PONTIFICIA UNIVERSIDAD CATOLICA DE CHILE

ESCUELA DE INGENIERIA

HYDROGEN PRODUCTION ECONOMICS: A COMPOUND REAL OPTIONS ANALYSIS

TOMÁS OVALLE PAROT

Thesis submitted to the Office of Research and Graduate Studies in partial fulfillment of the requirements for the Degree of Master of Science in Engineering

Advisor:

ENZO ENRIQUE SAUMA SANTIS

Santiago de Chile, (January, 2022)

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(To my parents, siblings and friends, who were very supportive).

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RESUMEN

Muchos países ya han desarrollado políticas y estrategias para una economía verde del hidrógeno y, en consecuencia, el sector privado ya ha iniciado proyectos para producirlo. Dada la gran incertidumbre que conlleva un proyecto de este tipo, este trabajo propone una metodología para estimar el valor de añadir tanto la flexibilidad de retrasar algunas de las inversiones asociadas al proyecto como la flexibilidad de ampliar la capacidad de generación de energía renovable y la capacidad de producción de hidrógeno como decisiones separadas. En concreto, utilizamos un método llamado Compound Least Squares Monte Carlo, que puede servir para aplicar el análisis de opciones reales a los procesos de decisión de inversión en varias etapas. Ilustramos la metodología propuesta utilizando un caso hipotético, basado en el norte de Chile. Nuestros resultados numéricos muestran que, en el 86,74% de los casos, es óptimo invertir en una planta de producción de hidrógeno, realizando una inversión multietapa en energías renovables y luego en capacidad de producción de hidrógeno verde en el 100% de estos escenarios. En el resto de los casos, nuestros resultados sugieren invertir únicamente en capacidad de generación de energía renovable. Además, el Valor Actual Neto esperado del proyecto que permite las inversiones compuestas es un 1.186,5% más rentable que un enfoque que obliga al inversor a tomar todas las decisiones de inversión en un solo período.

Palabras clave: *Hidrógeno verde, Producción de hidrógeno, Least Square MonteCarlo, Opciones reales, Energías renovables*

ABSTRACT

Many countries have already developed policies and strategies for a green hydrogen economy and, accordingly, the private sector has already started projects to produce it. Given the large uncertainty that a project of this type entails, this paper proposes a methodology to estimate the value of adding both the flexibility of delaying some of the investments associated with the project and the flexibility of expanding the renewable-energy generation capacity and the hydrogen-production capacity as separate decisions. Specifically, we use a method called Compound Least Squares Monte Carlo, which can be used as a way to apply real options analysis to multi-stage investment decision processes. We illustrate the proposed methodology using a hypothetical case, based on Northern Chile. Our numerical results show that, in 86.74% of the cases, it is optimal to invest in a hydrogen production plant, making a multi-stage investment in renewables and then green hydrogen production capacity in 100% of these scenarios. In the rest of the cases, our results suggest investing only in renewable energy generation capacity. Furthermore, the expected Net Present Value of the project allowing compound investments is 1,186.5% more profitable than an approach that forces the investor to make all investment decisions in the first period.

Keywords: *Green hydrogen, Hydrogen production, Least Square MonteCarlo, Real Options, Renewable energy*

1. INTRODUCTION

The world is moving towards the decarbonization of energy systems. One strategy for pursuing this goal that has been encouraged by several governments is green hydrogen as a low-carbon fuel (IRENA, 2018).

Hydrogen (H_2) is the simplest and most abundant element in the universe, although it is not naturally found in its pure state. There are different ways to produce H_2, some of them with significant Greenhouse Gas (GHG) emissions. H_2 can be extracted from fossil fuels and biomass, from water through electrolysis, or a combination of both mechanisms. Currently, the main source of H_2 production is natural gas, which accounts for 75% of annual world production (70 million tons of H_2). The second source of H_2 is coal. A small fraction of H_2 production is from oil or electricity. Less than 0.1% of current H_2 production is through electrolysis (IEA, 2019). The advantage of the electrolysis is that by splitting the H_2 from the oxygen in the water molecules can produce H_2 in a GHG-emission-free manner. However, this process requires a considerable amount of electricity to feed the electrolysis H_2 production plants. Thus, H_2 production through electrolysis is green only if the electricity comes from renewable sources.

The cost and production potential of green H_2 depend on the availability of electricity from renewable sources. This is because the electricity cost is the main operating cost of a H_2 production plant (IEA, 2019). As a reference, in 2020 the average cost of producing H_2 by electrolysis was of the order of 3 USD/kg H_2 in China using renewable sources (without including renewable energy investments) and close to 5 USD/kg H_2 when using only grid electricity (without including grid investments) (IEA, 2019).

The International Renewable Energy Agency (IRENA) estimates that the cost of producing green H_2 using solar power will drop to 33% of the current value by 2050 (IRENA, 2019a). The two primary drivers are a 25% reduction in renewable energy costs by 2050 and a 50% reduction in the cost of electrolyzers by 2050.

The Hydrogen Council performed an analysis of 35 representative uses of H_2 and predicted that 22 of them will be cost-competitive with other low-carbon alternatives by 2030 and these uses correspond to approximately 15% of global energy consumption. These factors imply an important future role for H_2 as an energy carrier (Hydrogen Council, 2020).

The growing interest in the development of a H_2 economy can be seen in the efforts of many countries to develop an energy strategy that incentivizes green H_2 production. As illustrated in Fig. 1, the entire European Union and other twelve countries already have a green H_2 strategy, with nineteen others in the process of drafting a strategy, and several others in preliminary discussions (World Energy Council, 2021).

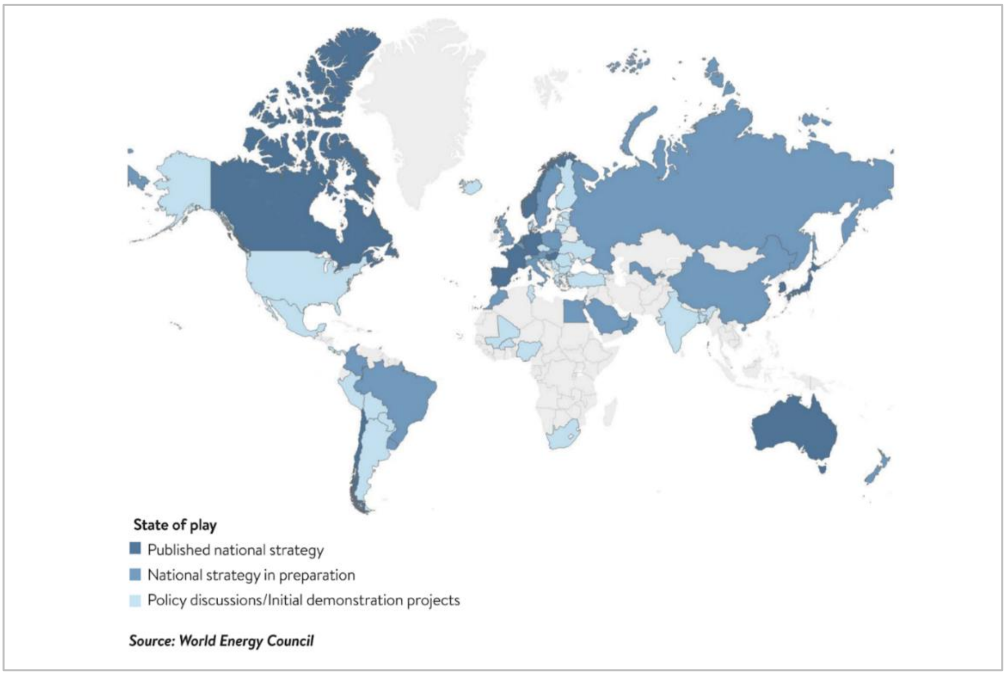

Fig. 1. Overview map of the countries activities towards developing a H_2 strategy

Nonetheless, there are still many uncertainties affecting the financial viability of H_2 production projects. Real Options (RO) analysis is a methodology commonly used when performing economic evaluations in the presence of uncertainty. A widely used RO analysis method is the Least Squares Monte Carlo (LSM) algorithm, proposed by Longstaff and Schwartz (2001) to value American options by simulation.

In this paper, we employ a LSM-based methodology that provides an estimate of the value of adding the flexibility of delaying some of the investments and the flexibility of expanding the renewable-energy generation capacity and the H_2 production capacity in a compound manner. The "compound" feature of the methodology refers to the possibility that the investor makes investment decisions as many times as desired within an investment horizon, in a multi-stage manner. For this reason, we call this method the Compound Least Squares Monte Carlo (CLSM).

The hypothesis of this thesis is that given the uncertainties that arise in energy projects, in this case, in the implementation of a green hydrogen plant, the most convenient method for project valuation is the CLSM method mentioned above. In accordance with the proposed hypothesis, the general objective of this thesis is to develop an economic valuation of the implementation of a green hydrogen plant that allows quantifying the advantage of analyzing the project with flexibilities in the economic evaluation, i.e., with the CLSM methodology.

Our methodology assumes that the investor has the option of investing in different levels of renewable-energy generation capacities and different levels of electrolyzer capacities at different times during the investment horizon. The investor is able to invest in multiple periods during the investment horizon, with the only constraint that the capacity of renewable-energy generation and/or H_2 production can only increase.

The returns from these investments on renewable energy and/or electrolyzer capacity depend on a number of variables that affect the incomes and costs associated with these investments, such as the electricity price, the H_2 price, the up-front cost of renewable-energy generation, and the up-front cost of electrolyzers. Given the large uncertainty of these variables with respect to their future behavior, we model them as Geometric Brownian Motion (GBM) processes.

For our case study applied to Northern Chile, we evaluate the proposed methodology in assessing the value of adding flexibility in the implementation of a H_2 production plant. We consider Northern Chile because of its high solar potential (the highest in Latin America and second-highest worldwide) and potential for achieving the lowest average costs in producing green H_2 according to a study performed by InvestChile

(CORFO, 2019a). Our numerical results show that it is always economic to make some investments in renewable-energy generation capacity, H_2 production capacity, or both. In 86.74% of the scenarios, investing in both renewable-energy generation capacity and H_2 production capacity in a compound manner (i.e., making investments in two or more steps) yields the highest realized payoff for the investor. In the remainder of the simulated scenarios, the highest realized payoff is achieved by investing only in renewable-energy generation capacity because selling renewable-energy power becomes more profitable than selling H_2. We also compare different project valuation methods (rigid investment, LSM and, CLSM), concluding that the flexibility to postpone investment yields economic benefits in the vast majority of cases. Furthermore, when the compound flexibility to expand renewable generation and electrolyzer capacity in a multi-stage way is allowed, these economic benefits become even larger.

The rest of the paper is organized as follows. Section 2 presents a review of the relevant literature. Section 3 explains the CLSM assessment methodology proposed and the main assumptions made in the model. Section 4 illustrates the proposed methodology in a case study based on real-world data and presents our results. Given the large uncertainty associated with these projects, a comprehensive sensitivity analysis is performed in Section 5. Specifically, Section 5 presents 16 sensitivity analyses, where we vary the most relevant model parameters, studying the impact of these changes in the investment strategies (i.e., rigid, flexible, and compound investments) and the project net present values (NPV). Finally, Section 6 presents our conclusions.

2. LITERATURE REVIEW

In this section, we present a literature review on three relevant topics related to this paper. First, we analyze the state of the art in electrolysis H_2 production. Then, we review the methodology of real options analysis and its application to energy-related studies. Finally, we analyze different real options methods applied to green H_2 production projects.

2.1 Electrolysis Hydrogen Production

The electrolysis process is a technique of decomposing water (H_2O) into oxygen and hydrogen using electric current (Speight, 2020). Depending on the source of the current used, the H_2 obtained is classified into gray or green. We assume that, if the electricity used is not from a 100% renewable source, the output is “gray hydrogen.” Conversely, when electric power comes from a 100% renewable source, the output is “green hydrogen”.

Due to the decreasing costs of renewable electricity, particularly from solar photovoltaics (PV) and wind power, there is a growing interest in producing green H_2 by electrolysis (Nikolaidis & Poullikkas, 2017). Hurtubia & Sauma (2021) analyze the economic and environmental consequences of supplementing the power supply of a green H_2 production plant (running only using renewable energy) with electricity from the grid during the time the renewable energy is not available. Yukesh Kannah et al. (2021) provide insights into the techno-economic analysis of various H_2 production methods, identifying the main factors governing the cost of H_2 production, such as feedstock and capital cost.

Glenk & Reichelstein (2019) model the production of H_2 from renewable energy through a power-to-gas process, from an investor's perspective, applying their model to Germany and Texas. Kurtz et al. (2018) study the economic feasibility of integrating H_2 as an alternative in the US transportation sector. Liu et al. (2020) conduct a comprehensive feasibility study on the production and utilization of wind-power-generated green H_2. Mohsin et al. (2018) consider large-scale applications using surplus renewable energy and natural gas pipeline transportation in China, while Xie et al. (2021) perform a similar study, but applied to a hydrogen-powered data center. At a more system-wide level, Pan et al. (2020) propose a bi-level mixed-integer optimization model to measure the impact of the H_2 production on the power-system expansion planning, emphasizing the role of H_2 in an energy system.

Although there are an increasing number of economic studies related to H_2, only few of them (mentioned later) apply a real options approach to deal with the large uncertainty that exists in these types of projects. In the next subsections we show that using a real options approach may help in assessing the variability that is intrinsic to these type of projects.

2.2 Real Option Analysis in Energy Related Projects

As mentioned, there is large uncertainty about the future energy markets due to technological change and climate policy goals for the energy sector. When making project investment decisions, an investor would prefer to make sequential decisions in response to the evolution of the associated markets. This is exactly where the rigid discounted cash flow method differs from real options analysis, as a method for evaluating investment projects. In rigid discounted cash flow, the investor takes a passive attitude once the initial investment is made, while, in real options analysis, some flexibilities (such as postponing, expanding, or abandoning the project) are incorporated, reflecting the investor's option to strategically react throughout the project (Hassi et al., 2022).

Real options analysis has been applied in multiple studies related to power systems. Binder et al. (2017) consider the option to upgrade or reconfigure hybrid electric system configurations in response to economic and technological changes that are uncertain at the beginning of the project horizon. Schachter & Mancarella (2016) consider the option to delay or accelerate investment decisions, waiting until at least some of the uncertainties are resolved and changing the system design of the project involving smart grids and low carbon energy systems. Locatelli et al. (2016) evaluate the strategy of waiting for a change in the market conditions before investing in energy storage systems in the UK. Moon & Baran (2018) incorporate the option to defer the investment in the use of residential PV systems, while Hassi et al. (2022) add the option of expanding the capacities of a residential PV-storage system in multiple decision stages.

In addition, real options analysis has been repeatedly applied in case studies related to the energy area. Mariscal et al. (2020), Henao et al. (2017), Pringles et al. (2014) and Rios et al. (2019) use it to assess the value of adding flexibility to Transmission Expansion Planning (TEP) projects, showing that traditional methods usually recommend suboptimal investment decisions due to the large uncertainty in deregulated power markets. Similar type of analyses using real options are performed by Lee (2011) in the case of a wind power project and by Santos et al. (2014) for a hydroelectric power plant.

2.3 Real Options Analysis and Hydrogen Projects

The large uncertainty associated to the factors affecting H_2 projects (such as the price of electricity, the price of H_2, the PV module investment cost and the electrolyzer investment cost) has led to an increasing interest in real options analysis for the valuation of these projects. This is mainly because real options analysis incorporates flexibilities in the investment decision process, allowing the investor to react strategically to new information throughout the project investment horizon. However, upon our knowledge, only two works have used real options to assess H_2 production investment decisions.

One of the first papers that combine these topics is Kroniger & Madlener (2014), who investigate the economic feasibility of H_2 production and storage using excess electricity generated with wind power plants. For the analysis, they applied Monte Carlo simulation and real options analysis to evaluate two possible scenarios. These authors are the first to apply Monte Carlo methods to a hybrid wind power and H_2 storage system, finding significant benefits of applying the proposed approach. A potential shortcoming of their method is that real options are not evaluated in a compound way, which, according to Machiels et al. (2020), corresponds to a significant research gap in large projects' evaluations, giving an incomplete overview of these megaprojects.

More recently, Van den Boomen et al. (2021) apply compound real options analysis to optimize time-varying expansion strategies for a H_2 pipeline network in the port of Rotterdam under an uncertain demand development. They do not emphasize the option value, but rather the path to be taken by the investor. Furthermore, Van den Boomen et al. use a decision tree analysis methodology, which can present complexities in the tree formation and difficulties in reading and interpreting the results, as opposed to the Monte Carlo simulation method that offers more accurate and realistic results (Machiels et al., 2020).

In this paper, we use an extension of the LSM method of Longstaff and Schwartz (2001), called Compound Least Squares Monte Carlo (CLSM), first used by Hassi et al. (2022). In our context, CLSM is used to evaluate the implementation of a green H_2 production plant, in which the investor has the option (but not the obligation) to invest in multiple stages and in multiple combinations of renewable-energy generation capacity and electrolyzer capacity levels within an investment horizon.

3. METHODOLOGY

We consider an investor with access to grid electricity, and who is interested in developing a H_2 production plant. For simplicity, we will consider that only PV solar power is available to be installed near this plant and in addition to the access to the energy from the grid. The investor can invest in the technology needed to produce power and/or H_2 (i.e., PV modules and/or electrolyzers[1], respectively) several times, always scaling up to higher capacities. Investments are made within the so-called "investment horizon" (T_{inv}). The investor is assumed to continue to use the same PV-solar-power and electrolyzer capacities installed at the end of T_{inv}, during a so-called "valuation horizon" ($T - T_{inv}$).

According with this investment framework, there are several possible states of installed capacity in the plant, which result from the combination of the different capacity levels of solar PV power and electrolyzers. We assume that the investor is free to install only PV capacity (in this case, she can only sell power), only electrolyzers (in this case, she can only sell gray H_2, produced using grid power), or a combination of both (in this case, she can sell power and H_2); and she can move from any state to another with higher capacity levels during the investment horizon. She starts in a state "S_0" where there are no PV modules nor electrolyzers installed. Then, over the investment horizon, she can choose to invest only once (following a "Single Transition Path") and remain in that state for the rest of the valuation horizon, or she can choose to make investments in multiple periods (following a "Multiple Transition Path") and remain in the final state for the rest of the valuation horizon. Consequently, the investor has many paths she can take, investing in capacity associated to one or more states, always scaling up within the investment horizon.

[1] We assume the electrolyzer has a 100% usage, either as on-grid or off-grid, as in (Kroniger & Madlener, 2014).

To account for the large uncertainty existing in a H_2 production investment decision, Geometric Brownian Motion (GBM) processes were used to model the price of electricity ($E(t)$), the price of H_2 ($H(t)$), the PV module investment cost ($M(t)$) and the electrolyzer investment cost ($Z(t)$). Equations (1) – (4) describe these processes:

$$dE(t) = E(t) \cdot \alpha_E \cdot dt + E(t) \cdot \sigma_E \cdot dW_{EH} \tag{1}$$

$$dH(t) = H(t) \cdot \alpha_H \cdot dt + H(t) \cdot \sigma_H \cdot dW_{EH} \tag{2}$$

$$dM(t) = M(t) \cdot \alpha_M \cdot dt + M(t) \cdot \sigma_M \cdot dW_M \tag{3}$$

$$dZ(t) = Z(t) \cdot \alpha_Z \cdot dt + Z(t) \cdot \sigma_Z \cdot dW_Z \tag{4}$$

where α, σ, and dW correspond to the drift, the volatility, and the increment of the Wiener processes, respectively. We used the same increment of the Wiener process (dW_{EH}) for the electricity price and the H_2 price because of the existing strong correlation between them.[2] The starting point of the GBM is estimated based on data from existing studies. In Section 4, we estimate the parameters of the GBMs used in our case study with data from the Chilean power market. For illustrative purposes, Fig. 2 shows the evolution of the relevant variables of the GBMs in 20 of the scenarios used in that case study.[3]

[2] More than half of the H_2 production cost is due to the cost of electricity (IEA, 2019).
[3] In the context of the problem we are dealing with in this work, the values of the variables modelled with GBMs never reach negative values, which we verified in the case study presented in Section 4. If this were the case in a different context, we could easily solve this issue applying logarithms to equations (1)-(4) in order to completely eliminate the possibility of obtaining negative values.

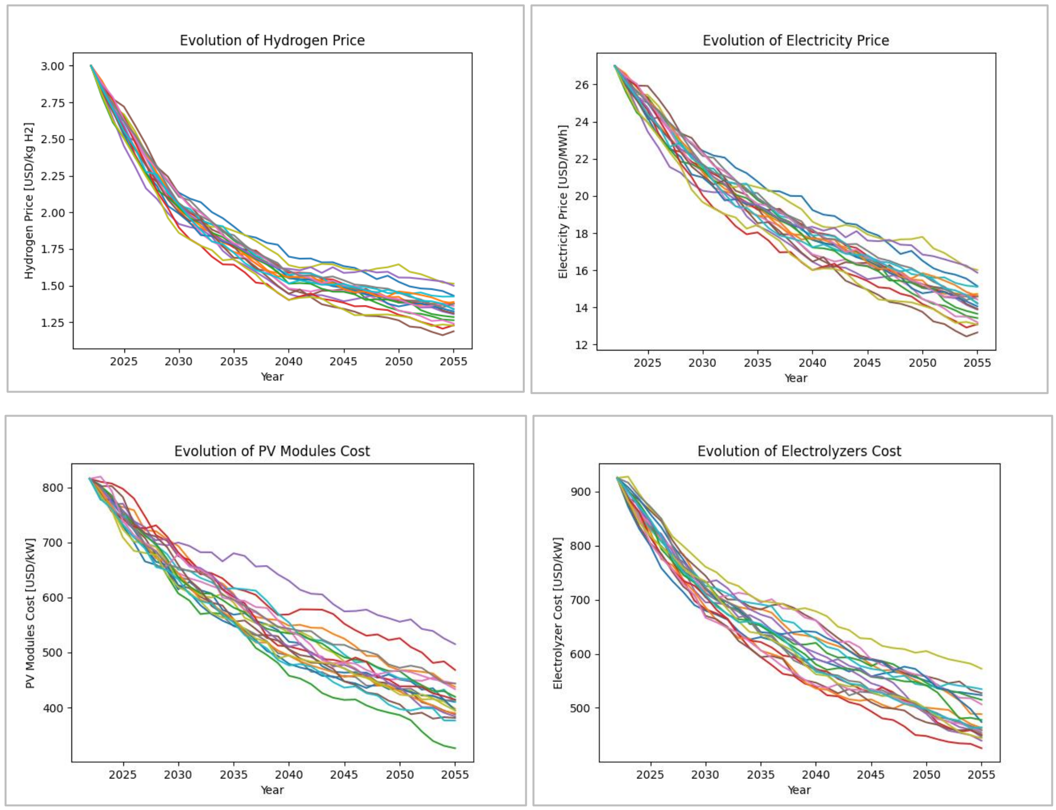

Fig. 2. Evolution of prices and investment costs (using 20 scenarios, for illustrative purposes).

3.1 Rigid Benefits and Costs

The investor benefits from being in a certain state at time *t* can come from the sale of power and/or the sale of H_2. If the investor only has PV solar power capacity installed, then she can only obtain benefits from selling power. If the investor only has H_2 production capacity installed, then she can only obtain benefits from selling gray H_2. Finally, if the investor has PV solar power capacity and H_2 production capacity installed, then she can obtain benefits from selling green H_2 (produced by electrolysis using electricity from the PV solar power installed, i.e., off-grid production), gray H_2 (produced by electrolysis using electricity from the grid, i.e., on-grid production), and power (in case of having a surplus of PV solar power generation).

The investor costs associated with being in a certain state at time *t* are related with the initial capacity investment cost, the investment costs associated with the replacement of PV modules and electrolyzers after reaching their lifetime, and the salvage investment costs at the end of the valuation horizon, as well as the operating costs, mainly involving the cost of the electricity used for producing gray H_2.

3.1.1 Rigid Benefits

Formally, moving from one state S_i to another state S_j will confer benefits that are computed as the equivalent of the net present value of the annual cash flows of moving from state S_i to state S_j from time $\hat{t}$ until the end of the valuation horizon (T). This value will be called the rigid benefit and, assuming a discount rate *r*, is obtained as follows:

$$RB_{S_i \to S_j}^{\hat{t}} = \sum_{t=\hat{t}}^{T} (B_{S_j}^{t} - B_{S_i}^{t}) \cdot e^{-r\,(t-\hat{t})} \tag{5}$$

where $B_{S_i}^{t}$ corresponds to the benefits obtained in state *i* at time *t*.

As mentioned before, benefits (profits) in a state S_i come from three components: power, gray H_2 and green H_2 sales. These components vary depending on the state: (i) in the case of having only PV modules, power is sold during the hours that solar power is produced; (ii) in the case of having only electrolyzers, gray H_2 is produced 24 hours a day and is sold using electricity from the grid; and (iii) when the investor has both renewable generation and electrolyzer capacity, three scenarios can occur depending on the capacities of the PV modules and the electrolyzers:

- If the installed capacity of the PV modules is equal to that required by the electrolyzers, then the investor sells green H_2 during the hours PV solar power is generated and gray H_2 during the hours when the electrolyzer is connected to the grid (because PV solar power is not available).
- If the installed capacity of the PV modules is larger than that required by the electrolyzers, then the investor sells the surplus of electricity produced by the PV modules and the green H_2 produced during the hours PV solar power is generated, as well as gray H_2 during the hours the electrolyzer is connected to the grid (because PV solar power is not available).
- If the installed capacity of the PV modules is smaller than that required by the electrolyzers, then the investor sells green H_2 during the hours solar energy is generated and gray H_2 during all hours (selling some gray H_2 during the same hours PV solar power is generated, by being connected to the grid, and selling full-capacity gray H_2 during the time the electrolyzer is only connected to the grid (because PV solar power is not available). [4]

Consequently, the benefits per state are calculated as follows:

$$B_{S_i}^t = (EB_{S_i}^t + GHB_{S_i}^t + VHB_{S_i}^t) \cdot 365 \tag{6}$$

where $EB_{S_i}^t$, $GHB_{S_i}^t$ and $VHB_{S_i}^t$ correspond to the daily profit from the sales of electricity, gray H_2, and green H_2 in state S_i, respectively. We simply multiply by 365 to obtain the annual profit in state S_i. This means that we are assuming that each day

[4] As mentioned before, it is always convenient that the electrolyzer is operated with 100% usage; i.e., 100% of the hours of the day (Kroniger & Madlener, 2014). For this reason, all the cases consider some gray H_2 production.

of plant operation is the same throughout the year.[5] The first component in the right-hand side of (6) is computed as:

$$EB_{S_i}^t = (Q_{S_i} - U_{S_i})^+ \cdot E^t \cdot hr_{E,S_i} \tag{7}$$

where $(*)^+$ represents the maximum value between 0 and *, Q_{S_i} corresponds to the power generation capacity of the PV modules $[MW]$ in S_i, U_{S_i} is the power capacity used by the electrolyzers $[MW]$ in S_i, E^t is the electricity price $[\frac{USD}{MWh}]$, and hr_{E,S_i} is the number of hours with PV solar power generation in S_i during a day of plant operation.

The second component in the right-hand side of (6) is computed as:

$$GHB_{S_i}^t = H_{S_i} \cdot P^t \cdot hr_{G,S_i} \cdot \frac{1}{LHV^t} \tag{8}$$

where H_{S_i} is the H_2 production capacity of the electrolyzers $[MW]$ in S_i, P^t is the price of H_2 in $[\frac{USD}{kg\ H_2}]$, hr_{G,S_i} is the number of hours producing gray H_2 in S_i during a day of plant operation, and LHV^t corresponds to the H_2 Lower Heating Value $[\frac{MWh}{kg\ H_2}]$ (i.e., the amount of energy needed to produce 1 kg of H_2).

Finally, the third component in the right-hand side of (6), the daily profit from the sales of green H_2 in state S_i is computed as:

[5] In this model, for simplicity reasons, we are assuming that each day of plant operation is the same throughout the year and, consequently, the amount of solar power generated and/or H_2 produced every day is fixed, for a given state. However, the model could be easily extended to account for solar radiation variability throughout the year by considering different values of $EB_{S_i}^t$, $GHB_{S_i}^t$ and $VHB_{S_i}^t$ depending on the season or month of the year considered.

$$VHB_{S_i}^{t} = H_{S_i} \cdot (P^t + V^t) \cdot hr_{V,S_i} \cdot \frac{1}{LHV^t} \tag{9}$$

where H_{S_i}, P^t, and LHV^t have the same meaning as before, V^t corresponds to a premium on the H_2 price $[\frac{USD}{kg\ H_2}]$ that is added when green H_2 is sold (as compared to the sale of gray H_2), and hr_{V,S_i} is the number of hours producing green H_2 in S_i during a day of plant operation. To estimate the premium V^t that is added to the H_2 price, we approximate this value with the social cost of emitting a kg of GHG emissions, which is estimated as:

$$V^t = EF^t \cdot LHV^t \cdot EC^t \tag{10}$$

where EF^t corresponds to the emission factor of the grid electricity system considered $[\frac{kg\ CO_2}{MWh}]$ (i.e. the amount of GHG released into the atmosphere given a certain energy consumption), LHV^t corresponds to the H_2 Lower Heating Value $[\frac{MWh}{kg\ H_2}]$ (as explained before), and EC^t is the GHG emission cost, which we will assume is the same as the carbon dioxide tax $[\frac{USD}{kg\ CO_2}]$. This tax depends on the country considered.

3.1.2 Rigid Costs

The costs associated with moving from state S_i to state S_j at time $\hat{t}$ ($RC_{S_i \to S_j}^{\hat{t}}$) are divided into four components, as follows.

$$RC_{S_i \to S_j}^{\hat{t}} = SC_{S_i \to S_j}^{\hat{t}} + \sum_{t=\hat{t}}^{T} (REC_{S_i \to S_j}^{t}) \cdot e^{-r\,(t-\hat{t})} - SV_{S_i \to S_j}^{\hat{t}} \cdot e^{-r\,(T-\hat{t})} + \sum_{t=\hat{t}}^{T} (OC_{S_j}^{t} - OC_{S_i}^{t}) \cdot e^{-r\,(t-\hat{t})} \tag{11}$$

$SC^{\hat{t}}_{S_i \to S_j}$ is the initial setup cost and corresponds to the investment that is needed when changing states, within the investment horizon. This investment cost can correspond to the purchase of PV modules or electrolyzers.

The $REC^{t}_{S_i \to S_j}$ corresponds to the replacement cost of the PV modules and electrolyzers, which is incurred because the lifespan of the equipment is sometimes shorter than the valuation horizon. This replacement cost is subject to the same GBM processes describing the investment costs of PV modules or electrolyzers, and it is incurred between $\hat{t}$ and T each time the investor must replace them.

The $SV^{\hat{t}}_{S_i \to S_j}$ is the salvage value that the investor obtains from the components of the equipment at the end of the valuation horizon. Specifically, this value is computed as the product of the investment cost of the PV module and/or electrolyzer at time T and the remaining fraction of the lifespan in that period.

Finally, apart from the investment costs, we assume an operating cost, $OC^{t}_{S_i}$. The operating cost is between 60% and 80% of the total cost of H_2 production in the electrolysis process, while the remaining cost is almost entirely the capital cost of the electrolyzer (CORFO, 2018). The operating cost of a H_2 production plant is mainly the cost associated with the electricity used in the production of H_2. The Balance-of-Plant costs and water treatment costs represent a very small share (<5%) of the operating cost of a H_2 production plant, and, therefore, we consider them to be negligible (CORFO, 2018). Thus, the operating cost $OC^{t}_{S_i}$ is computed as follows:

$$OC^{t}_{S_i} = (U_{S_i} - Q_{S_i})^{+} \cdot E^{t} \cdot hr_{G,S_i} \cdot 365 \tag{12}$$

where U_{S_i}, Q_{S_i}, E^{t}, and hr_{G,S_i} have the same meaning as before.

3.2 Project Valuation

This section provides more details on the Compound Least Squares Monte Carlo (CLSM) methodology for project valuation. For an enhanced understanding, we compare it with two other traditional project valuation methodologies. The first one is rigid valuation, where all investments are made in the first period. The second is the traditional LSM methodology, which gives the single option to postpone an investment. These two traditional methodologies are first introduced and then compared with the CLSM methodology, which gives the investor the flexibility to postpone the investments and to expand the initial capacities in power generation and H_2 production in a multi-stage manner.

3.2.1 Rigid Valuation

As mentioned above, a rigid valuation methodology evaluates an investment in a single state, with a certain capacity of PV solar generation and electrolyzers, and only in year 0, remaining for the rest of the valuation horizon (T) in that same state.

Therefore, the Rigid Net Present Value ($RNPV^0_{S_0 \to S_j}(n)$) for a certain transition from state S_0 to state S_j and each scenario n in year 0 is computed as the difference between the rigid benefits ($RB^0_{S_0 \to S_j}(n)$) and costs ($RC^0_{S_0 \to S_j}(n)$):

$$RNPV^0_{S_0 \to S_j}(n) = RB^0_{S_0 \to S_j}(n) - RC^0_{S_0 \to S_j}(n) \tag{13}$$

Accordingly, the $RNPV_{S_0 \to S_j}$ matrix of all scenarios (N) is as follows:

$$RNPV_{S_0\to S_j} = \begin{bmatrix} RNPV^0_{S_0\to S_j}(0) \\ \vdots \\ RNPV^0_{S_0\to S_j}(N) \end{bmatrix} \tag{14}$$

Thus, the Expected Rigid Net Present Value is obtained by calculating the average among all scenarios.

3.2.2 Single Flexibility Valuation

In this methodology, it is assumed that the investor can invest in a single state, with certain capacity of PV solar generation and electrolyzers, but in any year of the investment horizon (i.e., any time t between 0 and T_{inv}). Analogous to the rigid valuation methodology, a similar matrix of RNPV can be calculated, but instead of doing it only for $t = 0$, it is done for every year between 0 and T_{inv}. Therefore, $RNPV^t_{S_i\to S_j}(n)$, in this case, is:

$$RNPV^t_{S_i\to S_j}(n) = RB^t_{S_i\to S_j}(n) - RC^t_{S_i\to S_j}(n) \tag{15}$$

Then, the $RNPV_{S_i\to S_j}$ matrix is:

$$RNPV_{S_i\to S_j} = \begin{bmatrix} RNPV^0_{S_i\to S_j}(0) & \dots & RNPV^{T_{inv}}_{S_i\to S_j}(0) \\ \vdots & \ddots & \vdots \\ RNPV^0_{S_i\to S_j}(N) & \cdots & RNPV^{T_{inv}}_{S_i\to S_j}(N) \end{bmatrix} \tag{16}$$

Then, for each scenario n, the LSM method applied to the $RNPV_{S_i \to S_j}$ matrix yields the optimal time t^* to invest. This is done by comparing, at each period t, the NPV of investing at t with the continuation value (i.e., the value of having the option, but not the obligation to invest in the future). Thus, the flexible NPV in a given scenario n ($FNPV_{S_i \to S_j}(n)$) is computed as the discounted value of the corresponding element of the $RNPV_{S_i \to S_j}$matrix in the optimal investment time in that scenario:

$$FNPV_{S_i \to S_j}(n) = RNPV^{t^*}_{S_i \to S_j}(n) \cdot e^{\,(-t^* \cdot r)} \tag{17}$$

Finally, the Expected Flexible Net Present Value is obtained by calculating the average among all scenarios.

3.2.3 Compound Flexibility Valuation

In the CLSM methodology, the investor can invest in multiple states and in multiple years within the investment horizon, always increasing the capacity of PV modules and/or electrolyzers. For the investment valuations where only one transition is made (that is, when the investor invests only in a single state during the investment period), the valuation methodology becomes the same as the single flexibility methodology. In contrast, when evaluating investments where more than one state transition are made within the investment horizon, a Compound Net Present Value (CNPV) matrix is needed, with elements computed as follows:

$$CNPV^{t}_{S_i \to S_j \to S_f}(n) = RNPV^{t}_{S_i \to S_j}(n) + CV^{t}_{S_j \to S_f}(n) \tag{18}$$

where $RNPV^t_{S_i \to S_j}(n)$ is defined in (15) and $CV^t_{S_j \to S_f}$ corresponds to the continuation value, calculated using the LSM method, which represents the expected net present value of moving from state S_j to S_f in the future, considering all possible transitions that may occur between both states ($S_j \to S_f$; $S_j \to S_k \to S_f$; $S_j \to S_k \to S_l \to S_f$, and investments within all the investment horizon).

Then, for each scenario n, the LSM method applied to the $CNPV^t_{S_i \to S_j \to S_f}$ matrix yields the optimal times ${t^*}_{S_i \to S_j}$, ${t^*}_{S_j \to S_f}$, etc., in which it is economic to invest. Thus, for a path with more than one transition, the Flexible Net Present Value in a given scenario n ($FNPV^t_{S_i \to S_j \to S_f}(n)$) is computed as the discounted values of the corresponding elements of the $RNPV_{S_i \to S_j}$matrix in the optimal investment times in that scenario:

$$FNPV^t_{S_i \to S_j \to S_f}(n) = RNPV^{{t^*}_{S_i \to S_j}}_{S_i \to S_j}(n) \cdot e^{\,(-{t^*}_{S_i \to S_j} \cdot r)} + RNPV^{{t^*}_{S_j \to S_f}}_{S_j \to S_f}(n) \cdot e^{\,(-{t^*}_{S_j \to S_f} \cdot r)} \tag{19}$$

Finally, the Optimal Flexible Net Present Value of a certain scenario n can be obtained by calculating the maximum FNPV among all the possible investment paths that can be realized, considering all single-transition and multiple-transition paths, as described in (20).

$$OPNPV(n) = Max\ [FNPV^t_{S_i \to S_j}(n);\ FNPV^t_{S_i \to S_j \to S_f}(n)] \tag{20}$$

Finally, the Expected Compound Flexible Net Present Value is obtained by calculating the average among all scenarios.

4. CASE STUDY: H_2 PRODUCTION PLANT IN THE CHILEAN MARKET

We consider an investor interested in developing a H_2 production plant in the north of Chile, with significant PV solar power potential and close to the electric grid. We assume she has the option to invest in two different capacity levels of PV solar power generation (P_{min} and P_{max}) and in two different capacity levels of electrolyzers (E_{min} and E_{max}). In the particular case study analyzed here, we consider the following capacities: $P_{min} = 80MW$; $P_{max} = 160MW$; $E_{min} = 50MW$; and $E_{max} = 100MW$ [6]. As mentioned in the methodology section, we assume she can invest once or several times during the investment horizon. Thus, we consider 9 possible states: $No\ Investment\ (S_0)$; P_{min}; P_{max}; E_{min}; E_{max}; $P_{min} + E_{min}$; $P_{min} + E_{max}$; $P_{max} + E_{min}$; and $P_{max} + E_{max}$. The states and possible transitions among them are shown in Fig. 3; transitions among states are only allowed when moving towards a higher-capacity state.

[6] We considered the minimum capacity of the H_2 production plant to be 1% of the H_2 production estimated in (Chilean Ministry of Energy, 2020) in Chile for 2025 and the maximum capacity of the H_2 production plant to be twice the size of our minimum capacity of the H_2 production plant.

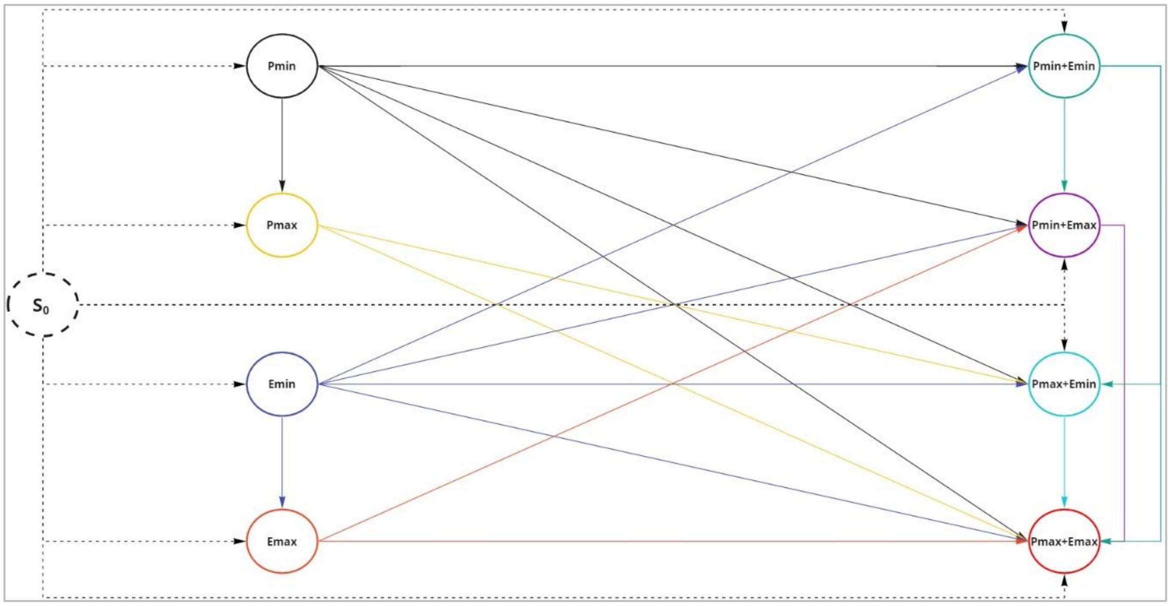

Fig. 3. Possible states and transitions

The investor starts in an initial state S_0 where there are no PV modules nor electrolyzers installed. Then, during the investment horizon, she can choose to invest in a single state and remain there for the rest of the valuation horizon or continue to make investments in multiple states. Consequently, she can take 51 different possible paths in total. For example, all possible paths that pass through P_{max} are: $S_0 \rightarrow P_{max}$; $S_0 \rightarrow P_{max} \rightarrow P_{max} + E_{min}$; $S_0 \rightarrow P_{max} \rightarrow P_{max} + E_{max}$; $S_0 \rightarrow P_{max} \rightarrow P_{max} + E_{min} \rightarrow P_{max} + E_{max}$.

We used an investment horizon of 10 years (i.e., $T_{inv} = 10$) and a valuation horizon of 25 years (i.e., $T = 25$). The lifespan of the PV modules is considered to be 20 years, a conservative financial lifetime of PV modules (Chilean National Energy Commission, 2020), while 10 years is used for the lifespan of electrolyzers (IRENA, 2020)[7]. In addition, we used an annual discount rate (r) of 6%, which is also used in related studies (IEA, 2021; Chilean Ministry of Energy, 2020). We simulate 25,000 scenarios (i.e., $N = 25{,}000$) for each GBM considered to represent the uncertainty associated with the project.

4.1 Parameters Associated with the Benefit and Cost Calculations

The price of electricity and the price of H_2, which are important for the calculation of the investor's revenues (and the investor´s operating costs in the case of price of electricity), are modelled using GBM processes for each scenario. In modelling the GBM for the electricity price, the initial value used for the electricity price is 27 $\frac{USD}{MWh}$, which was obtained by calculating the average of the levelized cost of energy (LCOE) in Chile in 2022 at the national level (Chilean Ministry of Energy, 2020). The drifts used in the GBM were varied using three stages (2022-2030 / 2030-2040 / 2040-2055) and were estimated using the average of the electricity price projections of the same study (Chilean Ministry of Energy, 2020), decreasing linearly over the years. For instance, the values obtained for the years 2030, 2040 and 2055 are 74.9%, 59.3% and 45.8% of the initial value, respectively. For the volatility calculation, we use the volatility of the price projections of four relevant studies: (CORFO, 2019b); (IRENA, 2019a); (IRENA, 2020); and (Chilean Ministry of Energy, 2020), obtaining an average value of 7.35%.

Regarding the GBM associated with the H_2 price, the initial price used is 3 $\frac{USD}{kg\ H_2}$, which corresponds to the conservative scenario for 2022 in (Chilean Ministry of Energy, 2020). We also consider an expected decrease of the H_2 price of 59.7%, 42.9%, and 36% of the initial price in 2030, 2040 and 2055, respectively, decreasing linearly over

[7] Ten years corresponds to the average between the lifespan of electrolyzers in 2020 and the expected lifespan of electrolyzers in 2050.

the years –which is calculated according to the price projections in (Chilean Ministry of Energy, 2020), and a volatility of 7.247%, which is the average volatility of the H_2 price projections in these four studies: (Hydrogen Council, 2020); (IRENA, 2019a); (Chilean Ministry of Energy, 2020); and (Strategy&, 2020).

Regarding the premium paid for the sale of green H_2, we use the estimation described in (10). In this calculation, we consider an initial emissions factor of 383 $\frac{kg\ CO_2}{MWh}$, which corresponds to the current value in the main Chilean power grid (Chilean National Energy Commission, 2021), a final emissions factor of 100 $\frac{kg\ CO_2}{MWh}$ in 2055, and a linear interpolation between both values in the intermediate years. For the H_2 Lower Heating Value, we use the value projections in (IRENA, 2020); resulting in the values 50.7 $\frac{MWh}{kg\ H_2}$ for 2022, 42.6 $\frac{MWh}{kg\ H_2}$ for 2055, and a linear interpolation between both values in the intermediate years. Finally, for the emissions cost calculation, we use 5 $\frac{USD}{kg\ CO_2}$ until 2030, which corresponds to the current Chilean carbon tax value, and then we assume this value linearly increases up to 50 $\frac{USD}{kg\ CO_2}$ by 2040 and then up to 75 $\frac{USD}{kg\ CO_2}$ by 2055.

The number of hours in which electricity (hr_{E,S_i})[8], gray H_2 (hr_{G,S_i}) and/or green H_2 (hr_{V,S_i}) is sold, as well as the number of hours with electricity consumption (hr_{G,S_i}) to produce gray H_2, depends on the investment state. Table 1 summarizes the values associated with each investment state. Electricity is sold if there is only solar PV panels or surplus power, green H_2 is sold when the electricity feeding the electrolyzers is off-grid, and gray H_2 is sold when it is on-grid. The numbers in Table 1 represent hours while the available capacity is represented in parenthesis. For instance, in state P_{max}+E_{min}, energy is sold only from the surplus capacity ($P_{max} - P_{min}$), since a capacity of P_{min} is used during the 9 hours that the solar PV modules operate for the generation

[8] This value defines the plant factor (PF) of the PV solar power plant, which corresponds to the percentage of hours of the day that the PV modules generate electricity. In this case, PF = 9/24 = 37.5%

of green H_2 (E_{min}). The remaining time (15 hours), gray H_2 is generated using energy from the grid (at a capacity of E_{min}).

Table 1. Parameters used for the hours

State	hr_{E,S_i}	hr_{G,S_i}	hr_{V,S_i}
P_{min}	9 (P_{min})	0	0
P_{max}	9 (P_{max})	0	0
E_{min}	0	24 (E_{min})	0
E_{max}	0	24 (E_{max})	0
P_{min} + E_{min}	0	15 (E_{min})	9 (E_{min})
P_{min} + E_{max}	0	15 (E_{max}); 9 (E_{max} - E_{min})	9 (E_{min})
P_{max} + E_{min}	9 (P_{max} - P_{min})	15 (E_{min})	9 (E_{min})
P_{max} + E_{max}	0	15 (E_{max})	9 (E_{max})

The investment costs of PV modules and electrolyzers, which are important for the calculation of the investor's costs, are modelled using GBM processes for each scenario. In modelling the GBM for the PV module investment cost, we use an initial value of 816 $\frac{USD}{kW}$, which corresponds to the 2022 PV module price projection used in (Chilean Ministry of Energy, 2019b). The values for years 2030, 2040 and 2055 are 76.9%, 60% and 46.2% of the initial value, respectively (Palma-Behnke et al., 2019), decreasing linearly over the years; and the volatility is 8.978%, which is the average volatility of the cost projections from these three studies: (CORFO, 2018); (Palma-Behnke et al., 2019); and (IRENA, 2019b). In modelling the GBM for the electrolyzer investment cost, we use an initial value of 925 $\frac{USD}{kW}$ (Chilean Ministry of Energy, 2019a), an expected decrease of 74.6%, 60% and 46.6% of the initial price in 2030, 2040 and 2055, respectively, decreasing linearly over the years –obtained from (IRENA, 2019a), and a volatility of 7.002%, which is calculated as the average volatility of the cost projections from these four studies: (Chilean Ministry of Energy, 2019a); (IRENA, 2019a); (IRENA, 2020); and (Strategy&, 2020).

In summary, the values of the initial price, the drifts, and the volatilities used in the GBM modelled are summarized in Table 2.

Table 2. Summary of the parameters used in modelling the GBM

	Initial Price (2022)	**Drift 2022-2030**	**Drift 2030-2040**	**Drift 2040-2055**	**Volatility**
Electricity Price	$27 \frac{USD}{MWh}$	3.56%	2.30%	1.70%	7.350%
Hydrogen Price	$3 \frac{USD}{kg\ H_2}$	6.24%	3.27%	1.15%	7.247%
PV Module Cost	$816 \frac{USD}{kW}$	3.23%	2.45%	1.73%	8.978%
Electrolyzer Cost	$925 \frac{USD}{kW}$	3.60%	2.14%	1.68%	7.002%

4.2 Numerical Results

This section presents the results obtained in the case study. First (4.2.1), we show the expected NPV and the frequency of each path, after performing 25,000 simulations. Then (4.2.2), we show the frequency of selecting each end node as the optimal decision, and the transitions made in each case. Finally (4.2.3), the NPV values obtained for each type of project valuation in every state are presented.

As a summary of the results, the average NPV (called project NPV) obtained, with the CLSM methodology, for the case study is USD 24,949,418. This was obtained as the result of averaging all the NPVs of the simulated scenarios. This value is 1,187% more profitable than investing in the most frequent terminal state (P_{max}+E_{max}) at $t = 0$ and 118.7% more profitable than investing in state P_{max} at $t = 0$, which corresponds to the most profitable state if the investor is forced to invest only at time $t = 0$.

The results show that for all states, except for those with the only option of investing in PV modules (P_{min} and P_{max}), having the option to choose whether to invest or not yields economic benefits. Performing the project valuation with the flexibility to postpone the investments and to expand the capacities of the PV modules and electrolyzers in multiple steps is strictly more profitable than the rigid valuation in 86.74% of the simulated scenarios and equally profitable relative to rigid valuation in the rest of the simulated scenarios.

4.2.1 Path Selection

Table 3 shows the frequency each relevant path is chosen among the 25,000 simulations. As mentioned before, there are 51 alternative paths; however, results show that only 6 of them are optimally chosen in the different scenarios simulated. Column 2 in Table 3 refers to the frequency a certain path is chosen. Column 3 corresponds to the average NPV of each path. Columns 4, 5, and 6 show the states through which the investor moves (and the median investment time in parentheses). Finally, column 7 shows the terminal state of the path and the frequency at which that state was chosen between parentheses. For example, the row for path 3 in Table 3 recommends investing in path 3 in 0.05% of the scenarios, with an average NPV of USD 23,889,626, and, most frequently, investing in state P_{min} in the eighth year and adding the investment in P_{max} and E_{max} in the ninth year. In addition, the last column shows the frequency (59.54%) with which the terminal state of this path (P_{max}+E_{max}) was the same as other paths, in this case from 3 to 6.

Table 3. Path selection when using the CLSM method

N° Path (1)	**Freq [%] (2)**	**Average NPV [USD] (3)**	**1st Transition (4)**	**2nd Transition (5)**	**3rd Transition (6)**	**Terminal State (7)**
1	13.26	18,341,177	P_{max} (1)			P_{max} (13.26%)
2	27.20	24,525,245	P_{max} (1)	P_{max} + E_{min} (2)		P_{max}+E_{min} (27.20%)
3	0.05	23,889,626	P_{min} (8)	P_{max} + E_{max} (9)		P_{max}+E_{max} (59.54%)
4	46.06	26,767,701	P_{max} (7)	P_{max} + E_{max} (8)		
5	1.21	24,128,021	P_{min} (8)	P_{max} (9)	P_{max} + E_{max} (10)	
6	12.22	26,293,351	P_{max} (7)	P_{max} + E_{min} (8)	P_{max} + E_{max} (9)	

Our results show that, in all scenarios, it is economic to make an investment (because the sum of column 2 is 100%); i.e., choosing state S_0 is never optimal. Only in 13.26% of the scenarios do the results recommend investing only in PV solar power generation (Path 1 in Table 3). And there is no case in which the optimal investment decision is only to invest in electrolyzers. This is because, in the eventual situation that the investor can only produce and sell gray H_2, she does not cover the investment costs plus the operating costs associated with purchasing the electricity needed in these states (E_{min} and E_{max}). This is exactly the reason why electrolysis H_2 production using fossil fuels (i.e., gray H_2) is very small today and, especially, why worldwide interest is primarily in electrolysis H_2 production in those countries with large renewable energy potential, such as Chile.

Summarizing our results, in 86.74% of the cases, it is economic to invest in some capacity to produce H_2, making a compound investment in 100% of these scenarios (Paths 2-6 in Table 3). This means that currently developing a H_2 production plant is less profitable than having sequential investments (i.e., investing first in a PV solar power plant and investing later in some electrolyzer capacity, after some uncertainties are revealed). This result implies that investing today in solar PV is an enabler for pursuing the optimal investment path in electrolysis H_2 production plant in the future.

The path with the highest NPV, equal to $26,767,701, is precisely the most frequently recommended path (Path 4 in Table 3), which, in general, involves investing in the maximum capacity of PV modules in the seventh year, and then investing the following year in the maximum capacity of electrolyzers. In this manner, the investor can take advantage of the economic benefits from selling green H_2 when investment and operational costs decrease.

In general, the results show that, when the investor faces a scenario that favors selling solar PV energy (Paths 1-2 in Table 3), the investment in PV modules should be made as soon as possible because a PV solar power plant is profitable. However, in both Paths 1 and 2, a NPV (column 3) lower than that of the project NPV (i.e., weighted average NPV) is obtained because selling green H_2 is more profitable on average. In fact, the NPV of path 1 (that only sells electricity) is 68.52% of that of path 4 (the most frequently optimal path), while that of path 2 (that includes green H_2 sales with minimum capacity) is 91.62% of that of path 4.

When the investor faces a scenario in favor of selling H_2, the investment must be delayed because, at current costs, it is not economic to invest in a H_2 production plant.

Accordingly, the investment is made in the maximum capacity of electrolyzers in 58.28% of the scenarios (Path 4 and 6 in Table 3), starting in the seventh year in state P_{max} and then moving to the terminal state P_{max}+E_{max}. In 12.22% of those scenarios, there is an intermediate investment of electrolyzers, going from P_{max} to P_{max}+E_{min} and then to P_{max}+E_{max}. For these scenarios, the path NPVs are higher than that of the project NPV because they correspond to the best-case scenarios for the implementation of a H_2 production plant of maximum capacity, given a large revenue from the sale of H_2 and the premium considered in the sale of green H_2, which makes these scenarios much more profitable than only selling electricity.

4.2.2 State Transitions

Fig. 4 shows the optimal recommendations of transitions occurring according to the simulations. The width of the arrows is proportional to the transition frequency. As it can be seen, only five states of the nine possible states are shown because the remaining states do not appear in the simulated scenarios. Within these five states, only three represent terminal states because the frequency is greater than 0% (P_{max}; P_{max}+E_{min}; P_{max}+E_{max}, also shown in column 7 of table 3), while the other two are transient states (counting the initial state, where no investment is made).

The figure makes it evident that moving to state P_{max} is economic in almost all cases. However, in most cases, this is only a transition state (i.e., only 13.26% of the times, it is economic to remain in that state until the end of the valuation horizon), with state P_{max}+E_{max} being the next most recommended transition. It is also remarkable that, in 59.54% of the scenarios, it is in the investor's best interest to invest in state P_{max}+E_{max} as the terminal state.

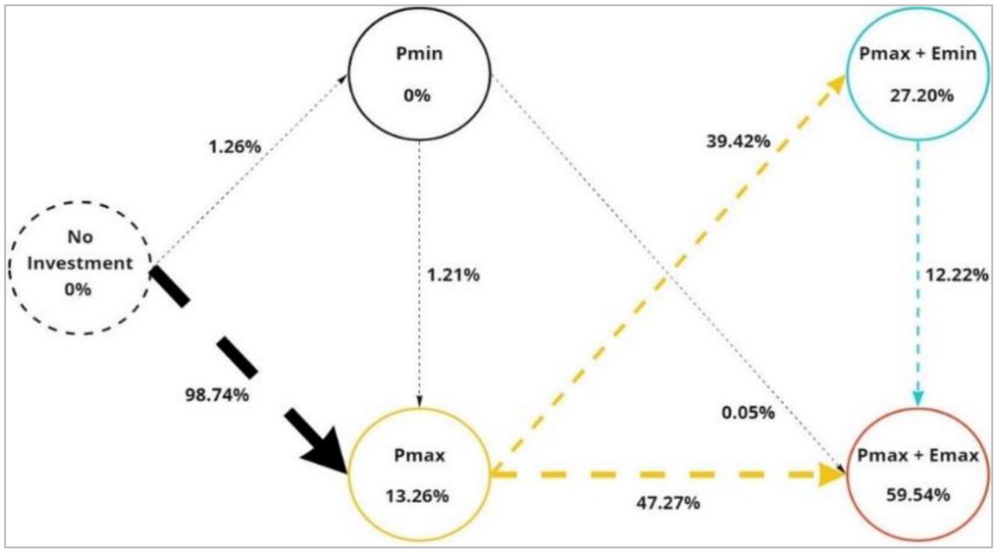

Fig. 4. Scheme representation of state transitions

4.2.3 Value of Single and Compound Flexibility

Table 4 shows a comparison of the NPVs obtained with the different economic valuation methods. Column 1 shows the different states considered. Column 2 corresponds to the number of paths that have that state (S_i) as a terminal state. Column 3 shows the rigid NPV, which corresponds to the NPV of moving from state S_0 to state S_i, where the investor is obliged to invest at time $t = 0$. Column 4 shows the single flexible NPV, corresponding to having the option, but not the obligation, to move from state S_0 to state S_i anytime within the investment horizon (T_{inv}). Column 5 shows the compound flexible NPV, corresponding to the NPV of starting in state S_0 and staying or ending in state S_i, having the option, but not the obligation, to make one or more transitions between states, within the investment horizon (T_{inv}). Column 6 corresponds to the single flexibility value, calculated as the difference between columns 4 and 3. Column 7 corresponds to the compound flexibility value, calculated as the difference between columns 5 and 3. Finally, column 8 corresponds to the difference between the compound and single flexibility value, computed as the difference between columns 7 and 6.

Table 4. Expected NPV and flexibility value in each state

State (1)	**N° Paths** (2)	**Rigid NPV [USD]** (3)	**Single Flex NPV [USD]** (4)	**Compound Flex NPV [USD]** (5)	**Single Flex Value [USD]** (6)	**Compound Flex Value [USD]** (7)	**Dif. Comp - Single Flex [USD]** (8)
$\mathbf{P_{min}}$	1	10,375,783	10,375,783	10,375,783	0	0	0
$\mathbf{P_{max}}$	2	21,012,930	21,012,930	21,012,930	0	0	0
$\mathbf{E_{min}}$	1	-9,708,072	0	0	9,708,072	9,708,072	0
$\mathbf{E_{max}}$	2	-19,241,838	0	0	19,241,838	19,241,838	0
$\mathbf{P_{min} + E_{min}}$	3	779,704	12,278,436	14,382,368	11,498,732	13,602,664	2,103,932
$\mathbf{P_{min} + E_{max}}$	8	-8,754,061	9,905,615	10,177,062	18,659,676	18,931,123	271,447
$\mathbf{P_{max} + E_{min}}$	8	1,839,476	15,103,185	21,547,585	13,263,709	19,708,109	6,444,400
$\mathbf{P_{max} + E_{max}}$	26	2,102,700	22,857,524	26,963,393	20,754,824	24,860,693	4,105,869

As the results of Table 4 show, there are three states where the rigid valuation of the project is negative; that is, being obligated to invest in those states at time $t = 0$ is unprofitable. In two of these (E_{min} and E_{max}), it is actually never economic to invest directly, even when having flexibility in the time of the investment. This happens because, as explained before, the sale of H_2 is not profitable enough by itself to recover all costs in these states. In the case of the P_{min}+E_{max} state, the investor does make the investment when having flexibility because it is not economic to invest in the PV modules and the maximum capacity of electrolyzers at $t = 0$, but having the flexibility to postpone the investments until more favorable conditions occur makes the flexible project profitable.

In the remainder of the states, there are large benefits from flexibility. Postponing investment and/or expanding the capacities during the investment horizon have value. Considering both flexibilities leads always to more (or equally) profitable investment decisions than single flexibility option, which can be seen in the values in column 8 (which are all non-negative). This is expected because the compound flexible NPV includes the single flexible NPV and adds more scenarios where transitions can be made among states in a compound manner. Comparing, for example, the rigid NPV of the most recommended terminal state (i.e., P_{max}+E_{max}) with the case of adding flexibility, adding the ability to postpone the investment increase the expected profitability of the project substantially relative to the rigid investment decision. If the possibility of expanding power generation and H_2 production capacities in a multi-stage manner are added, then the CLSM methodology leads to investment decisions that are even more profitable (in fact, 1,282% more profitable) than with rigid investment decisions.

5. SENSITIVITY ANALYSES

Given the large uncertainty associated with the implementation of these types of projects, we conducted sensitivity analyses to show how the results change if certain model parameters are varied. Given their relevance in the investor’s decisions, the parameters selected were: (i) H_2 price drift (α_H); (ii) Electricity price drift (α_E); (iii) PV Module investment cost (price) drift (α_M); (iv) Electrolyzer investment cost (price) drift (α_Z); (v) Volatilities of the GBM of H_2, electricity, PV modules, and electrolyzers $(\sigma_H, \sigma_E, \sigma_M, \sigma_Z)$; (vi) Discount rate (r); (vii) CO_2 tax $[\frac{USD}{kg\ CO_2}]$; and (viii) Power Plant Factor (PF). For comparison purposes, we use the same simulations of the GBM used before, but varied the selected parameters by plus and minus 25%.

The results obtained are summarized in Table 5. For each sensitivity analysis performed, Table 5 shows the frequency with which a certain path was taken. The colors in Table 5 represent, from dark red to dark green the path frequency (from least, 0%, to most, 100%). It can be seen that, in general, there are four paths that dominate, with results above the 50^{th} percentile (which are P_{max}; $P_{max} \rightarrow P_{max}+E_{min}$; $P_{max} \rightarrow P_{max}+E_{max}$; and $P_{max} \rightarrow P_{max}+E_{min} \rightarrow P_{max}+E_{max}$).

Table 5. Path frequencies for sensitivity analyses

Transition	FREQUENCIES [%]																
1st	P_{min}	P_{max}	E_{min}	P_{min} + E_{min}	P_{max} + E_{max}	P_{min}	P_{min}	P_{max}	P_{max}	E_{max}	P_{min} + E_{max}	P_{max} + E_{min}	P_{min}	P_{min}	P_{max}	P_{min}	No Investment
2nd						P_{min} + E_{min}	P_{max} + E_{max}	P_{max} + E_{min}	P_{max} + E_{max}	P_{max} + E_{max}	P_{max} + E_{max}	P_{max} + E_{max}	P_{max}	P_{min} + E_{max}	P_{max} + E_{min}	P_{max}	
3rd													P_{max} + E_{max}	P_{max} + E_{max}	P_{max} + E_{max}	P_{max} + E_{min}	
4th																P_{max} + E_{max}	
Base Case		13.26					0.05	27.20	46.06				1.21		12.22		
H_2 Drift (-25%)					0.01				87.91						12.08		
H_2 Drift (+25%)		100															
Electricity Drift (-25%)		99.99						0.01									
Electricity Drift (+25%)					0.01		0.05		97.94				0.25		1.75		
PV Module Drift (-25%)		19.42					0.01	57.90	16.09				0.46		6.12		
PV Module Drift (+25%)		4.24			0.03		0.06	6.92	79.26				0.99		8.50		
Electrolyzer Drift (-25%)		53.14						15.17	27.15				0.23		4.31		
Electrolyzer Drift (+25%)		1.03			0.01		0.12	20.67	62.68				2.97		12.52		
Volatilities (-25%)		9.85					0.02	27.22	45.22				1.22		16.47		
Volatilities (+25%)	0.01	19.60		0.01	0.09	0.01	0.11	22.37	51.12	0.01			1.11	0.01	5.53	0.01	0.01
Discount Rate (-25%)		0.04						23.33	69.67				0.97		5.98	0.01	
Discount Rate (+25%)	0.02	5.68		0.69	7.90	0.73	0.06	2.22	81.44		0.01	0.08			0.32		0.85
CO_2 Tax (-25%)		49.21					0.01	19.54	26.51				0.24		4.49		
CO_2 Tax (+25%)		1.27					0.08	18.82	63.18				3.34		13.30	0.01	
Plant Factor (-25%)	0.01		0.01	0.49	0.22	10.32	0.10	0.05	68.16						0.01		20.63
Plant Factor (+25%)		0.45						69.80	29.63						0.12		

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We compare the NPVs in the rigid and compound valuations and the terminal state for each sensitivity analysis. Our results are presented in Table 6, where column 2 shows the project NPV for each sensitivity analysis and column 3 compares the profitability of each case with respect to the base case (which corresponds to the results presented in the previous section). Column 4 shows the most frequent terminal state, column 5 shows the rigid NPV of that terminal state (TS), computed as in Table 4, and column 6 shows the percentage of simulations where compound paths were chosen.

Table 6. Results of the sensitivity analyses

	NPV [USD] (2)	**NPV Difference with respect to Base Case [%] (3)**	**Terminal State (TS) (4)**	**Rigid NPV of TS [USD] (5)**	**Compound Paths [%] (6)**
Base Case	24,949,418		$P_{max}+E_{max}$	2,102,700	86.74
H_2 Drift (-25%)	64,565,647	158.79	$P_{max}+E_{max}$	44,777,106	99.99
H_2 Drift (+25%)	21,292,699	-14.66	P_{max}	21,012,930	0
Electricity Drift (-25%)	29,267,410	17.31	P_{max}	28,929,066	0.01
Electricity Drift (+25%)	35,686,377	43.03	$P_{max}+E_{max}$	14,294,783	99.99
PV Module Drift (-25%)	24,498,087	-1.81	$P_{max}+E_{min}$	676,314	80.58
PV Module Drift (+25%)	27,242,974	9.19	$P_{max}+E_{max}$	3,163,014	95.73
Electrolyzer Drift (-25%)	22,446,975	-10.03	P_{max}	21,012,930	46.86
Electrolyzer Drift (+25%)	28,421,657	13.92	$P_{max}+E_{max}$	5,815,036	98.96
Volatilities (-25%)	24,356,275	-2.38	$P_{max}+E_{max}$	2,094,232	90.15
Volatilities (+25%)	27,101,442	8.63	$P_{max}+E_{max}$	2,128,629	80.28
Discount Rate (-25%)	52,691,205	111.19	$P_{max}+E_{max}$	26,555,372	99.96
Discount Rate (+25%)	9,234,509	-62.99	$P_{max}+E_{max}$	-16,987,316	84.86
CO_2 Tax (-25%)	22,479,644	-9.90	P_{max}	21,012,930	50.79
CO_2 Tax (+25%)	28,588,672	14.59	$P_{max}+E_{max}$	5,776,859	98.73

Plant Factor (-25%)	4,830,803	-80.64	P_{max}+E_{max}	-36,760,215	78.64
Plant Factor (+25%)	58,170,869	133.16	P_{max}+E_{min}	38,253,143	99.55

Table 6 shows that in all cases the NPV of the project is positive, considering all possible paths and the investor's possibility of being able to postpone the investment and expand capacities in a multi-stage manner (column 2). That is, it is always economic to invest when compound investments are allowed. Moreover, in 11 cases (rows of Table 6), it is economic to make compound investments in more than 80% of the scenarios (this is shown in column 6), which shows that flexibility still adds large value when parameters change.

Table 6 also shows that, when there is a 25% decrease in the drift of the H_2 price and when the drift of the electricity price increases by 25%, profits increase relative to the base case because the sale of H_2 is more profitable. In the first case, this is mainly due to the increased income benefit from the sale of green and gray H_2 while the rest of the costs remain constant, and, in the second case, this is due to the low production cost of gray H_2.

In contrast, if there is a 25% increase in the H_2 price drift or if the electricity price drift decreases by 25%, the results show that the investor would be better off focusing on the sale of the renewable energy generated by the PV modules (state P_{max}). In the first case, it is because the low price of H_2 makes a H_2 plant less profitable. The second case is more profitable than the base case because selling PV electricity becomes more lucrative given the higher price of electricity.

One interesting analysis is the variation in the power plant factor (PF), which determines the efficiency of the PV modules installed. The results show that, if the PF decreases by 25%, the NPV decreases by 80.64% relative to the base case. In 20.63%

of the scenarios, it would not be economic to invest (remaining at S_0 is preferred). However, this situation is unlikely to occur in our case study since the plant factor in northern Chile is currently much higher than the roughly 28% obtained in this pessimistic case, where the project NPV is still positive. Increasing the plant factor by 25%, which many observers believe is likely to occur, will bring large benefits to the investor, being 133.16% more profitable than the base case.

The discount rate affects the discounted cash flows of the project. For the base case ($r = 6\%$), the value of a cash flow discounted one year is equivalent to 94.17% of its original value, and after 25 years is 22.31%. For comparison, if the discount rate is increased by 25% ($r = 7.5\%$), these values are 92.77% and 15.33%, and, if it is decreased 25% ($r = 4.5\%$), these values are 95.60% and 32.47%. Therefore, there are large profit differences when discounting the flows at these three discount rates.

The analysis of variations in investment costs for PV modules and electrolyzers and the CO_2 tax, plus and minus 25%, bring changes of less than 15% with respect to the project NPV of the base case. Among these variations, the one that varies the most is the CO_2 tax because it directly influences the premium which affects the revenue from the sale of green H_2. Thus, if the CO_2 tax increases, there are more profits and the results are similar to the base case, but with higher revenues, while if it decreases, in half of the scenarios the results recommend focusing only on the business of a PV power plant (state P_{max}) because it becomes more profitable than selling H_2.

Regarding the variations in electrolyzer prices, differences in profitability are low because, as mentioned, the CAPEX cost of electrolyzers can vary between 15% and 35% of the cost of H_2 production. Therefore, given that revenues would remain the same, a lower investment cost will definitely be more profitable, while a higher investment cost in electrolyzers yields the recommendation to invest only in a PV plant (state P_{max}) in more than half of the cases.

The variations in the prices of the PV modules yield minor differences in the project NPV due to their long lifetime. Variations in the volatilities of the GBMs also have small impacts. Although the number of optimal paths for some scenarios becomes larger as volatilities increase, many of those path have low frequencies; and, therefore, no significant changes can be observed with respect to the base case results.

It is interesting to note that, roughly speaking, the variations that negatively affect the NPVs (i.e., the increase in the hydrogen drift and in the discount rate and the decrease in the plant factor, in the carbon tax, in the electrolyzer drift, in the PV module drift, and in the volatilities) have a smaller impact on the average magnitude of the changes in the NPVs than those that positively affect the NPVs (i.e., the decrease in the hydrogen drift, in the discount rate, and in the energy drift and the increase in the plant factor, in the energy drift, in the carbon tax, in the electrolyzer drift, in the PV module drift, and in the volatilities). This is due to the fact that this is a project where the income from the sale of electricity presents a trade off with the sale of H_2 in case it is more beneficial.

Fig. 5 graphically shows the project NPV for each of the sensitivity analyses performed.

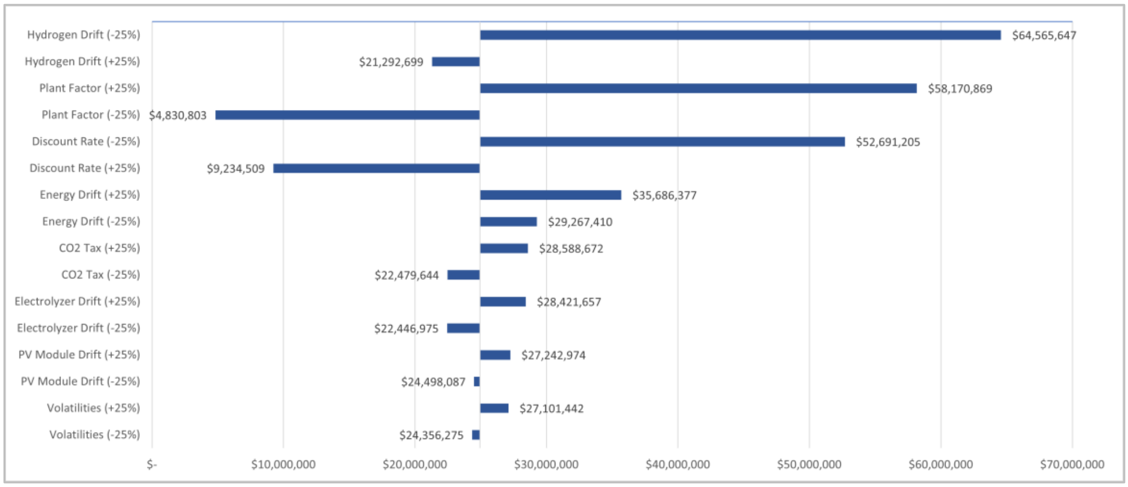

Fig. 5. NPV for each sensitivity analysis performed

Six of the 16 analyses performed show large variations (larger than 20%), and only 2 of them (Plant Factor -25% and Discount Rate +25%) affect the NPV negatively with respecto to the base case, although still maintain a positive NPV for the project. It is interesting to note that in each of the analyses performed, except for the two mentioned above, the average NPV when allowing the flexibilities are higher than the NPV obtained in the best-case scenario when the investor is forced to invest at $t = 0$ (USD 21,012,930). Thus, as mentioned before, adding flexibility to the investment decisions still adds large value when parameters change.

6. DISCUSSION AND CONCLUSIONS

One promising way to achieve a low carbon electricity supply is to use green H_2 production and its derivatives as fuels. This is likely why many countries have already adopted policies and strategies for a H_2 economy. Thus, it is interesting to study the incentives of the private sector to invest in this technology because it has the potential to bring large economic and environmental benefits in the future. Because the cost at which H_2 can be produced is likely to decrease in line with the cost of electricity (main operation cost for electrolysis), this is a timely and important issue.

In this paper, we propose a methodology that estimates the value of an investment project in a H_2 production plant, the optimal path to follow and the years when it is economic to invest, considering that the private investor has the flexibility to postpone the investment and/or to expand plant capacity in a multi-stage manner. For this, the investor can invest in PV modules and electrolyzers on their own or by combining them as many times as she wants and when it is most economic to do so. This methodology, called CLSM, allows consideration of the flexibilities of postponing the investment and capacity expansion decisions, which brings significant benefits because it rules out suboptimal investment decisions that can be taken when ignoring the flexibilities and uncertainties that a project of this type entails.

We applied the CLSM method to a hypothetical case in northern Chile, where we used real data to estimate the value of the flexibilities considered. The results are encouraging, since performing the project valuation having the flexibility to postpone the investments and to expand the capacities of the PV modules and electrolyzers in multiple steps, is strictly more beneficial (1,186.5%) than the rigid valuation, as expected in the hypothesis. Moreover, results imply that it is economic to invest in a H_2 production plant in 86.74% of the simulated scenarios. In 100% of those cases, it is preferable to implement these investments it in a compound way; that is, considering the flexibility of postponing the investment and investing in two or more steps to reach the terminal state. In addition, the sensitivity analyses carried out shows that investments in the project should always be made, varying for some cases the final state in which the investments should occur. In this sense, it is important to emphasize the added value that flexibility gives to the projects related to H_2 production.

For future work, it would be interesting to deepen on the economic analysis of this type of projects since there are still many variables that affect that can be specified with the passing of time and the improvement of the technology. In addition, it is important to emphasize the added value that gives the flexibility for the valuation of projects in the studies to be carried out related to hydrogen and the energy area.

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