Hydrogen Production Economics: A Compound Real Options and Policy Analysis

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A B S T R A C T

We study the decision to invest in a hydrogen production plant that accounts for the uncertainty in future values of the economic variables driving this decision. We provide a methodology for quantifying the benefits and costs of introducing flexibility in the timing and magnitude of investments in renewable-energy generation capacity and the hydrogen-production capacity. We use a compound real options methodology to compare the amount of hydrogen production stimulated by two hypothetical carbon tax policies for Chile, one that starts low, but is monotonically increasing over time and a second that sets fixed tax rate that is equal to the average over time of the increasing tax. We find that the second carbon tax yields a 40 percent increment in expected hydrogen production and a 70 percent increase in the expected net present value from these investments. We also compare these outcomes with two different levels of the volatility in electricity prices, one 50 percent higher than the other, and find small changes in expected hydrogen production and the expected net present value of these investments across the two scenarios.

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

1. Introduction

Green hydrogen is an increasingly popular strategy for decarbonization. (IRENA, 2018). Hydrogen (H_2) is the simplest and most abundant element in the universe, although it is not typically found in its pure state. There are different ways to produce H_2 and some of them produce 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. Less than 0.1% of current H_2 production is through electrolysis (IEA, 2019). The advantage of electrolysis is that by splitting the H_2 from the oxygen in the water molecules H_2 can be produced in a GHG-emission-free manner. This process requires a considerable amount of electricity to feed the electrolysis H_2 production plants, but the H_2 produced is green only if the electricity comes from zero-carbon sources.

Consequently, the cost and output potential of green H_2 depends on the availability and cost of electricity from zero-carbon sources, typically wind and solar sources. This is because the electricity cost is the main operating cost of a H_2 production plant (IEA, 2019). Nevertheless, 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

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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 discussing a strategy (World Energy Council, 2021).

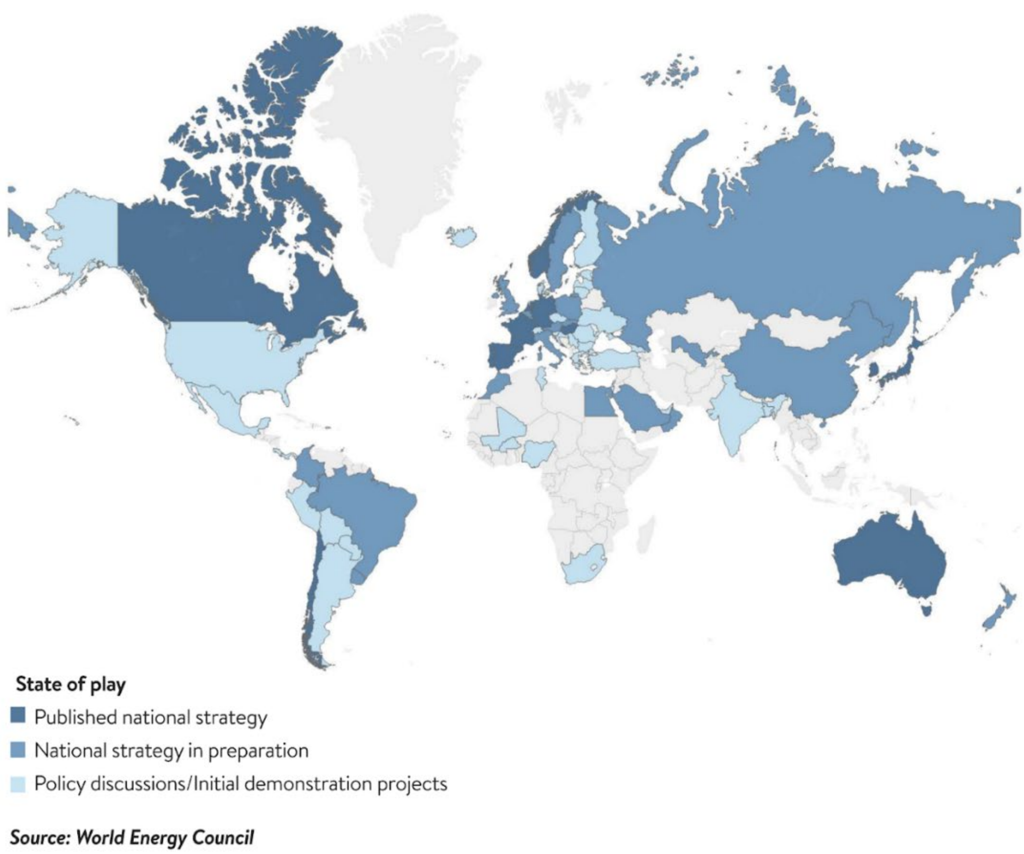

Fig. 1. Overview map of the countries activities towards developing a H_2 strategy

There are still many uncertainties affecting the financial viability of H_2 production projects. Real Options (RO) analysis is commonly used to evaluate irreversible investments in the presence of uncertainty. A widely used RO analysis method is the application of Least Squares Monte Carlo (LSM), proposed by Longstaff and Schwartz (2001) to value American options by simulation.

In this paper, we employ an LSM-based methodology to estimate the value of adding the flexibility of delaying some of the investments in renewable-energy generation capacity and in H_2 production capacity in a compound manner. The "compound" feature of the methodology refers to the possibility that the investor makes (incremental) 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).

Our methodology assumes that investments can occur in different amounts of renewable-energy generation capacity and different levels of electrolyzer capacity at different times during the investment horizon. Investments may occur in multiple periods during the investment horizon, with the only constraint that the accumulated capacity of renewable-energy generation and/or H_2 production cannot decrease over time. The realized returns from investments on renewable energy and/or electrolyzer capacity depend on a number of variables that affect the income and cost associated with these investments, such as the electricity price, the H_2 price, the up-front cost of renewable-energy generation capacity, and the up-front cost of electrolyzer capacity. To capture substantial uncertainty in future values of these variables, we model their evolution using Geometric Brownian Motion (GBM) processes.

For our Northern Chile case study, we apply our methodology to assess the value of adding flexibility in the implementation of a H_2 production plant. We study Northern Chile because of its abundant solar resources and potential for achieving the lowest average cost of producing green H_2 according to a study performed by InvestChile (CORFO, 2019a). For the case of Northern Chile, our modeling results show that it is always profitable to make some investments in renewable-energy generation capacity, H_2 production capacity, or both. For 86% of our base-case 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; not only once) 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 investments yields sizeable 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.

We use our methodology to compare the performance of two approaches to carbon tax policy design. A politically palatable approach to implementing a carbon tax is to start with a modest tax and commitment to increase it over time. In an uncertain environment this is likely to lead to less investment in renewable generation capacity and electrolyzer capacity because of the option to delay investments until the carbon tax is sufficiently high. We compare expected hydrogen production under this carbon tax policy to a fixed carbon tax set equal to average over time of the increasing tax and find a 40 percent increment in expected hydrogen production and a 70 percent increase in the expected net present value in these investments for the fixed carbon tax. This result supports the position that if investors have the option to delay some or all their spending on renewable generation and electrolyzer capacity, the politically palatable approach of setting a low carbon tax with commitment to increase it over time can significantly reduce the amount investment that ultimately takes place. We also use our methodology to compare the expected net present values and expected hydrogen production for two values of the volatility in electricity prices--one 50 percent higher than the other--and find small changes in expected hydrogen production and the expected net present value of these investments across these two values of price volatility.

The rest of the paper is organized as follows. Section 2 presents a review of the literatures on the economics of hydrogen production from electrolysis, the real options approach to modelling investments in energy infrastructure, and modeling investments in green hydrogen production in particular. Section 3 explains our the CLSM assessment methodology and the main assumptions of our model. Section 4 illustrates the proposed methodology in a case study based on real-world data from Chile and presents our modeling results. Section 5 described our comparison of the performance of the two different carbon tax policies and different levels of electricity price volatility. Given the large uncertainty associated with behavior of economic factors driving investments in these projects, a comprehensive sensitivity analysis is performed in Section 6. We present 16 sensitivity analyses that vary most of the model parameters quantifying the impact of these changes on the different investment strategies and net present values (NPV). Section 7 presents our conclusions.

2. Literature Review

This section reviews the literature on three topics. First, we analyze the state of the art in the economic modeling of electrolysis H_2 production. Then, we review the methodology of real options analysis and its application to energy sector investments. Finally, we survey real options methodologies applied to green H_2 production projects.

2.1 Electrolysis Hydrogen Production

The electrolysis process decomposes water (H_2O) into oxygen and hydrogen using an electric current (Speight, 2020). Depending on the source of the electric current, 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 photovoltaic (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 time when 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 conditions in 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 of 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. Xie et al. (2021) perform a similar study, but applied to a hydrogen-powered data center. 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 a few of them, described below, apply a real options approach to model the large uncertainty in the ex-post value of these projects. The next subsection argues that using a real options approach may help in assessing the impact of the variability in the ex-post value of these type of projects.

2.2 Real Options Analysis in Energy Related Projects

There is a large amount of uncertainty about the future energy market outcomes due to technological change and climate policy goals. Consequently, when making project investment decisions, an investor would prefer to make sequential decisions in response to the temporal resolution of these sources of uncertainty. 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 analysis, the investor makes a single initial investment decision, whereas in real options analysis, some flexibilities (such as postponing, expanding, or abandoning the project) are incorporated. These reflect the investor's option to strategically react to the resolution of uncertainty throughout the life of 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 capacity of a residential PV-storage system in multiple decision stages.

Real options analysis has been applied to many case studies related to the energy sector. 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 types 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

There are four major sources of uncertainty associated with valuing H_2 projects: the price of electricity, the price of H_2, PV module investment cost and electrolyzer capacity investment cost. These sources of uncertainty and the ability to sequence the investments allows the investor to react to new information throughout the project investment horizon. These factors support the application of real options analysis to H_2 production projects.

One of the first works 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. They apply Monte Carlo simulation and real options analysis to evaluate the financial viability of a hybrid wind power and H_2 storage system. Machiels et al. (2020) perform a literature review finding a potential benefit of using compound real options analysis to assess the economic feasibility of energy projects. Van den Boomen et al. (2021) apply compound real options analysis (based on decision tree analysis) to optimize time-varying expansion strategies for a H_2 pipeline network in the port of Rotterdam for an uncertain future demand.

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), to model investments in green H_2 production where 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 the investment horizon.

3. Methodology

We consider an investor with access to grid electricity, who would like to develop a H_2 production plant. For simplicity, we assume that only solar photovoltaic (PV) capacity can be installed near this plant in addition to energy from the grid. Investments can be made in the technology necessary to produce electricity and/or H_2 (i.e., PV modules and/or electrolyzers[2], respectively) several times, always scaling up to higher capacities of both technologies. Investments are made within the so-called "investment horizon" (T_{inv}). The investor is assumed to continue to use the same solar-power and electrolyzer capacities installed at the end of T_{inv}, during a so-called "valuation horizon" (T).

We assume there are several possible states of installed capacity for the H_2 plant which result from the combination of the different capacity levels of solar PV capacity and electrolyzers. We assume that investments can be made to install only solar PV capacity (in this case, only electricity is sold), only electrolyzers (in this case, only gray H_2 produced using grid power is sold), or a combination of both (in this case, electricity and green and gray H_2 can be sold). Investments can go from any state to another with higher capacity levels for both solar and electrolyzer capacity during the investment horizon. Investments start in a state "S_0" where there are no PV modules or electrolyzers installed. Then, over the investment horizon, the investor can choose to invest only once (following what we call 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.

Geometric Brownian Motion (GBM) processes are 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 ($Z(t)$) within the investment horizon. Equations (1) – (4) describe these processes:

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

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

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

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

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

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 empirically.[3] The three increments are assumed to be independently distributed. In Section 4, we calibrate 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 four GBMs in 20 of the scenarios used in that case study.[4]

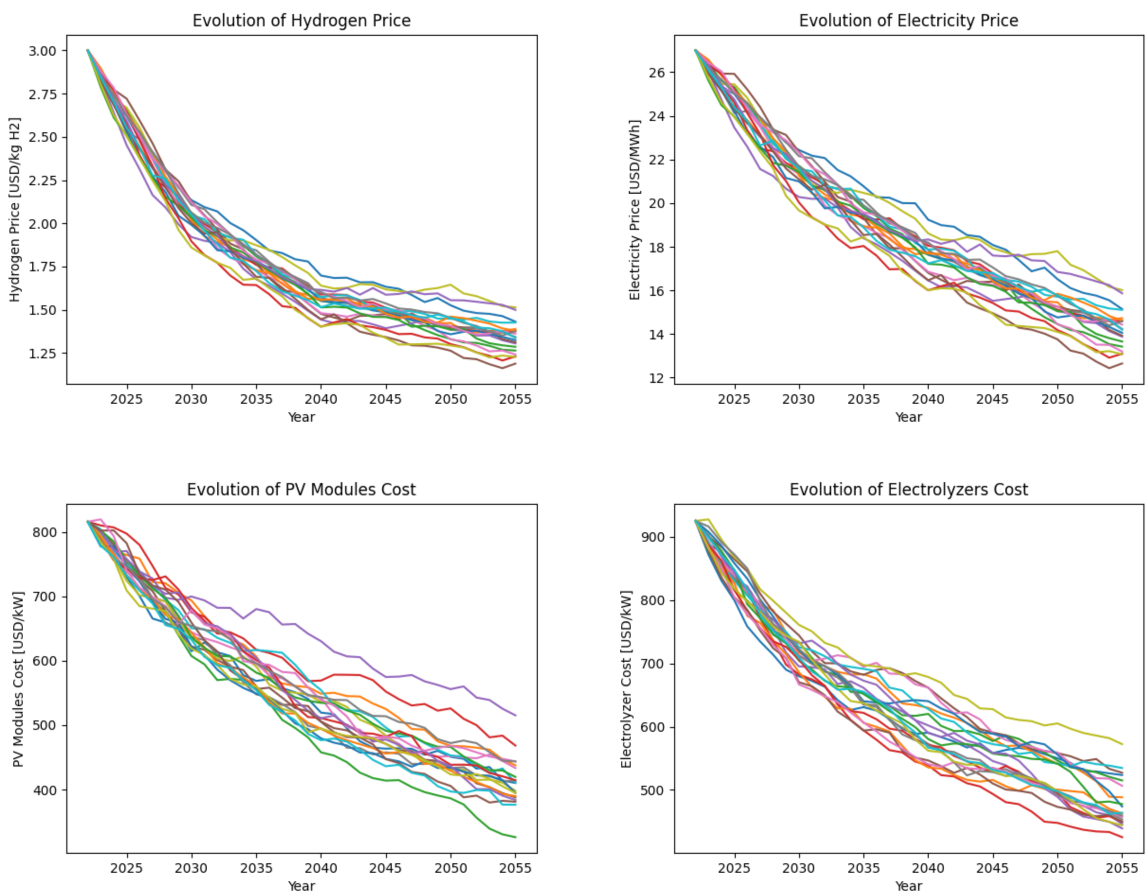

Fig. 2. Evolution of prices and investment costs (using 20 scenarios, for illustrative purposes).

3.1 Rigid Benefits and Costs

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

[3] More than half of the H_2 production cost is due to the cost of electricity (IEA, 2019).
[4] For our problem, the values of the variables modelled with GBMs never reach negative values., This is verified in the case study presented in Section 4.

The investor costs associated with being in a certain state at time t depend on the initial solar PV and electrolyzer capacity investment cost, the investment costs associated with the replacement of PV modules and electrolyzers after reaching the end of their useful lifetime, and the salvage 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.

Benefits and costs are considered "rigid" when the investor is obligated to make a single initial investment decision and remains in that state for the entire time horizon considered. We assign the name "flexible" benefits and costs to the benefits and costs obtained when some flexibilities (such as postponing, expanding, or abandoning the project) are incorporated, reflecting the investor's option to strategically react to the resolution of uncertainty throughout the life of the project.

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 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). Because it involves only one change in states, 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 S_i at time t.

The benefits (profits) in a state, S_i, come from three components: electricity, gray H_2, and green H_2 sales. These components vary depending on the state: (i) in the case of having only PV modules, electricity is sold during the hours that solar energy is produced; (ii) in the case of having only electrolyzers, gray H_2 is produced and sold 24 hours a day 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 solar energy is generated and gray H_2 during the hours when the electrolyzer is connected to the grid (because solar energy 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 solar energy is generated, as well as gray H_2 during the hours the electrolyzer is connected to the grid (because solar energy 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 solar PV energy 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 solar energy is not available). [5]

[5] As mentioned before, we assume the electrolyzer is operated 100% of the hours of the day as in Kroniger & Madlener, 2014. For this reason, all the cases with electrolyzer capacity have some gray H_2 production.

Consequently, the benefits for year t for state S_i 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 average 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.[6] 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 generation capacity of the PV modules $[MW]$ in S_i, U_{S_i} is the capacity used by the electrolyzers $[MW]$ in S_i, E^t is the grid electricity price $[\frac{USD}{MWh}]$, and hr_{E,S_i} is the number of hours selling electricity with solar PV 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 selling 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 electricity needed to produce 1 kg of H_2). The difference between H_{S_i} and U_{S_i} is the electrolyzer efficiency (that is, $H_{S_i} = U_{S_i} \cdot \varepsilon_{S_i}$, with ε_{S_i} being the electrolyzer efficiency in S_i).

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:

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

where H_{S_i}, P^t, and LHV^t have already been defined, 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:

[6] This is equivalent to assuming that each day of plant operation is the same throughout the year and, consequently, the amount of solar energy 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.

$$V^t = EF^t \cdot LHV^t \cdot EC^t \quad (10)$$

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

3.1.2 Rigid Costs

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

$$RC^{\hat{t}}_{S_i \to S_j} = SC^{\hat{t}}_{S_i \to S_j} + \sum_{t=\hat{t}}^{T} (REC^{t}_{S_i \to S_j}) \cdot e^{-r\,(t-\hat{t})} - SV^{\hat{t}}_{S_i \to S_j} \cdot e^{-r\,(T-\hat{t})} + \sum_{t=\hat{t}}^{T} (OC^{t}_{S_j} - OC^{t}_{S_i}) \cdot e^{-r\,(t-\hat{t})} \quad (11)$$

$SC^{\hat{t}}_{S_i \to S_j}$ 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 and/or electrolyzers.

The $REC^{t}_{S_i \to S_j}$ corresponds to the replacement cost of the PV modules and/or 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 average 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--less than 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:

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

where U_{S_i}, Q_{S_i}, E^t, and hr_{G,S_i} have been already defined.

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 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 electricity generation and H_2 production in a multi-stage manner.

3.2.1 Rigid Valuation

The rigid valuation methodology evaluates an investment in a single state, with a certain capacity of solar PV 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 in $t = 0$ and each scenario n 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, the investor can invest only in a single state, with certain amount of solar PV and electrolyzer capacity, 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:

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

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:

$$FNPV_{S_i \to S_j}(n) = RNPV_{S_i \to S_j}^{t^*}(n) \cdot e^{(-t^* \cdot r)} \quad (17)$$

Finally, the Expected Flexible Net Present Value is obtained by calculating the average across 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 is made within the investment horizon, a Compound Net Present Value (CNPV) matrix is calculated, with elements computed as follows:

$$CNPV_{S_i \to S_j \to S_f}^{t}(n) = RNPV_{S_i \to S_j}^{t}(n) + CV_{S_j \to S_f}^{t}(n) \quad (18)$$

where $RNPV_{S_i \to S_j}^{t}(n)$ is defined in (15) and $CV_{S_j \to S_f}^{t}$ 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 ($S_j \to S_f$; $S_j \to S_k \to S_f$; $S_j \to S_k \to S_l \to S_f$).

Then, for each scenario n, the LSM method applied to the $CNPV_{S_i \to S_j \to S_f}^{t}$ 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 ($FNPV_{S_i \to S_j \to S_f}^{t}(n)$) is computed as the discounted values of the corresponding elements of the $RNPV_{S_i \to S_j}$matrix considering the optimal investment times in that scenario:

$$FNPV_{S_i \to S_j \to S_f}^{t}(n) = RNPV_{S_i \to S_j}^{t^*{}_{S_i \to S_j}}(n) \cdot e^{(-t^*{}_{S_i \to S_j} \cdot r)} + RNPV_{S_j \to S_f}^{t^*{}_{S_j \to S_f}}(n) \cdot e^{(-t^*{}_{S_j \to S_f} \cdot r)} \quad (19)$$

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).

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

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

4. Case Study: H_2 Production Plant in the Chilean Market

We consider investment in a H_2 production plant in the north of Chile, with significant solar PV power potential, close to the electric grid. We assume there is the option to invest in two different capacity levels of solar PV power generation (P_{min} and P_{max}) and in two different capacity levels of electrolyzers (E_{min} and E_{max}). In the particular case analyzed here, we consider the following capacities: $P_{min} = 80MW$; $P_{max} = 160MW$; $E_{min} = 50MW$; and $E_{max} = 100MW$.[7] As mentioned in the methodology section, we assume investments may occur 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.

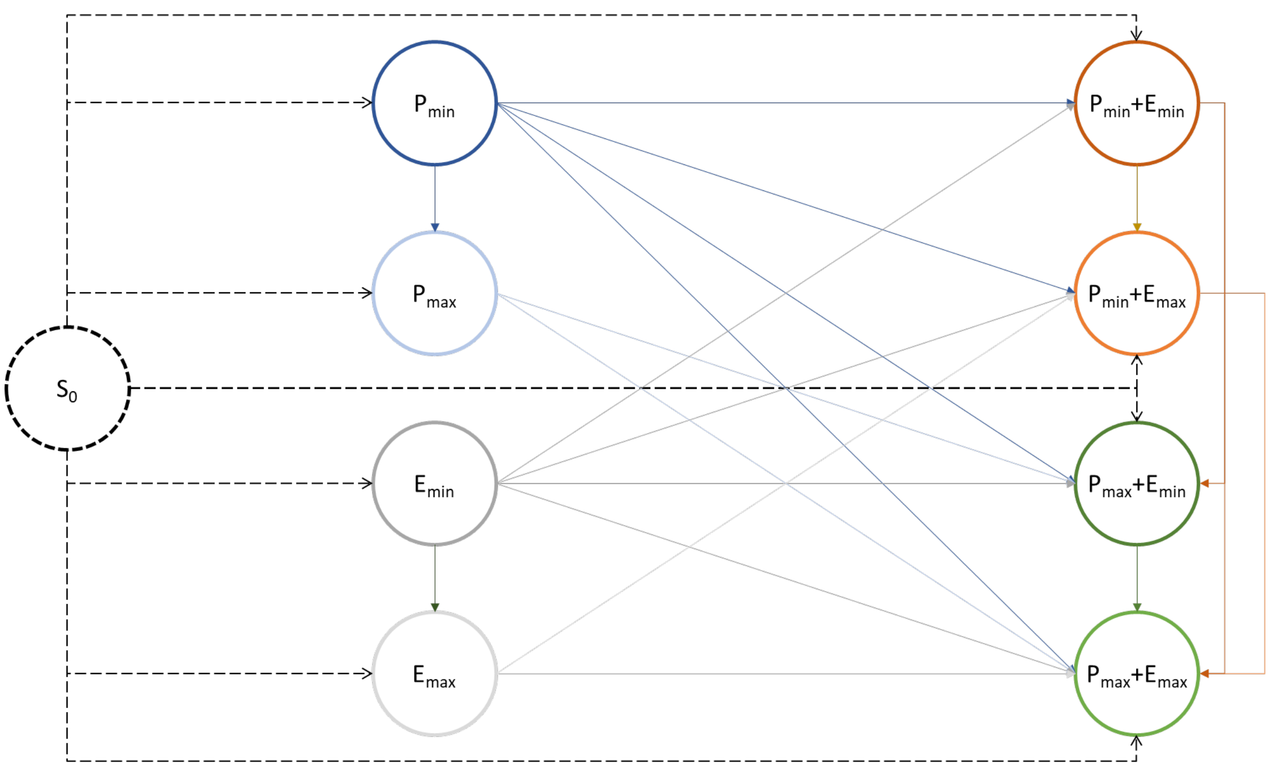

Fig. 3. Possible states and transitions

[7] 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. The difference between P_{min} and E_{min} is due to the electrolyzer efficiency (i.e., $E_{min} = 50\ MW = 80\ MW \cdot \varepsilon$, with ε being the electrolyzer efficiency). The same occurs between P_{max} and E_{max} .

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

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).[8] 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 10,000 scenarios (i.e., $N = 10{,}000$) for each of the four GBM driving the uncertainty in the underlying economic environment.

4.1 Parameters Associated with the Benefit and Cost Calculations

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 in 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%.

For the GBM associated with the H_2 price, the initial value 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 in the H_2 price of 59.7%, 42.9%, and 36% of the initial price in 2030, 2040 and 2055, respectively, decreasing linearly over 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.

For the premium paid to green H_2, we use the estimation described in equation (10). In this calculation, we consider an initial average emissions factor of 0.383 $\frac{ton\ CO_2}{MWh}$, which corresponds to the current value in the main Chilean power grid (Chilean National Energy Commission, 2021), a final average emissions factor of 0.100 $\frac{ton\ CO_2}{MWh}$ in 2055, and a linear interpolation between both values in the intermediate years. For the H_2 Lower Heating Value, we use the projections in (IRENA, 2020); resulting in the values 0.0507 $\frac{MWh}{kg\ H_2}$ for 2022, 0.0426 $\frac{MWh}{kg\ H_2}$ for 2055, and a linear interpolation between both values in the intermediate years. For the emissions cost calculation, we compare two cases: (i) one case where the emissions cost is linearly increasing, considering 5 $\frac{USD}{ton\ CO_2}$ until 2030, which corresponds to the current Chilean carbon tax value, and then we assume this value linearly increases up to 50 $\frac{USD}{ton\ CO_2}$

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

by 2040 and then up to 75 $\frac{USD}{ton\ CO_2}$ by 2055; and (ii) another case where the emissions cost is fixed over time, considering 38 $\frac{USD}{ton\ CO_2}$ in all years, which is the simple average tax over years of the previous case.

The number of hours in which electricity (hr_{E,S_i})[9], gray H_2 (hr_{G,S_i}) and/or green H_2 (hr_{V,S_i}) is sold depends on the investment state. Table 1 summarizes the values used for the hours in each investment state. Electricity is sold if there is solarPV panels and surplus energy, 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}, electricity is sold only from the surplus capacity ($P_{max} – P_{min}$), because a capacity of P_{min} is used during the 9 hours that the solarPV modules operate to produce green H_2 (E_{min}). The remaining time (15 hours), gray H_2 is generated using electricity 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. 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, decreasing linearly over the years, using the annual drifts presented in Table 2 (Palma-Behnke et al., 2019); 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 intervening 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.

[9] This value defines the plant factor (PF) of the solar PV 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%

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 for the case study with the parameters described in the previous section. First, we show the expected NPV and the frequency of each investment path, in the 10,000 simulations. Then we show the frequency of selecting each end node as the optimal decision, and the transitions made in each case. Finally, we present the NPV values obtained for each type of project valuation in every state.

As a summary of the results, the average NPV (called project NPV) obtained, with the CLSM methodology, for the case study is USD 25,356,231. This was obtained as the result of averaging all the NPVs of the simulated scenarios. This value is 822% more profitable than rigidly investing in the most frequent terminal state (P_{max}+E_{max}) at $t = 0$ and 18% more profitable than rigidly 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 85.75% 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 10,000 simulations. Although there are 51 possible investment paths, the results show that only 7 of them are optimally chosen in the different scenarios simulated. Column 2 in Table 3 presents the frequency a certain path is chosen. Column 3 presents the average NPV of each path. Column 4 presents the average (over all the simulations) of the total amount of hydrogen produced in the valuation horizon. Columns 5, 6 and 7 show the states through which the investor moves (and the median investment time in parentheses). Finally, column 8 shows the terminal state of the path and the frequency at which that state was chosen in parentheses. For example, the row for path 4 in Table 3 states that investment in path 4 occurs in 0.04 % of the scenarios, with an average NPV of USD 23,990,975, average H_2 production of 305.69 Mton, and, most frequently, investing in state P_{min} in the eighth year and adding the investment up to P_{max} and E_{max} in the ninth year. In addition, the last column shows the frequency, 57.1 %, in which the terminal state of this path (P_{max}+E_{max}) was the same as other paths, in this case from path 3 to path 7.

Table 3. Path selection when using the CLSM method

N° Path (1)	Freq [%] (2)	Average NPV [USD] (3)	Average H_2 prod. [Mton] (4)	1st Transition (5)	2nd Transition (6)	3rd Transition (7)	Terminal State (8)
1	14.25	18,916,804	0	P_{max} (1)			P_{max} (14.25%)
2	28.65	25,005,605	424.38	P_{max} (1)	$P_{max} + E_{min}$ (2)		$P_{max}+E_{min}$ (28.65%)
3	0.01	23,990,748	323.96	$P_{max} + E_{max}$ (8)			$P_{max} + E_{max}$ (57.10%)
4	0.04	23,990,975	305.69	P_{min} (8)	$P_{max} + E_{max}$ (9)		
5	44.04	27,287,759	322.92	P_{max} (7)	$P_{max} + E_{max}$ (8)		
6	0.99	24,622,870	287.06	P_{min} (8)	P_{max} (9)	$P_{max} + E_{max}$ (10)	
7	12.02	26,815,219	322.98	P_{max} (7)	$P_{max} + E_{min}$ (8)	$P_{max} + E_{max}$ (9)	

It is remarkable in the results that the path most often selected by investors (based on the highest NPV obtained), i.e., path 5, is not the same path that delivers the maximum level of average hydrogen production. This means that the most profitable investments from a private perspective do not necessarily lead to the largest expected hydrogen production. This result has important public policy consequences because government policies aimed at encouraging the hydrogen production may have misaligned goals with respect to the payoffs to private investors. In particular, from a governmental viewpoint, early installation of electrolyzers (like in path 2) is desirable due to the larger production of hydrogen obtained, but private investors prefer to wait until the technology is more mature and has a lower capital cost.

Our results also show that, in all scenarios, it is economic to make an investment (the sum of column 2 is 100%); i.e., choosing state S_0 is never optimal. Only in 14.25% of the scenarios do the results recommend investing only in solar PV 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 likely to be 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 85.75% of the cases, it is economic to invest in some capacity to produce H_2, making a compound investment in almost 100% of these scenarios (all paths other than 3 in Table 3). This means that currently developing a H_2 production plant (although this may have large environmental benefits in terms of avoided emissions) is less profitable than having sequential investments (i.e., investing first in a solar PV plant and investing later in some electrolyzer capacity, after some uncertainties are revealed). In fact, the NPV of path 2 (that includes electricity and green H_2 sales with minimum capacity) is 8.36% lower than (or equivalently, 91.64% of) the NPV of path 5, although the H_2 production under path 2 is the largest over the valuation horizon. 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 \$27,287,759, is precisely the most frequently recommended path from an investor perspective (Path 5 in Table 3), which, in general, involves building the maximum capacity of PV modules in the seventh year, and then investing the following year in the maximum capacity of electrolyzers. The investor can take advantage of the economic benefits from selling green H_2 when investment and operational costs decrease. However, this is not the path with the greatest environmental benefit because it does not yield the largest hydrogen production (assuming more hydrogen production leads to less GHG emissions).

4.2.2 State Transitions

Fig. 4 shows the optimal transitions occurring according to our 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 occur in the simulated scenarios. Within these five states, only three represent terminal states with a frequency greater than 0% (P_{max}; P_{max}+E_{min}; P_{max}+E_{max}, as shown in column 8 of Table 3), while the other two are transient states (counting the initial state, where no investment is made).

The figure shows that directly moving to state P_{max} is economic in almost all cases. However, in most cases, this is only a transition state (i.e., only 14.25% of the time, 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. In 57.10% of the scenarios, it is in the investor's best interest to invest in state P_{max}+E_{max} as the terminal state.

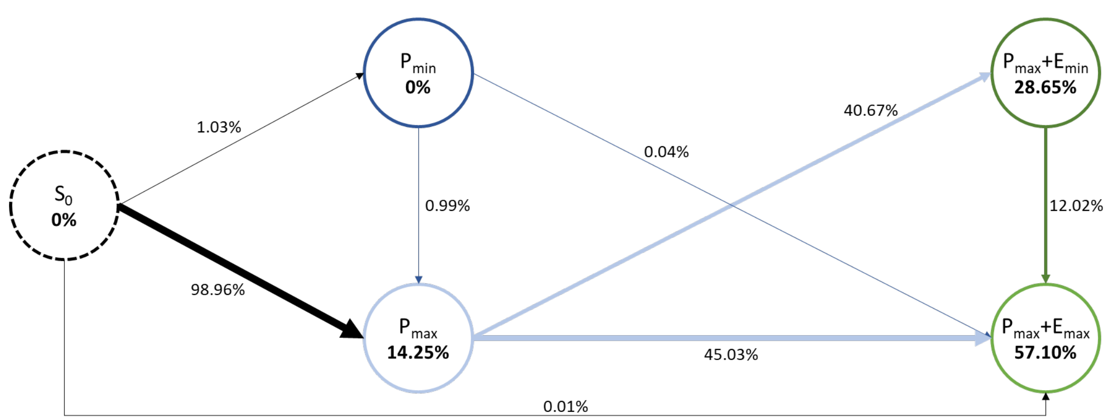

Fig. 4. Scheme representation of state transitions

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, when all investments must occur 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 at 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)
P_{min}	1	10,649,351	10,649,351	10,649,351	0	0	0
P_{max}	2	21,558,552	21,558,552	21,558,552	0	0	0
E_{min}	1	-9,706,422	0	0	9,706,422	9,706,422	0
E_{max}	2	-19,238,500	0	0	19,238,500	19,238,500	0
P_{min} + E_{min}	3	1,104,170	12,435,272	14,528,679	11,331,102	13,424,509	2,093,407
P_{min} + E_{max}	8	-8,427,907	10,069,172	10,330,410	18,497,079	18,758,317	261,238
P_{max} + E_{min}	8	2,484,620	15,416,769	22,071,311	12,932,149	19,586,691	6,654,542
P_{max} + E_{max}	26	2,749,532	23,177,830	27,262,959	20,428,298	24,513,427	4,085,129

As Column 3 of Table 4 shows, 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 in them, even when having flexibility in the timing of the investment. This happens because the sale of gray 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 not make the investment at $t = 0$ 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 (as shown in Columns 4 and 5).

Table 4 also shows that, in all states except for P_{min} and P_{max}, there are large benefits from flexibility. Postponing investment and/or expanding the capacities during the investment horizon have value. Considering compound flexibilities leads to more (or equally) profitable investment decisions than the 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 increases the expected profitability of the project substantially relative to the rigid investment decision. If the possibility of expanding solar generation and H_2 production capacities in a multi-stage manner is added, then the CLSM methodology leads to investment decisions that are even more profitable (in fact, 8.22 times more profitable) than with rigid investment decisions.

5. Policy Scenario Analysis

This section uses our modeling framework to compare carbon pricing and electricity pricing policies in terms of their ability to stimulate hydrogen production during the decision horizon. Our carbon tax policy analysis compares a carbon tax that is monotonically increasing over time to a fixed carbon tax equal to the average over time of the monotonically increasing tax. In the first case the carbon price is 5 $\frac{USD}{ton\ CO_2}$ until 2030, which is the current Chilean carbon tax. The tax then increases linearly up to 50 $\frac{USD}{ton\ CO_2}$ by 2040 and then up to 75 $\frac{USD}{ton\ CO_2}$ by 2055. In the second case the tax is fixed for all years at 38 $\frac{USD}{ton\ CO_2}$, which is the average of the carbon tax over all years for the monotonically increasing case. This carbon tax comparison is relevant because virtually all regions with carbon taxes start with a low tax and a commitment to increase it over time. However, a low initial tax that increases over time works against making investments in renewable generation capacity or electrolyzer capacity profitable until later in the decision horizon. This results in less profitable investment paths and less hydrogen production over the decision horizon.

We also assess the impact of two values of electricity price volatility on the level of hydrogen production. This comparison is relevant to the electricity market in Chile because it is currently considering transitioning from an audited cost-based wholesale market to an offer-based wholesale market. Allowing suppliers to submit offer prices rather than audited cost to set the electricity price is likely to lead to more volatile wholesale prices (Galetovic et al., 2015). Therefore, we consider a scenario that increases the volatility in the electricity price to 11.025%, which is a 50% increase over the baseline electricity price volatility of 7.35%.

Tables 3, 5, 6, and 7 present the results of these four scenarios. Table 3 shows the case of a monotonically increasing carbon tax and an electricity price volatility of 7.35%. Table 5 presents the case of monotonically increasing carbon tax and electricity price volatility of 11.025%. Tables 6 and 7 present the case of a fixed carbon tax and electricity price volatility of 7.35% and 11.025% respectively. A comparison of Table 3 to Table 6 and Table 5 to Table 7 demonstrates the impact of fixed carbon tax on the attractiveness of early investments in H_2 production facilities relative to the more politically palatable carbon policy of a low initial tax that monotonically increases, for both values of the electricity price volatility. In 100% of the sample paths in Tables 6 and 7, the first transition invests in the maximum amount of renewable generation capacity and the second transition invests in maximum amount of electrolyzer capacity. In contrast, Tables 3 and 5 find that seven transition paths are optimal with different frequencies, and not all of them end in the $P_{max}+E_{max}$ state. The expected hydrogen production in Tables 3 across the seven transition paths is 306 Mton. The corresponding value for Table 5 is 294 Mton. The expected hydrogen production in Tables 6 and 7 is 423 MTon, a 40% increase in expected hydrogen production over the levels in Tables 3 and 5. These results illustrate the downside of politically palatable carbon tax policies in stimulating the investments in H_2 production. An upfront commitment to fixed carbon tax throughout the decision horizon makes investments in green H_2 production facilities more profitable earlier in the decision horizon relative to monotonically increasing carbon tax that has higher values in the future.

The policy analysis of the impact of increasing electricity price volatility yields very small differences in the expected amount hydrogen production. The increase in electricity price volatility between Tables 6 and 7 yields no change in the expected amount of hydrogen production of 423 Mton. Comparing the results in Table 3 to those in Table 5 yields a small reduction in expected hydrogen production associated with the increase electricity price volatility from 306 Mton to 294 Mton.

Taken together these policy simulations point out the importance of the immediate commitment to a substantial carbon tax to obtaining significant investments in green H_2 production. Increases in the amount of electricity price volatility that could accompany the transition to an offer-based short-term market are not likely to drive significant changes in the investments in green H_2 production.

Table 5. Path selection (CLSM method), when emissions cost is linearly increasing and electricity price volatility is 11.025%

N° Path (1)	**Freq [%] (2)**	**Average NPV [USD] (3)**	**Average H_2 prod. [Mton] (4)**	**1st Transition (5)**	**2nd Transition (6)**	**3rd Transition (7)**	**Terminal State (8)**
1	17.36	27,329,697	0	P_{max} (1)			P_{max} (17.36%)
2	26.63	23,453,706	424.59	P_{max} (1)	$P_{max} + E_{min}$ (2)		$P_{max}+E_{min}$ (26.63%)
3	0.01	14,818,257	323.96	$P_{max} + E_{max}$ (8)			$P_{max} + E_{max}$ (56.01%)
4	0.05	19,622,279	305.69	P_{min} (8)	$P_{max} + E_{max}$ (9)		
5	44.77	26,226,071	323.29	P_{max} (7)	$P_{max} + E_{max}$ (8)		
6	1.33	21,220,186	287.12	P_{min} (8)	P_{max} (9)	$P_{max} + E_{max}$ (10)	
7	9.85	24,626,442	322.31	P_{max} (7)	$P_{max} + E_{min}$ (8)	$P_{max} + E_{max}$ (9)	

Table 6. Path selection (CLSM method), when emissions cost is fixed over time and electricity price volatility is 7.35%

N° Path (1)	**Freq [%] (2)**	**Average NPV [USD] (3)**	**Average H_2 prod. [Mton] (4)**	**1st Transition (5)**	**2nd Transition (6)**	**3rd Transition (7)**	**Terminal State (8)**
1	100	43,173,671	423.69	P_{max} (1)	$P_{max} + E_{max}$ (2)		$P_{max} + E_{max}$ (100%)

Table 7. Path selection (CLSM method), when emissions cost is fixed over time and electricity price volatility is 11.025%

N° Path (1)	**Freq [%] (2)**	**Average NPV [USD] (3)**	**Average H_2 prod. [Mton] (4)**	**1st Transition (5)**	**2nd Transition (6)**	**3rd Transition (7)**	**Terminal State (8)**
1	100	43,188,330	423.69	P_{max} (1)	$P_{max} + E_{max}$ (2)		$P_{max} + E_{max}$ (100%)

6. General sensitivity analysis

This section presents the results of sensitivity analyses to show how our results change if certain model parameters are varied. Given their relevance in the investor's decisions, the parameters selected are: (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) initial CO_2 tax $[\frac{USD}{ton\ CO_2}]$; and (viii) Power Plant Factor (PF). For comparison purposes, we use the same simulations of the GBM increments used before (in the base case, with increasing carbon tax, presented in Section 4), but varied the selected parameters by plus and minus 25%.

Table 8 summarizes our results. For each sensitivity analysis performed, Table 8 shows the frequency that certain transition path was taken. The colors in Table 8 represent, from dark red to dark green the path frequency (from least, 0%, to most, 100%). There are four paths that dominate, with results above the 50th percentile—these 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 8. Path frequencies for sensitivity analyses

Transition	FREQUENCIES [%]													
1st	P_{min}	P_{max}	P_{min} + E_{min}	P_{max} + E_{max}	P_{min}	P_{min}	P_{max}	P_{max}	E_{max}	P_{max} + E_{min}	P_{min}	P_{min}	P_{max}	
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}	P_{min} + E_{max}	P_{max} + E_{min}	No Investment
3rd											P_{max} + E_{max}	P_{max} + E_{max}	P_{max} + E_{max}	
4th														
Base Case		14.25		0.01		0.04	28.65	44.04			0.99		12.02	
H_2 Drift (-25%)								88.95					11.05	
H_2 Drift (+25%)		100												
Electricity Drift (-25%)		99.99					0.01							
Electricity Drift (+25%)						0.04		98.12			0.29		1.55	
PV Module Drift (-25%)		19.59					58.41	15.60			0.41		5.99	
PV Module Drift (+25%)		5.04		0.01		0.03	7.27	77.3			1.18		9.17	
Electrolyzer Drift (-25%)		55.25					14.76	25.73			0.19		4.07	
Electrolyzer Drift (+25%)		1.07		0.01		0.18	22.85	60.03			2.77		13.09	
Volatilities (-25%)		11.62				0.01	29.35	41.89			0.92		16.21	
Volatilities (+25%)		20.12		0.07		0.11	22.67	50.19			1.05	0.01	5.78	
Discount Rate (-25%)		0.04					22.92	70.04			1.12		5.88	
Discount Rate (+25%)	0.04	7.34	0.53	7.50	0.54	0.07	2.27	80.38	0.01	0.09	0.01		0.5	0.72
CO_2 Tax (-25%)		51.66					18.82	25.27			0.3		3.95	
CO_2 Tax (+25%)		1.47		0.01		0.08	21.12	60.33			3.13		13.86	
Plant Factor (-25%)			0.55	0.39	10.18	0.14	0.04	69.61					0.03	19.06
Plant Factor (+25%)		5.75					64.36	29.81					0.08	

We also compare the NPVs for the rigid and compound valuations and the terminal state for each sensitivity analysis. These results are presented in Table 9, where column 2 shows the project (average) NPV for each sensitivity analysis and column 3 compares the profitability of each case with respect to the base case presented in Section 4. 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 9. Results of the sensitivity analyses

	Project 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	25,356,231		$P_{max}+E_{max}$	2,749,532	86.74
H_2 Drift (-25%)	64,959,989	156	$P_{max}+E_{max}$	45,421,731	100
H_2 Drift (+25%)	21,826,843	-14	P_{max}	21,558,552	0
Electricity Drift (-25%)	29,799,621	18	P_{max}	29,474,295	0.01
Electricity Drift (+25%)	36,045,901	42	$P_{max}+E_{max}$	14,940,985	100
PV Module Drift (-25%)	24,993,094	-1	$P_{max}+E_{min}$	1,326,389	80.41
PV Module Drift (+25%)	27,557,362	9	$P_{max}+E_{max}$	3,805,312	94.95
Electrolyzer Drift (-25%)	22,944,166	-10	P_{max}	21,558,552	44.75
Electrolyzer Drift (+25%)	28,739,032	13	$P_{max}+E_{max}$	6,461,259	98.92
Volatilities (-25%)	24,723,172	-2	$P_{max}+E_{max}$	2,742,969	88.32
Volatilities (+25%)	27,561,087	9	$P_{max}+E_{max}$	2,769,464	79.81
Discount Rate (-25%)	53,173,423	110	$P_{max}+E_{max}$	26,817,017	99.96
Discount Rate (+25%)	9,495,623	-63	$P_{max}+E_{max}$	-16,606,110	83.87
CO_2 Tax (-25%)	22,976,556	-9	P_{max}	21,558,552	48.34
CO_2 Tax (+25%)	28,879,668	14	$P_{max}+E_{max}$	6,423,691	98.52
Plant Factor (-25%)	5,004,879	-80	$P_{max}+E_{max}$	-36,111,734	80.00
Plant Factor (+25%)	58,815,830	132	$P_{max}+E_{min}$	38,896,639	94.25

Table 9 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 9), it is economic to make compound investments in equal or more than 80% of the scenarios (this is shown in column 6), which shows that flexibility still adds large value when parameters change.

Table 9 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, 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 solar 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% relative to the base case. In 19.06% 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 because 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 132% 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 initial value of 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 largest occurs when varying the initial CO_2 tax [10] because it directly influences the premium paid in the sale of green H_2. Thus, if the CO_2 tax increases, there are more profits from selling H_2, while if it decreases, in half of the scenarios the results recommend focusing only on selling electricity (state P_{max}) because it becomes more profitable than selling H_2.

Variations in electrolyzer prices imply modest differences in H_2 profitability because, 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 be more profitable, while a higher investment cost in electrolyzers yields investment only in a solar 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 paths have low frequencies; and, therefore, no significant changes can be observed with respect to the base case results.

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[10] In this sensitivity analysis, the initial value of the carbon tax ($5\,\frac{USD}{ton\ CO_2}$ until 2030 in the base case) is increased and decreased by 25% (i.e., starting at $3.75\,\frac{USD}{ton\ CO_2}$ and $6.25\,\frac{USD}{ton\ CO_2}$, respectively). For the following years, we still consider an increasing carbon tax with the same slope as in the base case. That is, we still consider the same increasing carbon tax, but increased/decreased every year by $1.25\,\frac{USD}{ton\ CO_2}$.

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

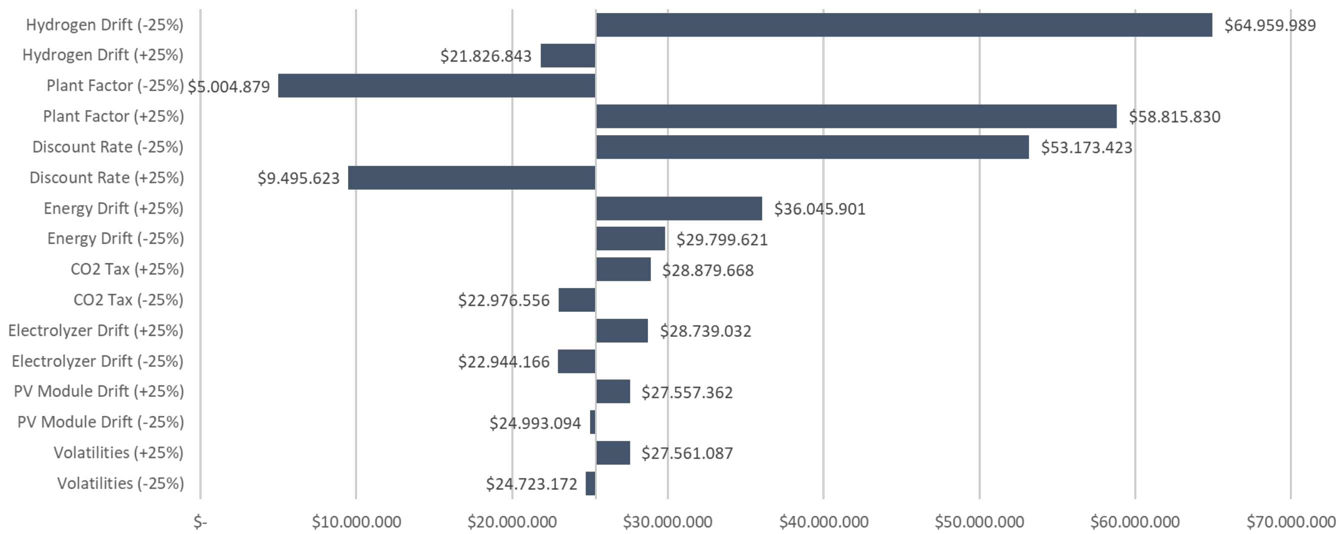

Fig. 5. NPV for each sensitivity analysis performed

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 respect 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 and Hydrogen Drift +25%, the average NPV when allowing for flexibilities are higher than the NPV obtained in the best-case scenario when the investor is forced to invest at $t = 0$ (USD 21,558,552). Thus, as mentioned before, adding flexibility to the investment decisions still adds large value even for different model parameter values.

7. Discussion and Conclusions

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 an investor has the flexibility to postpone the investment and/or to expand plant capacity in a multi-stage manner. 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 economic benefits to the investor because it rules out suboptimal investment decisions that ignore the flexibilities and the resolution of intertemporal 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 imply that it is economic to invest in a H_2 production plant in 85.75% of the simulated scenarios. In almost 100% of those cases, it is preferable to implement these investments 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.

It is remarkable in the results that the path mostly selected by investors (based on the highest NPV obtained) is not necessarily the same path that has the maximum expected hydrogen production. This means that the most profitable investments from a private perspective do not necessarily lead to the largest hydrogen production in the system.

Another policy relevant result is that establishing a sizeable stable carbon tax over time, which leads to a stable green H_2 price premium, leads to larger green hydrogen production than an equivalent policy where emissions cost is linearly increasing. Moreover, such a stable emissions cost policy induces a stronger economic incentive for investments in H_2 production facilities than the equivalent monotonically increasing carbon tax policy. This result suggests that linearly increasing over time the carbon tax (although politically convenient) may not be the best public policy to encourage green hydrogen production and to incentivize renewable energy and hydrogen production investments.

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