzer enter the stand-by state, and no hydrogen is produced. However, it does consume power to maintain pressure and temperature and be able to quickly enter on-state again. In this case, the variable  $z_{sb}^{t,h}$  will be set to 1.
3. Off state: no power is consumed nor hydrogen is produced. However, no flexibility exists as temperature and pressure are not being maintained, and the electrolyzer cannot resume production as quick as in stand-by state. Although ramps are high in AEMs and PEMs -in the order of 10% of nominal power per second [13], going from off state to on state means augmented degradation. If the electrolyzer is at off state, the variable  $z_{off}^{t,h}$  will be 0.

The three states are modeled with the following constraints:

$$z_{on}^{t,h} + z_{sb}^{t,h} + z_{off}^{t,h} = 1 \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H} \quad (2.2a)$$

$$z_{sb}^{t,h} + z_{off}^{t-1,h} \leq 1 \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H} \quad (2.2b)$$

While constraint (2.2a) ensures one and only one state at a given time, constraint (2.2b) forbids jumping from off state to stand-by state, as the algorithm could save the cold start-up cost by performing this operation. To count the number of cold start-ups, a new variable  $C_{coldstart}^{t,h}$  is defined as:

$$C_{coldstart}^{t,h} = z_{on}^{t,h} - z_{on}^{t-1,h} - z_{sb}^{t-1,h} \quad \forall t \in \mathcal{T} \setminus \{1\} \quad \forall h \in \mathcal{H} \quad (2.2c)$$

This counter is used in the objective function along with an economic cost per cold start induced to model the degradation of the electrolyzer properly.

## Electrochemical model

To be able to know how much hydrogen will be produced, one must know beforehand the efficiency of the electrolyzer. The most common approaches in the literature include setting a fixed parameter independent on the load factor of the electrolyzer or modelling a linear efficiency curve, such as in [6], [7], [13], [14] or [15]. Furthermore, when several subprocesses with non-linear dependency on the load factor are involved, as in Power-to-X systems, the model becomes byzantine, and the computational burden increases.

The difference between linear and non-linear modelling of the electrolyzer's efficiency curve has been studied in the literature, showing decisive differences in operation and subsequently in the revenues, such as in [16] and [17]. Specifically for Power-to-X systems, any change in operation of the electrolyzer will greatly affect the degradation and operation of the downstream chemical processes. Also, the electricity consumption of water electrolysis in Power-to-X systems can represent 95% of the total. Consequently, modelling water electrolysis efficiency as accurately as possible is critical in any algorithm involving Power-to-X operations.

To achieve this, a non-linear function will be used in this work. As efficiency and hydrogen production curves are currently difficult to obtain from manufacturers, the semi-empirical model developed originally in [18] and later enhanced in [19] to account for the effects of pressure is used. The reader is referred to those works for a deeper analysis of the underlying physics of electrolysis.

First, the current-voltage curve can be found as function of temperature  $T$ , current density  $i$  and pressure  $pr$  as follows:

$$U_{cell} = U_{rev} + [(r_1 + d_1) + r_2 \cdot T + d_2 \cdot pr] \cdot i + s \cdot \log \left[ \left( t_1 + \frac{t_2}{T} + \frac{t_3}{T^2} \right) \cdot i + 1 \right] \quad (2.3a)$$

where  $U_{rev}$  is the reversible potential, and  $r_i$ ,  $d_i$ ,  $t_i$  and  $s$  parameters obtained empirically. The second term is associated with ohmic over-potential, while the third one with the activation over-potential. Hence, the power consumption density of the cell can be computed as:

$$P_{cell} = U_{cell}(i, T, pr) \cdot i \quad (2.3b)$$

Then, the area needed to achieve the desired capacity  $Cap$  is:

$$A = \frac{Cap}{P_{cell}(i_{max}, T_{op}, pr_{op})} \quad (2.3c)$$

where  $i_{max}$  corresponds to the maximum current density and  $T_{op}$  and  $pr_{op}$  to the operating temperature and pressure, respectively. The power consumed in the whole stack thereby can be calculated as:

$$P_{stack} = P_{cell} \cdot A \quad (2.3d)$$

Finally, the hydrogen production per hour in the stack  $f_{H2}$  can be obtained with the expression for the gas flow rate:

$$f_{H2} = \frac{i}{2F} \cdot \eta_f \cdot A \cdot 3600 \quad (2.3e)$$

where  $n_f$  represents the Faradaic efficiency:

$$n_f = \left( \frac{i^2}{f_{11} + f_{12} \cdot T + i^2} \right) \cdot f_{21} + f_{22} \cdot T \quad (2.3f)$$

Now, one can obtain the current density  $i_{min}$  at operating temperature and pressure corresponding to the minimum power at on-state with expression (2.3b). Evaluating expression (2.3e) from the minimum current density  $i_{min}$  to the maximum current density  $i_{max}$ , the hydrogen curve for all the operating range of the electrolyzer is obtained, which may be included in the model as a quadratic polynomial:

$$f_{H2} = Q_2 \cdot p_{H2}^2 + Q_1 \cdot p_{H2} + Q_0 \quad (2.3g)$$

where  $Q_2$ ,  $Q_1$  and  $Q_0$  refer to the quadratic coefficients and  $p_{h2}$  to the power consumed by the electrolyzer to produce hydrogen. It must be recalled that at stand-by state there is electricity consumption but no hydrogen production.

Only linear problems guarantee convexity, which is fundamental for solving optimization problems in a quick and reliable manner [20]. However, one should note that this expression is non-linear and non-convex. To overcome this issue, the quadratic approximation is relaxed into a second order cone -which can be solved in polynomial time, following the method described in [21]. Accounting for the electrolyzer states, the result is a *mixed-integer second order cone problem* or MISOCP. The constraints modeling the hydrogen production as a function of the power consumption are as follows:

$$f_{H2}^{t,h} = Q_2^h \cdot \varepsilon^h + Q_1^h \cdot p_{H2}^{h,t} + Q_0^h \cdot z_{on}^{t,h} \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H} \quad (2.4a)$$

where  $\varepsilon$  is the auxiliary conic variable:

$$\varepsilon^h \geq (p_{H_2}^{h,t})^2 \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H} \quad (2.4b)$$

Now, the electricity consumption at any given time of the electrolyzer is:

$$p_{total}^{t,h} = p_{H_2}^{h,t} \cdot z_{on}^{t,h} + P_{sb}^h \cdot z_{sb}^{t,h} \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H} \quad (2.4c)$$

$$P_{H_2,min}^h \leq p_{H_2}^{h,t} \leq P_{H_2,max}^h \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H} \quad (2.4d)$$

so that the consumption equals the stand-by power if the electrolyzer is at stand-by state ( $P_{sb}^h \cdot z_{sb}^{t,h}$ ) and the power used to generate hydrogen if at on state ( $p_{H_2}^{h,t} \cdot z_{on}^{t,h}$ ). Constraint (2.4d) enforces the power consumed at on state to be within the limits of minimum  $P_{H_2,min}$  and maximum  $P_{H_2,max}$  production

Representing the hydrogen production curve calculated using the electrochemical model (2.3e) and the corresponding quadratic approximation (2.3g) gives the following figure:

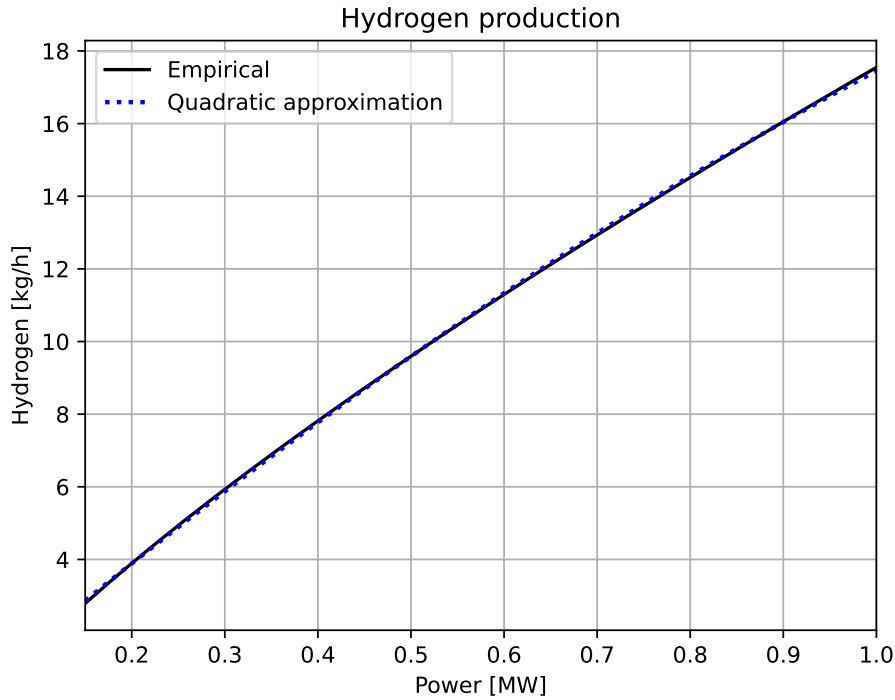


Fig. 2.3. Hydrogen production approximation

Dividing the hydrogen production curve obtained by each method by the power consumption in the whole stack at each intensity value gives the efficiency of the electrolyzer:

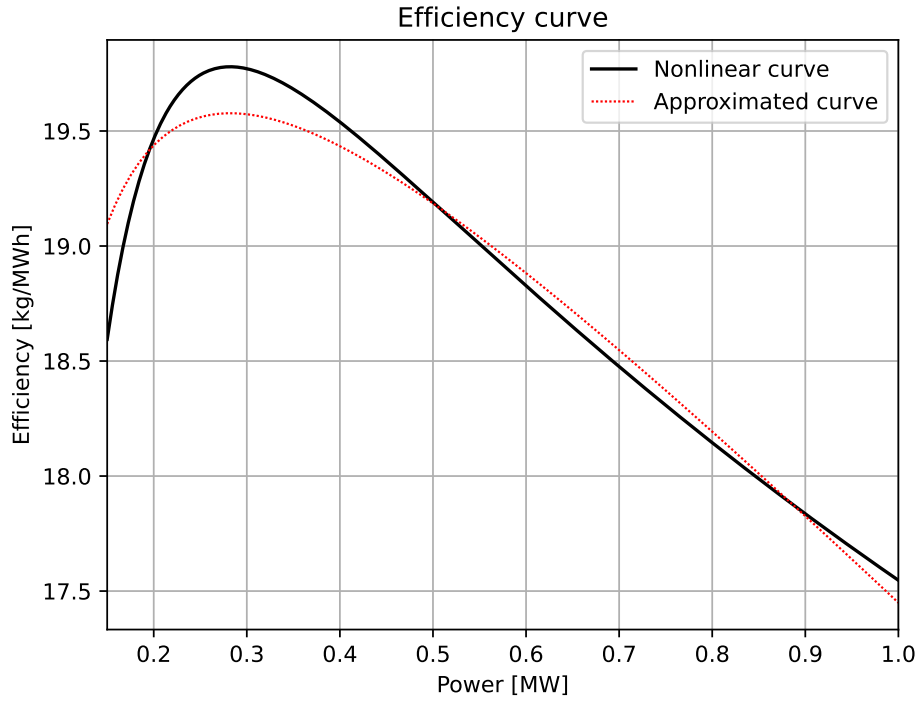


Fig. 2.4. Hydrogen efficiency approximation

### 2.2.2. Electricity production

The amount of electricity produced onsite to feed the electrolyzer can easily be modeled using a parameter for the maximum power, a production profile and some operating costs. If a non-renewable energy plant is used, one can set the capacity factor  $CF$  to 1 for the whole simulation horizon and include in the operating expenses the cost of the fuel. Additionally, the plant can be connected to the grid and get electricity when the generators are not available and sell when there is a surplus of energy.

The power generation  $p_{gen}^{t,g}$  of generator  $g$  at time  $t$  can be computed as:

$$p_{gen}^{t,g} \leq CF^{t,g} \cdot P^g \quad \forall t \in \mathcal{T} \quad \forall g \in \mathcal{G} \quad (2.5a)$$

where  $CF^{t,g}$  is the generator  $g$  capacity factor at time  $t$ , and  $P^g$  its maximum power output. The energy exchanged with the grid can be modelled with the following constraint:

$$-P_{export} \leq p_{grid}^t \leq P_{import} \quad \forall t \in \mathcal{T} \quad (2.5b)$$

where  $p_{grid}^t$  represents the power purchased from the grid if positive and sold to the grid if negative. Note that expression (2.5a) is not an equality constraint so that, in case of renewable generation, curtailment is allowed, and in case of conventional generation the power plant may or may not be at nominal power at any given time.



### 2.2.3. Energy Storage Systems

The model includes great flexibility for simulating a broad range of energy storage systems. Typical BESS can be modelled easily along with its degradation costs, as well as other technologies such as water pumping. The energy stored  $e^{t,s}$  in the ESS  $s$  during time  $t$  can be computed as:

$$e^{t,s} = e^{t-1,s} + \eta^s \cdot p_{in}^{t,s} - \frac{1}{\eta^s} \cdot p_{out}^{t,s} \quad \forall t \in \mathcal{T} \setminus \{1\} \quad \forall s \in \mathcal{S} \quad (2.6a)$$

$$e^{t,s} = E_{initial}^s \quad t = 1 \quad \forall s \in \mathcal{S} \quad (2.6b)$$

where  $e^{t-1,s}$  corresponds to the energy stored during the previous hour,  $\eta^s$  to the efficiency of the ESS, and  $p_{in}$  and  $p_{out}$  the energy entering and exiting the ESS, respectively. For the first hour, the energy inside the storage will be equal to the initial storage parameter  $E_{initial}$  chosen by the user, whereas during the rest of the time the state of charge follows a simple energy balance rule, with efficiency for both energy entering and exiting the system. Obviously, the energy stored in a certain hour must be between the minimum and the maximum storage allowed. Also, input power and output power must be below the limits imposed:

$$E_{min}^s \leq e^{t,s} \leq E_{max}^s \quad \forall t \in \mathcal{T} \quad \forall s \in \mathcal{S} \quad (2.6c)$$

$$p_{in}^{t,s} \leq P^s \quad \forall t \in \mathcal{T} \quad \forall s \in \mathcal{S} \quad (2.6d)$$

$$p_{out}^{t,s} \leq P^s \quad \forall t \in \mathcal{T} \quad \forall s \in \mathcal{S} \quad (2.6e)$$

### BESS degradation

Regarding degradation costs for BESS, the literature typically includes as input parameters the maximum allowed daily cycles, or minimum SOC. For example, in [7] it is assumed that the battery will not undergo in more than two cycles per day and that there is no transfer of energy between days.

However, there may exist certain situations where the model may want to surpass the minimum SOC -for instance, if degradation of the PEM membrane is reduced, or if there is a large difference in grid prices that compensates for the degradation cost. Hence, this data should be ideally results of the optimization problem, not input parameters. The degradation model developed in [22] follows this philosophy, and thus will be the one chosen for this work with some modifications explained later on. Note that the following constraints only apply for those ESS that have been marked as BESS.

$$\theta_{up}^{t,b} - \theta_{down}^{t,b} \leq 1 \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B} \quad (2.7a)$$

$$\theta^{t,b} - \theta^{t-1,b} = \theta_{up}^{t,b} + \theta_{down}^{t,b} \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B} \quad (2.7b)$$

$$p_{in}^{t,b} \leq P^b \cdot \theta^{t,b} \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B} \quad (2.7c)$$

$$p_{out}^{t,b} \leq P^b (1 - \theta^{t,b}) \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B} \quad (2.7d)$$

By this method, three binary variables will be implemented to count the number of cycles performed along the simulation horizon.  $\theta_{up}^t$  will be 1 when the charging process is being finished,  $\theta_{down}^t$  when the charging process is beginning, and  $\theta^t$  when the BESS is charging. This behaviour is modelled with constraint (2.7b), while constraint (2.7a) avoids that both variables are set to 1 in the same time slice. Finally,  $\theta^t$  is added in the constraints related with charging and discharging.

Including any of  $\theta_{up}^t$  or  $\theta_{down}^t$  in the objective function with an associated cost will result in a minimization of the cycles. However, the additional variable  $e_{end}^t$  is the one implemented in the objective function, which accounts for the energy remaining in the battery when a charging cycle is starting, i.e. when  $\theta_{down}^t$  is set to 1. This way, we do not only minimize cycles but also the DOD. Similarly, another variable  $e_{start}^{t,b}$  could be defined to penalize full charge.

$$e_{end}^{t,b} \leq E_{max}^b \cdot (1 - \theta_{down}^{t,b}) + e^{t,b} \cdot \theta_{down}^{t,b} \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B} \quad (2.7e)$$

A novel expression is presented in constraint (2.7e), which differs from the source. In the original formulation, degradation costs were incurred always, and the algorithm could reduce these costs only when  $\theta_{down}^{t,b} = 1$  by increasing  $e_{end}^t$ , i.e., by reducing the DOD at each cycle. This could lead to situations where the battery prefers to perform more cycles to be able to reduce costs more frequently. For this reason, this model will only incur in degradation costs when a charging phase starts. Hence, the degradation cost term in the objective function will be:

$$\min_{\substack{t \in \mathcal{T} \\ b \in \mathcal{B}}} (E_{max}^b - e_{end}^{t,b}) \cdot C_{deg}^b \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B} \quad (2.7f)$$

where  $C_{deg}^b$  is the degradation cost associated with a particular BESS.

The algorithm will look to maximize the value of  $e_{end}^{t,b}$ , whose maximum according to constraint (2.7e) can be:

- A.  $E_{max}^b$  when the battery is not on a charging phase start ( $\theta_{down}^{t,b} = 0$ ). Thus, degradation costs will be zero.
- B.  $e^{t,b}$  -the energy remaining in the battery, when the battery is on a charging phase start. Thus, the algorithm will look maximize  $e^{t,b}$ , that is, to reduce the DOD. As a side effect, the algorithm will also try to avoid setting  $\theta_{down}^{t,b}$  to 1 to be in situation A. as long as possible, so the number of cycles will be also minimized.

## Hydrogen storage

Hydrogen storage tanks are modeled similarly to the rest of the ESS in the system, following constraints (2.6) with the efficiency set to 1 and variables measuring power and energy now measuring mass flows and mass, respectively. However, the hydrogen is

stored in the tanks at a certain pressure, thus a compressor is needed. To estimate the electrical consumption of the compressor, adiabatic operation is assumed [13]:

$$p_c^t = K_c \cdot f_{h \rightarrow tank}^t \quad \forall t \in \mathcal{T} \quad (2.8a)$$

where  $f_{h \rightarrow tank}$  corresponds to the hydrogen going from the electrolyzer to the tank, and  $K_c$  is the power consumption of the compressor, which is computed with the following expression:

$$K_c = \frac{R \cdot T_{in}}{2(\gamma - 1)\eta_c} \left( \left( \frac{Pr_{out}}{Pr_{in}} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right) \quad (2.8b)$$

Here, the temperature  $T_{in}$  and the pressure  $Pr_{in}$  of hydrogen correspond to the operating temperature and pressure of the electrolyzer,  $Pr_{out}$  to the pressure desired in the storage tank,  $\gamma$  to the adiabatic efficiency,  $R$  to the ideal gas constant and  $\eta_c$  to the efficiency of the compressor.

## Derivatives production

The final operation of Power-to-X processes is the production of derivatives, which can go from ammonia for fertilizers to synthetic fuels for aviation (SAF), ships (methanol) and cars (e-gasoline). To obtain these derivatives specific reactions are needed -for the case of ammonia production it is known as Haber-Bosch, for methane/methanol as Sabatier, and for hydrocarbons production as Fischer-Tropsch.

Modeling reactors that perform these transformations in optimization problems is challenging, as chemical reactions suffer from non-linear phenomena [16]. Nonetheless, as explained before, in Power-to-X processes water electrolysis frequently represents the vast majority of electrical consumption, achieving 95% of the total in the case of ammonia production, for instance [23]. For this reason, the variation of electricity consumption for derivatives production with the load factor will be assumed as constant.

Reactors involving chemical reactions in presence of catalysts at high temperatures and pressure are very vulnerable to cold starts, which induce great stress on the components and reduce their lifetime. To avoid this, the reactors will work within a pre-defined load range.

$$F_{min,reactor} \cdot Cap_{reactor} \leq f_{derivative}^t \leq Cap_{reactor} \quad \forall t \in \mathcal{T} \quad (2.9a)$$

$$f_{derivative}^t = \left( \sum_{h \in \mathcal{H}} f_{H2}^{t,h} - f_{h \rightarrow tank}^t + f_{tank \rightarrow reactor}^t \right) \cdot K_{H2,reactor} \quad \forall t \in \mathcal{T} \quad (2.9b)$$

where  $F_{min,reactor}$  is the minimum load factor of the reactor, i.e. 20% in the case of a Haber-Bosch reactor and  $K_{H2,reactor}$  the amount of hydrogen consumed in one hour for the synthesis of a unit of mass of the derivative product. Also, the production of the derivative must equal the desired demand of such product. For this model, it has been decided that the annual equivalent hours of the reactor will be used as an input parameter, so the production of the derivative product must be:

$$\sum_{t \in \mathcal{T}} f_{derivative}^t = Cap_{reactor} \cdot EQ_{hours} \quad \forall t \in \mathcal{T} \quad (2.9c)$$

Finally, the energy balance of the whole Power-to-X system:

$$\sum_{\substack{s \in \mathcal{S} \\ g \in \mathcal{G} \\ h \in \mathcal{H}}} p_{in}^{t,s} + p_{total}^{h,t} + p_c^t + K_{e,reactor} \cdot f_{derivative}^t = \sum_{\substack{s \in \mathcal{S} \\ g \in \mathcal{G}}} p_{out}^{t,s} + p_{gen}^{t,g} + p_{grid}^t \quad \forall t \in \mathcal{T} \quad (2.9d)$$

where  $K_{e,reactor}$  is the electricity consumption of the reactor per unit of mass of hydrogen produced.

A variable  $p_{ens}$  can be included in the right hand-side of the constraint to account for the energy not served, avoiding an infeasible problem due to the lack of hydrogen supply and thus allowing the solver to reach a solution. The variable will give the amount of hydrogen lacking to supply the demand of derivatives at each hour -if any, and the user will know how much capacity of electrolysis and/or generators should be added. The objective function should also include the cost of energy not served, which must be set arbitrarily high for the algorithm not to avoid using the electrolyzers.

### 2.3. Objective function

As explained in 2.1, a minimization cost algorithm will be designed in this work, so the objective function must account for all the economic costs the plant will incur by modifying its operation. Those are:

1. Variable costs: more energy generated by the installed generators lead to higher variable cost. The same applies for the ESS, but taking into account both the energy charged and discharged.
2. Degradation costs: more usage of the battery means more degradation, obviously depending on the conditions of the cycles described in 2.2.3. For the electrolyzer, the cold-starts will impact the degradation of the membrane, so the cold start counter  $c_{coldstart}$  must be also be included.
3. Exchanges with the grid: as costs are trying to be minimized, energy purchased from the grid should have a positive sign, while energy sold will have a negative one, as it is a profit. Note that the same variable  $p_{grid}$  is being used for imports and exports, being lower than zero for imports. Thus, its term in the objective will have positive sign.

The cost must be minimized for all the simulation horizon -in this case, for a year, so the objective function must sum every term not only for all the elements in the system but also for each hour of the year.

$$\min \sum_{g,s,b,h,t} p_{ens}^t \cdot \lambda_{ens} + p_{grid}^t \cdot \lambda_{grid} + p_{gen} \cdot \lambda_{var}^g + (p_{out}^{t,s} + p_{in}^{t,s}) \cdot \lambda_{var}^s + (E_{max}^b - E_{end}^{t,b}) \cdot \lambda_{deg}^b + c_{coldstart}^{t,h} \cdot \lambda_{deg}^h \quad (2.10)$$

## 2.4. Implementation

The designed model is implemented in Python using the library Pyomo, a well-known package for optimization problems. To solve the problem, Pyomo calls a solver -in this case, Gurobi, which requires academic license. However, open source solvers capable of solving non-linear problems are also available, such as CBC (COIN-OR Branch-and-cut solver). If a solution is found, the solver returns the results to Pyomo, which can then be treated to be displayed to the user.

A diagram of the algorithm can be found below:

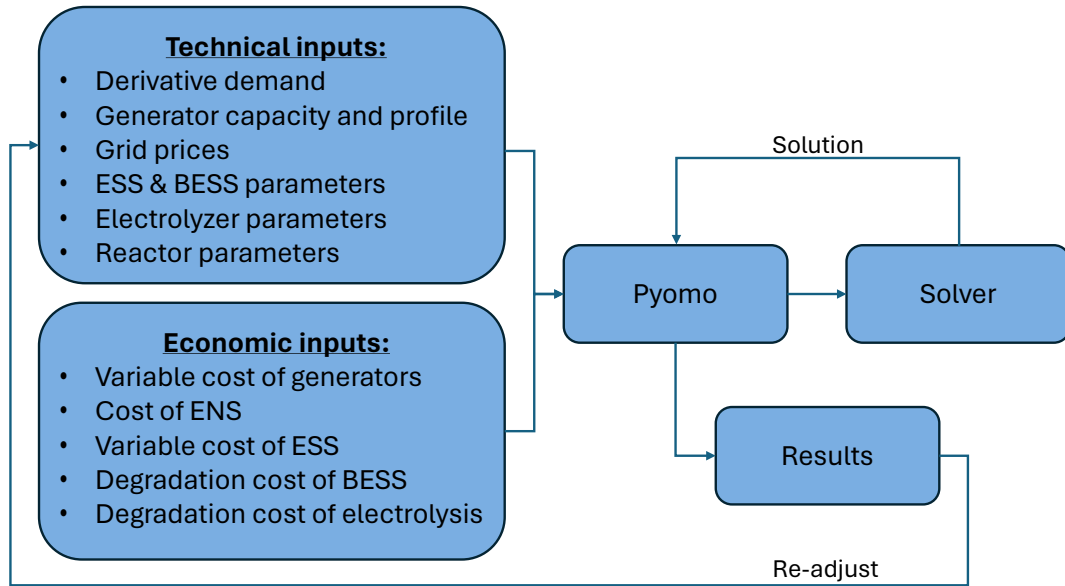


Fig. 2.5. Flow chart of the optimization algorithm

Firstly, the user sets the input parameters, which can be related with technical characteristics of the equipments or economic costs. Afterwards, the input parameters are sent to Pyomo, where the model itself is built. The mathematical formulae are then sent to the chosen solver, and the results of the optimization problem are sent back to Pyomo again. Finally, the results are displayed to the user.

If the solution found does not meet the expected results, the user may re-adjust the

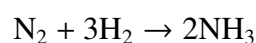
input parameters, for example, the installed capacity of generators, and re-run the simulation until the desired result is obtained.

### 3. CASES STUDY

In this chapter, several examples of Power-to-X systems will be analyzed, to showcase the capabilities and flexibility of the algorithm developed. First, a green ammonia production plant will be simulated, and then, although not related with derivatives production, a hydrogen production plant for injection into the European Hydrogen Backbone. The objective will be to compare the cost of several configurations and obtain the optimum sizing attending to different criteria.

#### 3.1. Synthesis of ammonia

Ammonia  $\text{NH}_3$  is a critical chemical in modern industrial processes, playing a pivotal role in the production of fertilizers, pharmaceuticals, and various industrial chemicals. The synthesis of ammonia is predominantly carried out via the Haber-Bosch process, a method that has been the cornerstone of industrial ammonia production since its development in the early 20th century. This process combines nitrogen  $\text{N}_2$  from the air with hydrogen  $\text{H}_2$  derived from natural gas, under high pressure and temperature in the presence of a catalyst:



Despite its efficiency and scalability, the Haber-Bosch process is energy-intensive and contributes significantly to global carbon dioxide  $\text{CO}_2$  emissions due to its reliance on fossil fuels for hydrogen production.

In response to the pressing need for sustainable industrial practices, there is growing interest in integrating renewable energy sources into ammonia production. Electrolysis of water to produce hydrogen represents a promising alternative to the conventional steam methane reforming method. By utilizing renewable electricity, such as solar or wind power, water can be split into hydrogen and oxygen, providing a green hydrogen source for the Haber-Bosch process. This hybrid approach not only mitigates  $\text{CO}_2$  emissions but also aligns with global efforts to transition towards a low-carbon economy.

The versatility of ammonia extends beyond its primary role in agriculture, where it is a key ingredient in nitrogen-based fertilizers. Thanks to the Haber-Bosch process, ammonia is being explored as a potential energy carrier and a carbon-free fuel, especially in the context of hydrogen economy developments. Its ability to store and transport hydrogen efficiently makes it an attractive candidate for addressing energy storage and distribution challenges.

The primary challenges associated with integrating green electrolysis into the Haber-Bosch process stem from the variability and intermittency of renewable power inputs. Chemical reactors, such as those used in the Haber-Bosch process, are particularly sensi-

tive to fluctuations in power supply. Frequent shutdowns or substantial deviations from a stable power input can significantly impact the operational lifespan of reactor components [16].

To mitigate these issues, Haber-Bosch reactors are typically designed to operate within specific load parameters. They are unable to function below a minimum load threshold, which is generally around 30% of their capacity. Additionally, the rate at which these reactors can increase their load is constrained, typically limited to an increment of no more than 15% per hour. Several options are commercially available right now to overcome these issues:

1. Electricity storage: adding electricity storage, particularly battery energy systems is a good choice to mitigate the variability of renewable energies, specially in the power domain. However, for great amounts of energy they become more CAPEX intensive than other options, thus hurting the viability of the project.
2. Hydrogen storage: hydrogen storage is less intensive in initial investment, so it is more common. Hydrogen tanks allow the system to have a hydrogen buffer, so even if the hydrogen production is variable the hydrogen entering the reactor will be constant.
3. Hydrogen pipelines: if the electricity generation and electrolysis plants cannot be located nearby the consumption point, i.e. the Haber-Bosch reactor, a pipeline will be needed. This pipeline has great utility as it can also function as a hydrogen buffer, thus mitigating any variable output of the electrolyzer.
4. Grid connection: relying on the grid to smooth hydrogen production is usually the way-to-go in pre-feasibility studies. However, green and low carbon hydrogen certifications are strict -specially in the European Union, and rigid conditions must be fulfilled [24]. These include consuming from the grid only when the wholesale price is below 0.36 times the price of the CO<sub>2</sub> credit or 20 EUR/MWh, so relying exclusively on the grid can only be done in countries with high share of renewable production or projects starting operation not anytime soon.
5. Complementary Power Purchase Agreement (PPA): if the system includes on-site electricity production, it is recommended to search for a complementary PPA, this is, generation plants that have a complementary profile to that of the on-site plant. For example, if the project includes an on-site PV plant, it is advisable to find a wind PPA with a generation profile as different as possible, so the electrolyzer can maintain a minimum load and produce hydrogen that is automatically green.

Evidently, there is no single solution and usually several of them are chosen. As of right now, the most used solutions are complementary PPA, hydrogen storage via tanks or pipelines and grid connection ensuring that the energy taken from the grid is green.



### 3.1.1. Data

Firstly, to produce the hydrogen curve, the model explained in section 2.2.1 will be used along with the empirical parameters obtained in [19] and [18].

Parameter	Value	Unit
$T_{op}$	30	Pa
$P_{op}$	90	°C
$i$	5000	$A\ m^{-2}$
$U_{rev}$	1.175	V
$r_1$	$4.45153 \times 10^{-5}$	$\Omega\ m^2$
$r_2$	$6.88874 \times 10^{-9}$	$\Omega\ m^2\ C^{-2}$
$d_1$	$-3.12996 \times 10^{-6}$	$\Omega\ m^2$
$d_2$	$4.47137 \times 10^{-7}$	$\Omega\ m^2\ bar^{-1}$
$s$	0.33824	V
$t_1$	-0.01539	$m^2\ A^{-1}$
$t_2$	2.00181	$m^2\ C\ A^{-1}$
$t_3$	15.24178	$m^2\ C^2\ A^{-1}$
$f_{11}$	478645.74	$A^2\ m^{-4}$
$f_{12}$	-2953.15	$A^2\ m^{-4}\ C^{-1}$
$f_{21}$	1.03960	-
$f_{22}$	-0.00104	$C^{-1}$

TABLE 3.1. EMPIRICAL DATA FOR HYDROGEN PRODUCTION CURVE

The data for the Haber-Bosch reactor and the electrolyzer will be from anonymized real-life projects. The electricity consumption of the Haber-Bosch reactor includes the air separation unit, the feed compressor, the ammonia chiller, the ammonia recycle compressor, the ammonia storage and the ammonia facility and service (building, control room, etc.).

Parameter	Value	Unit
<b>Haber-Bosch Reactor</b>		
Capacity	54	tons/hour
H <sub>2</sub> -NH <sub>3</sub> mass ratio	5.6	p.u.
Electricity consumption	0.695	MWh/ton
Minimum load	35	%
Ramp Rate	15	%/min
Equivalent annual hours	5000	h
<b>Electrolyzer</b>		
Capacity	500	MW
Minimum power	100	MW
Stand-by power	0.1	MW
Cold start-up cost	50	EUR
<b>Hydrogen storage</b>		
$\eta_c$	75	%
$P_{in}$	30	Pa
$P_{out}$	200	Pa
$T_{in}$	90	°C
Initial SOC	50	%
Minimum SOC	10	%
Maximum SOC	90	%
Cold start-up cost	50	EUR
<b>BESS</b>		
Capacity	4	h
Efficiency	90	%
Degradation cost	700	EUR/MWh
O&M cost	0	EUR/MWh
<b>Electricity generation units</b>		
PV O&M cost	0.05	EUR/MWh
Wind O&M cost	0.42	EUR/MWh
<b>Others</b>		
Grid connection capacity	0	MW

TABLE 3.2. INPUT DATA FOR AMMONIA SYNTHESIS CASE STUDY

Finally, several configurations will be simulated. The first one will rely on on-site PV production along with BESS to mitigate the variable power supply, the second one will use a wind PPA as-produced of 50 EUR/MWh to complement the variability of sun, and the final option will use imports from the grid.

	PV (MWp)	Wind PPA (MW)	BESS (MWh)
<b>Scenario 1</b>	80	-	5
<b>Scenario 2</b>	50	80	-
<b>Scenario 3</b>	50	-	-

TABLE 3.3. SCENARIOS FOR AMMONIA SYNTHESIS

To select the optimal sizing of the plant, the Net Present Value (NPV) of the Expenses Before Interest Taxes Depreciation and Amortization (EBITDA), the Internal Rate of Return (IRR) and the Levelized Cost Of Ammonia (LCOA) will be used, as per the following formulae:

$$NPV = \sum_{t=1}^n \frac{\text{Revenues}_t - \text{CAPEX}_t - \text{OPEX}_t}{(1 + r)^t} \quad (3.1)$$

$$0 = \sum_{t=1}^n \frac{\text{Revenues}_t - \text{CAPEX}_t - \text{OPEX}_t}{(1 + IRR)^t} \quad (3.2)$$

Where the operational expenditures are affected by the inflation, and include the model's BESS degradation output. To simulate the entire project lifetime, a calendar of deployment of CAPEX, OPEX and revenues is developed. The capital expenditures happen on the year 0 and year 10. Assuming the typical PEM stack lifetime ranges from 60,000 to 70,000 hours, the augmentation event will happen at year 10. On the other hand, operational expenditures are incurred every year of operation. Revenues also happen from year 1 until the end of the project's lifetime, which for all cases will be 20 years. The input parameters for the financial model of each scenario are shown below:

Parameter	Value	Unit
<b>BESS</b>		
Modules and installation CAPEX	25	kEUR/MWh
EPC cost	20	% of CAPEX
<b>PV Plant</b>		
Modules, Inverters and auxiliaries CAPEX	450	kEUR/MW
EPC costs	21	% of CAPEX
OPEX	20	kEUR/MWp/year
<b>Wind (PPA)</b>		
PPA duration	20	years
PPA price	50	EUR/MWh
<b>Hydrogen production</b>		
Stacks CAPEX	1000	kEUR/MW
EPC Costs	20	%
Water cost	10	EUR/tonH <sub>2</sub>

TABLE 3.4. INPUT DATA FOR AMMONIA SYNTHESIS CASE STUDY

### 3.1.2. Results

In scenario 1, the battery performs the task of supplying the power demand of the electrolysis when the PV plant is not available. The following graph shows this situation:

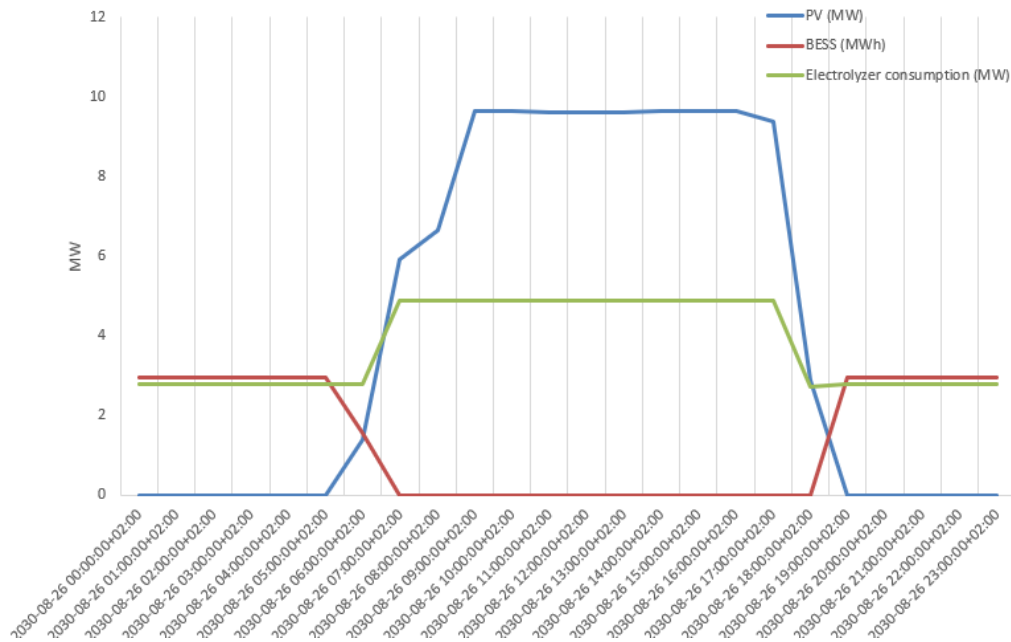


Fig. 3.1. Hydrogen production in scenario 1

In the central hours of the day, the PV is able to both supply the electrolysis and also

provide energy to the BESS. For the BESS to be able to do this, the storage must be huge. As we will see later, this hurts the IRR of the project.

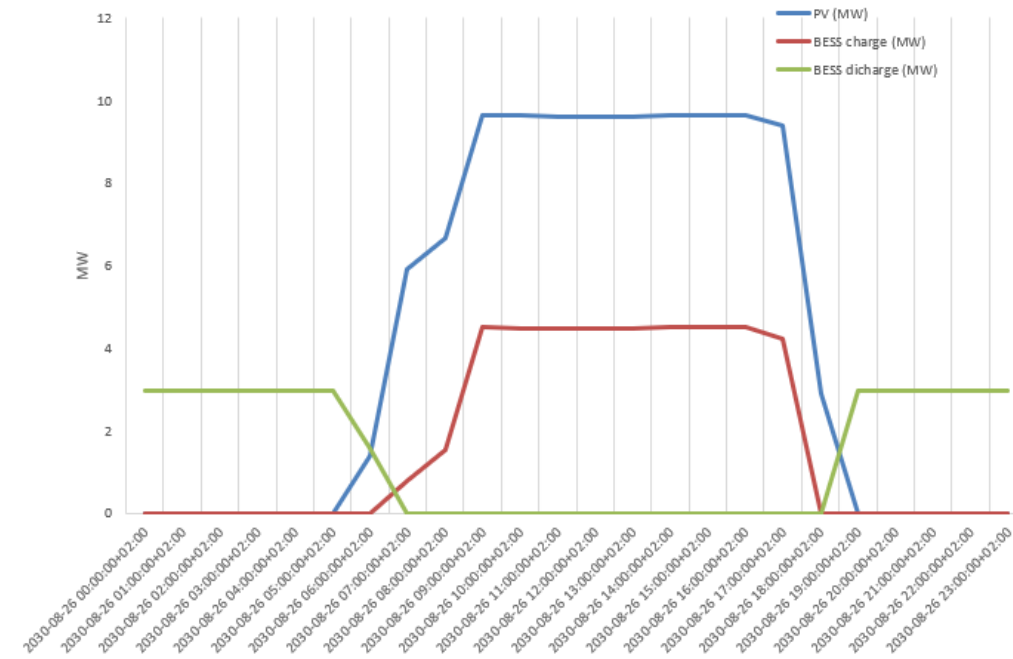


Fig. 3.2. BESS in scenario 1

Regarding scenario 2, the wind PPA takes the role of supplying the plant when no sun is available:

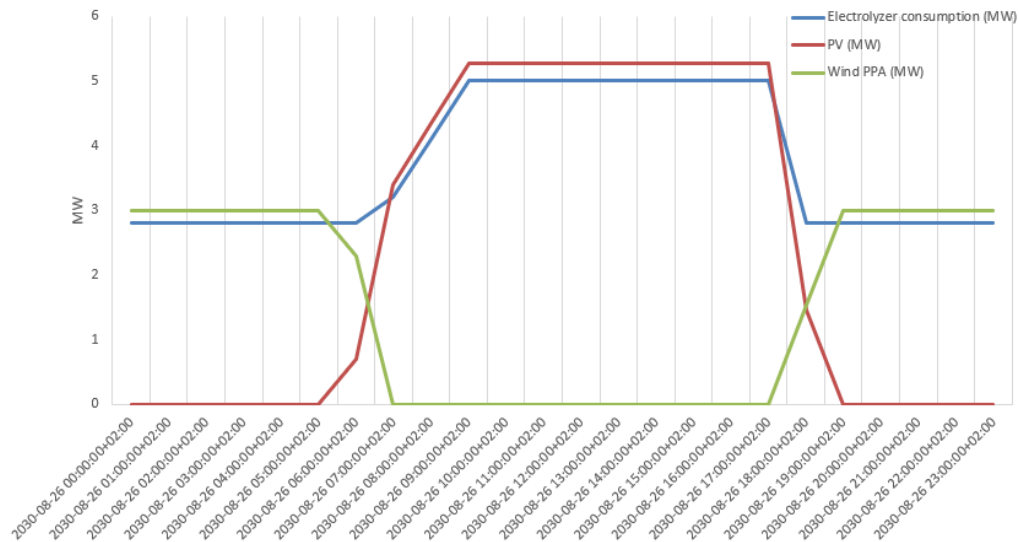


Fig. 3.3. Hydrogen production in scenario 2

A similar profile is observed in scenario 3, but the energy purchased from the grid is not at a fixed price, however. The results of the 3 scenarios are shown below:

	<b>Pre-tax IRR (%)</b>	<b>NPV of EBITDA (kEUR)</b>
<b>Scenario 1</b>	2.70	89,201.33
<b>Scenario 2</b>	7.68	104,802.88
<b>Scenario 3</b>	9.91	113,177.69

TABLE 3.5. SCENARIOS FOR AMMONIA SYNTHESIS

As it can be noted, only the third scenario -the one depending on grid imports, has an IRR above the discount rate used in the financial model. It is obvious that electrochemical storage is still too expensive, and cannot be made profitable neither by performing arbitrage nor increasing the electrolyzer's load factor. The Wind PPA scenario, although still below the discount rate, offers more certainty in the results, as a fixed price is being signed.

Regarding scenario 3, the following should be noted:

1. Grid prices: the grid prices used in this scenario correspond to a Spanish energy mix with high penetration of renewables, specially PV, and not a significant increase in demand. This means that grid prices are lower than what is observed today. Any change in renewable installation tendencies can affect grid prices prediction, and thus the profitability of the project.
2. Regulatory framework: as electrolysis is not a well established process, there are regulatory uncertainties when consuming from the grid. It is still unclear if electrolyzers will have to pay the so-called *cargos* to consume from the grid or will be exempt similar to BESS projects. Any political change could greatly affect this point.
3. Green hydrogen: strict rules apply in the EU from 2030 onwards for the classification of each type of hydrogen, such as the additionality rule explained before. Thus, it is possible that a certain amount of the hydrogen produced could not be labelled as green and thus should be sold at a lower price, hurting profits. Hydrogen will always be green when consuming from the grid in countries where renewable annual production is higher than 90%, such as Norway or Finland.

These results are on a par with what is observed in the industry. Although grid wholesale market offers good opportunities to buy and sell energy at advantageous prices and increase the profitability of hydrogen projects, relying on the grid is too risky, so developers typically prefer to sign PPA and protect themselves against the risks of wholesale prices.

Other industrial processes could be simulated, as the production of e-fuels. For the Fischer-Tropsch process, it could be interesting to add two electrolyzers (which the model allows for). One could perform what is known as co-electrolysis, which can break down

water to hydrogen and carbon dioxide into carbon monoxide in the same single process, obtaining syngas in just one step. For this, a high temperature and low flexibility electrolyzer can be used, as the Solid-Oxide Cells (SOEC). Another one with more flexibility, such as PEM or AEM could be added on top to absorb the variable wholesale grid prices and renewable supply.

### 3.2. Injection into European Hydrogen Backbone

The European Hydrogen Backbone or EHB is an initiative first developed in the European Union's Hydrogen Strategy published in 2020, and further improved in the REPowerEU package. It aims at leveraging the existing natural gas infrastructure where possible to enable widespread use of hydrogen as clean energy carrier, building also new pipelines where needed.

The objective will be not only to provide hydrogen to all the European countries, but also to set up a liquid and competitive market for green and low carbon hydrogen, as it exists for other energy carriers. While no clear dates are given, it is expected that the first injections of hydrogen in the EHB will not happen until 2030.

In this section an electrolysis plant with injection to the EHB will be simulated, as a showcase of the flexibility of the developed algorithm. Being connected to an off-taker such as the EHB is a great advantage, as the pipeline connecting our electrolysis plant with the injection point can serve as buffer, so additional storage may not be needed.

#### 3.2.1. Data

To simulate a plant with no derivative production, the reactor can be set to have an efficiency of 100% and no electricity consumption. The hydrogen will pass through this process with no losses, as if it did not exist.

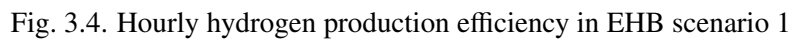
To preserve the duration of the membranes of the electrolyzer, a demand of hydrogen corresponding to 4,000 equivalent hours of annual operation will be set. The rest of input parameters will be the ones showcased in tables 3.1, 3.2 and 3.4.

The following scenarios will be simulated:

	<b>PV (MWp)</b>	<b>Wind PPA (MW)</b>	<b>Import capacity (MW)</b>
<b>Scenario 1</b>	20	-	5
<b>Scenario 2</b>	10	30	-

TABLE 3.6. SCENARIOS FOR EHB INJECTION

Firstly, the hydrogen production efficiency curve can be found below. Note that during peak hours of PV production, the electrolyzer reaches nominal condition. However, the efficiency is lower than at non-peak hours -as it has been explained before, electrolysis has better efficiency at lower load factors.



1. The year of operation is no sooner than 2030, when electrolyzers must comply with hourly matching. This means that the hydrogen will only be green if the energy used to produce that hydrogen is 100% of renewable origin and has been generated during the same hour.
2. The ETS emission allowance price is 140 EUR per ton of CO<sub>2</sub>, thereby setting the limit for producing green hydrogen from grid imports at 50.4 EUR/MWh.
3. The country where the plant is built has not a renewable production larger than 90%. If it was the case, all hydrogen produced from grid imports would be considered green.

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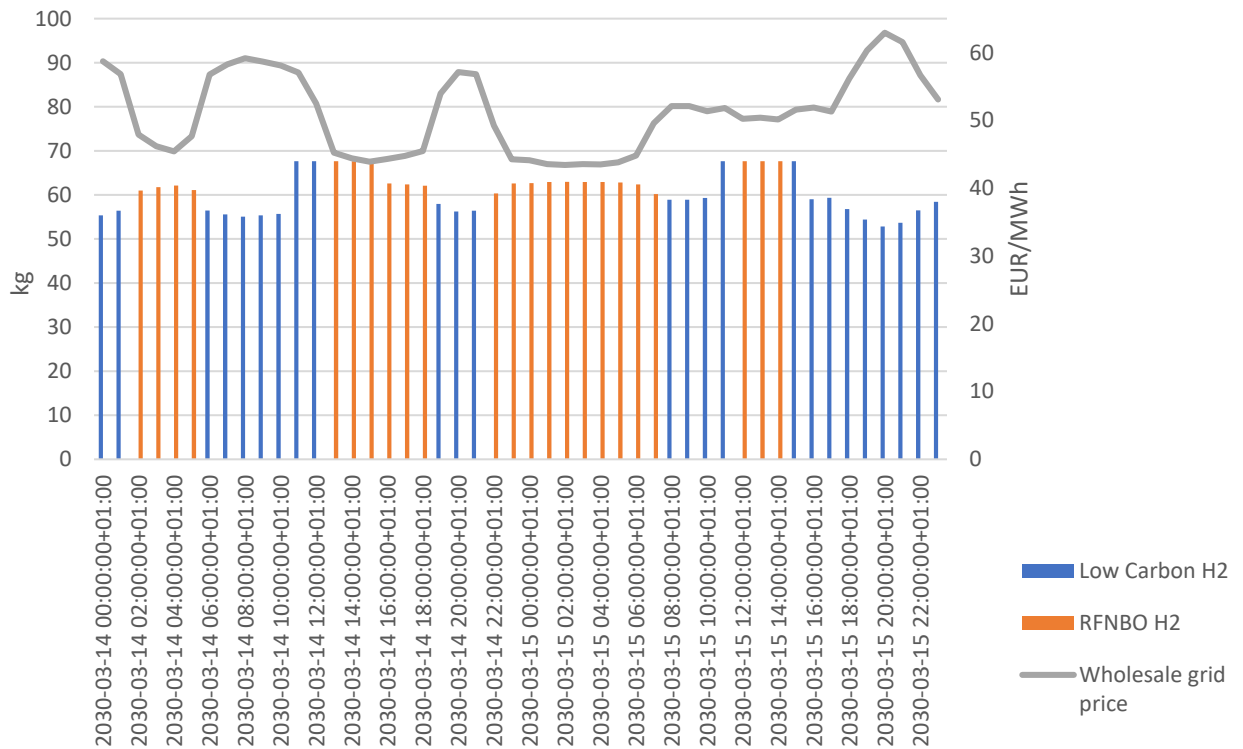


Fig. 3.5. RFNBO and LC hydrogen production in EHB scenario 1

During the year, the amount of Low Carbon hydrogen produced represents roughly 15% of the total.

To see at which price the hydrogen should be sold, it is useful to calculate the Levelized Cost of Hydrogen (LCOH). This can be easily done with the financial model developed for the ammonia study cases. Firstly, the hourly dispatch is simulated for a year, and the yearly results are extrapolated for the project's lifetime. Secondly, the Net Present Value of both energy terms and monetary terms are calculated. Thirdly, the contribution of each component is computed by dividing the total NPV of that component by the NPV of the hydrogen production, and by summing them, the total LCOH is obtained.

Component	Value	Contribution
Solar	2.96 EUR/kg	51%
Grid imports	1.20 EUR/kg	21%
Hydrogen production	1.59 EUR/kg	28%
<b>Total</b>	<b>5.74 EUR/kg</b>	<b>100 %</b>

TABLE 3.7. LCOH IN EHB SCENARIO 1

A Hydrogen Purchase Agreement with a value of 5.74 EUR/kg is the bare minimum the promoter should sign in order to see an IRR equal to the discount rate. For reference, the maximum bid at the latest European Hydrogen Bank auction was of 4.5 EUR/kg [25]. Now, if we add a wind PPA of 30 MW at 45 EUR/MWh and reduce the on-site PV to 10 MW, the LCOH calculation results are:

<b>Component</b>	<b>Value</b>	<b>Contribution</b>
Solar	1.48 EUR/kg	27%
Wind PPA	2.39 EUR/kg	44%
Hydrogen production	1.59 EUR/kg	29%
<b>Total</b>	<b>5.45 EUR/kg</b>	<b>100 %</b>

TABLE 3.8. LCOH IN EHB SCENARIO 2

In scenario 2 not only the LCOH is reduced by 0.30 EUR/kg, but also the risk of the project is mitigated thanks to the lower merchant exposure. It is important to remark that contrary to scenario 1, every kilogram of produced hydrogen can be sold as RFNBO.

It seems clear by this point that hydrogen projects should rely on PV and a complementary renewable PPA to maintain a high load factor, while reducing to the minimum the grid imports.

## 4. CONCLUSIONS

The developed algorithm and its subsequent implementation in Pyomo and Gurobi show that the states of the electrolyzer and its non-linear efficiency curve can be both included in the same model, providing optimal hourly dispatch solutions in polynomial time.

Thanks to the low time needed to reach a solution paired with the high accuracy of the electrolysis model, contrary to the state-of-the-art implementations, the algorithm could be used in real time operations, helping reduce the degradation of the stacks and thus increase profitability. This feature may be crucial for future implementation in EMS, enabling more uses of the algorithm outside pre-feasibility studies.

On the other hand, the techno-economic assessments developed for the studied cases highlight that green hydrogen projects are either non-profitable or depend on cheap wholesale grid prices to reach profitability. However, dependency on grid prices is risky and investors try to avoid it due to their high volatility, as it has been seen during these past years. Any change in the forecasted grid prices will have great impact on both operation and profitability. The addition of a Power Purchase Agreement complementing the on-site renewable production is a great way of not only protecting against inflation and price volatility, but also of increasing the electrolyzer's load factor, reducing cold starts and increasing the lifetime of the stacks.

The adoption of hydrogen as a clean energy carrier, which is a major part in the European Union's road towards net-zero goals by 2050, is still doubtful. The solutions to promote the construction of hydrogen projects could be:

1. To grant financial aids to help promoters reach profitability. This could go from direct grants for the purchase of electrolyzers, to tax exemptions.
2. To establish a clear, straight-forward regulatory framework to help electrolyzers produce hydrogen while consuming from the grid. Current regulation is conversant and imposes huge restrictions on the production of green hydrogen from grid imports.
3. To reduce electrolysis projects risks by stabilizing electricity wholesale prices. Huge efforts are currently being made by regulatory bodies and countries to solve the volatility of prices seen on recent years.
4. Advances in development of PEM and AEM membranes, such as taking advantage of economics of scale to reduce the prices of the stacks or comprehending better its dynamics to increase their lifetime. Although current Chinese developers offer electrolyzers below market prices, their response to variable renewable supply is still not fully understood.

#### **4.1. Future lines of work**

The developed formulation serves as a good and flexible base to build up more precise models. Further improvements include:

1. Include stochastic phenomena and/or robust optimization. This would allow achieving optimal solutions for different grid prices scenarios or renewable production forecasts, thereby enabling investors to better visualize the risks of the project.
2. Increment the amount of variables to be optimized. In this work, the chosen variable has been annual variable cost, but the user may want to maximize hydrogen production, minimize the levelized cost of hydrogen or reduce to the minimum the usage of grid imports.
3. Include multi-objective optimization, to optimize at the same time several variables -for instance, minimize degradation while also obtaining the highest hydrogen output possible.
4. Model several markets, so the algorithm can perform arbitrage between the commodities being traded. For example, the model could choose from trading electricity, hydrogen, or the derivatives at each hour, depending on the prices of each commodity.
5. Increase the resolution of the model. Instead of simulating time-steps of 1 hour, the model could function on a minute-by-minute basis. This would enable the modelling of electrolysis ramps, which are critical in slower and less flexible electrolyzers.

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## A. FULL PROBLEM

$$\begin{aligned}
\min \quad & \sum_{g,s,b,h,t} p_{ens}^t \cdot \lambda_{ens} + p_{grid}^t \cdot \lambda_{grid} + p_{gen} \cdot \lambda_{var}^g \\
& + (p_{out}^{t,s} + p_{in}^{t,s}) \cdot \lambda_{var}^s + (E_{max}^b - E_{end}^{t,b}) \cdot \lambda_{deg}^b + c_{coldstart}^{t,h} \cdot \lambda_{deg}^h \\
\text{s.t.} \quad & \sum_{\substack{s \in \mathcal{S} \\ g \in \mathcal{G} \\ h \in \mathcal{H}}} p_{in}^{t,s} + p_{total}^{h,t} + p_c^t + K_{e,reactor} \cdot f_{derivative}^t = \sum_{\substack{s \in \mathcal{S} \\ g \in \mathcal{G}}} p_{out}^{t,s} + p_{gen}^{t,g} + p_{grid}^t + p_{ens}^t, \quad \forall t \in \mathcal{T}, \\
& \sum_{t \in \mathcal{T}} f_{derivative}^t = Cap_{reactor} \cdot EQ_{hours}, \quad \forall t \in \mathcal{T}, \\
& f_{derivative}^t = \left( \sum_{h \in \mathcal{H}} f_{H2}^{t,h} - f_{h \rightarrow tank}^t + f_{tank \rightarrow reactor}^t \right) \cdot K_{H2,reactor}, \quad \forall t \in \mathcal{T}, \\
& F_{min,reactor} \cdot Cap_{reactor} \leq f_{derivative}^t \leq Cap_{reactor}, \quad \forall t \in \mathcal{T}, \\
& z_{on}^{t,h} + z_{sb}^{t,h} + z_{off}^{t,h} = 1, \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H}, \\
& z_{sb}^{t,h} + z_{off}^{t-1,h} \leq 1, \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H}, \\
& c_{coldstart}^{t,h} = z_{on}^{t,h} - z_{on}^{t-1,h} - z_{sb}^{t-1,h}, \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H}, \\
& f_{H2}^{t,h} = Q_2^h \cdot \varepsilon^h + Q_1^h \cdot p_{H2}^{h,t} + Q_0^h \cdot z_{on}^{t,h}, \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H}, \\
& \varepsilon^h \geq (p_{H2}^{h,t})^2, \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H}, \\
& p_{total}^{t,h} = P_{H2}^{h,t} \cdot z_{on}^{t,h} + P_{sb}^h \cdot z_{sb}^{t,h}, \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H}, \\
& P_{H2,min}^h \leq p_{H2}^{h,t} \leq P_{H2,max}^h, \quad \forall t \in \mathcal{T} \quad \forall h \in \mathcal{H}, \\
& p_c^t = K_c \cdot f_{h \rightarrow tank}^t, \quad \forall t \in \mathcal{T}, \\
& -P_{export} \leq p_{grid}^t \leq P_{import}^t, \quad \forall t \in \mathcal{T}, \\
& p_{gen}^{t,g} = CF^{t,g} \cdot P^g, \quad \forall t \in \mathcal{T} \quad \forall g \in \mathcal{G}, \\
& e^{t,s} = e^{t-1,s} + \eta^s \cdot p_{in}^{t,s} - \frac{1}{\eta^s} \cdot p_{out}^{t,s}, \quad \forall t \in \mathcal{T} \quad \forall s \in \mathcal{S}, \\
& e^{t,s} = E_{initial}^s, \quad t = 1 \quad \forall s \in \mathcal{S}, \\
& E_{min}^s \leq e^{t,s} \leq E_{max}^s, \quad \forall t \in \mathcal{T} \quad \forall s \in \mathcal{S}, \\
& p_{in}^{t,s} \leq P^s, \quad \forall t \in \mathcal{T} \quad \forall s \in \mathcal{S}, \\
& p_{out}^{t,s} \leq P^s, \quad \forall t \in \mathcal{T} \quad \forall s \in \mathcal{S}, \\
& \theta_{up}^{t,b} - \theta_{down}^{t,b} \leq 1, \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B}, \\
& \theta^{t,b} - \theta^{t-1,b} \leq 1, \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B}, \\
& \theta_{up}^{t,b} - \theta_{down}^{t,b} = \theta_{up}^{t,b} + \theta_{down}^{t,b}, \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B}, \\
& p_{in}^{t,b} \leq P^b \cdot \theta^{t,b}, \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B}, \\
& p_{out}^{t,b} \leq P^b (1 - \theta^{t,b}), \quad \forall t \in \mathcal{T} \quad \forall b \in \mathcal{B},
\end{aligned}$$



$$e_{end}^{t,b} \leq E_{max}^b \cdot (1 - \theta_{down}^{t,b}) + e^{t,b} \cdot \theta_{down}^{t,b},$$

$$\forall t \in \mathcal{T} \quad \forall b \in \mathcal{B}$$

## B. VARIABLES, PARAMETERS AND INDICES

Variable	Description	Unit
$f_{derivative}$	Derivative product produced	kg/h
$f_{derivative}$	Hydrogen produced	kg/h
$p_{in}$	Energy entering the ESS	MWh
$p_{out}$	Energy exiting the ESS	MWh
$e$	Energy stored in the ESS	MWh
$\theta_{up}$	Charging phase finish counter	-
$\theta_{down}$	Discharging phase start counter	-
$\theta$	Charging state binary	-
$e_{end}$	Energy at end of discharge	MWh
$p_{gen}$	Energy produced by the generators	MWh
$p_{grid}$	Energy exchanged with the grid	MWh
$f_{h \rightarrow tank}$	Hydrogen from electrolyzers to the tanks	kg/h
$f_{tank \rightarrow reactor}$	Hydrogen from the tank to the reactor	kg/h
$z_{on}$	On state binary	-
$z_{sb}$	Standby state binary	-
$z_{off}$	Off state binary	-
$C_{coldstart}$	Cold start binary	-
$p_{H2}$	Power consumed to produce hydrogen	MW
$p_{total}$	Total electrolyzer power consumption	MW
$p_c$	Compression power consumption	MW
$\varepsilon^h$	Conic auxiliary variable	-

TABLE B.1. TABLE OF VARIABLES

Parameter	Description	Unit
$Cap_{reactor}$	Reactor's capacity	kg/h
$EQ_{hours}$	Annual equivalent hours of the reactor	h
$K_{e,reactor}$	Power consumption of the reactor	MW/kg
$K_{H_2,reactor}$	Hydrogen consumption of the reactor	kg <sub>H2</sub> /kg
$F_{min,reactor}$	Minimum load of the reactor	p.u.
$Q_2$	Quadratic approximation coefficient	-
$Q_1$	Quadratic approximation coefficient	-
$Q_0$	Quadratic approximation coefficient	-
$P_{sb}$	Electrolyzer standby power	MW
$P_{H_2,min}$	Electrolyzer minimum on power	MW
$P_{H_2,max}$	Electrolyzer maximum on power	MW
$P_{export}$	Export power capacity	MW
$P_{import}$	Import power capacity	MW
$CF$	Capacity factor	p.u.
$\eta^s$	Efficiency	p.u.
$E_{initial}^s$	Initial energy level in the ESS	MWh
$E_{min}^s$	Minimum ESS energy level	MWh
$E_{max}^s$	Maximum ESS energy level	MWh
$P$	Installed power	MW
$\lambda_{ens}$	Cost of energy not served	EUR/MW
$\lambda_{grid}$	Wholesale market electricity price	EUR/MW
$\lambda_{deg}$	Cost of degradation	EUR/MW
$\lambda_{var}$	Variable cost	EUR/MWh

TABLE B.2. TABLE OF PARAMETERS

Parameter	Description	Set
$t$	Time slice	$\mathcal{T}$
$g$	Electricity generation unit	$\mathcal{G}$
$s$	Energy Storage System unit	$\mathcal{S}$
$b$	Battery Energy Storage System unit	$\mathcal{B}$
$h$	Electrolysis unit	$\mathcal{H}$

TABLE B.3. TABLE OF INDICES

## C. ACRONYMS

AEM	Anion Exchange Membrane
BESS	Battery Energy Storage System
CAPEX	Capital Expenditures
CF	Capacity Factor
DOD	Depth Of Discharge
EHB	European Hydrogen Backbone
EMS	Energy Management System
ENS	Energy Not Served
EPC	Engineering Procurement and Construction
ESS	Energy Storage System
EU	European Union
IRR	Internal Rate of Return
LC	Low Carbon
LCOH	Levelized Cost of Hydrogen
LP	Linear Programming
MILP	Mixed Integer Linear Programming
MISOCP	Mixed Integer Second Order Cone Programming
NPV	Net Present Value
OPEX	Operational Expenditures
PEM	Proton Exchange Membrane
PPA	Power Purchase Agreement
PtX	Power to X
PV	Photovoltaic
RFNBO	Renewable Fuel of Non-Biological Origin
SAF	Sustainable Aviation Fuel
SCADA	Supervisory Control and Data Acquisition
SOC	State of Charge
SOEC	Solid Oxide Electrolyzer Cell

TABLE C.1. ACRONYMS