Integration of Membrane Technology into Hydrogen Production Plants With CO₂ Capture: An Economic Performance Assessment Study

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Abstract

An economic performance evaluation framework for hydrogen production (HP) plants with integrated catalytic membrane reactor (CMR) modules is presented (HP-CMR) in light of their enhanced environmental performance prospects. A detailed comprehensive Net Present Value (NPV) model is first developed in order to assess the economic viability of HP-CMR plants, while irreducible sources of market and regulatory uncertainty are identified and their effect on the plant's economic performance is explicitly taken into account through Monte-Carlo techniques. As a result, the proposed economic performance evaluation framework for an HP-CMR plant allows the derivation of distribution profiles of economic performance outcomes rather than single-point value estimates that often lead to unsatisfactory valuation assessments by overlooking significant uncertainty effects over the plant's lifetime. Within the above framework, the HP-CMR plant is comparatively assessed against the conventional HP plant with and without Carbon Capture and Sequestration (CCS) systems. It is shown that future regulatory action on CO₂ emissions leads to comparatively appealing distribution profiles of economic performance outcomes for HP-CMR plants in the presence of uncertainty, thus offering a window of opportunity for this new technology option to emerge as a viable one for hydrogen production in a carbon-constrained world. Finally, the provision of a set of incentives is considered that could potentially facilitate the demonstration stage of the HP-CMR technology option on the commercial scale.

Keywords

Hydrogen production; CO₂ capture; Catalytic membrane reactor; Economic performance assessment under uncertainty; Monte-Carlo simulation

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1. Introduction

Global energy demand growth patterns accompanied by climate change mitigation challenges have provided significant stimulus to creative thought and attendant research activities aiming at the development and successful demonstration of advanced clean energy technology options worldwide. Indeed, according to the U.S. Energy Information Agency, energy demand in the U.S. increases by 0.4% annually [1], and in light of the current state of affairs in the field of energy production, energy supply security considerations, cost advantages as well as relatively low technology risks have traditionally favored the expansion of the use of fossil fuels worldwide to meet demand growth in the near/medium-term [2,3,4]. Within the above context, hydrogen represents an energy carrier with the potential to reliably contribute to a robust global energy system as a complementary option to electricity as well as liquid fuels use in an environmentally responsible manner provided that the pertinent hydrogen production technologies (both the conventional and the more advanced ones recently proposed) can reach appealing techno-economic performance levels in the presence of fuel market and regulatory uncertainties [2,3,4]. In particular, as shown in Figure 1, its use in the chemical and petrochemical industry is essential with a global share of 54% in the production of ammonia, 35% for upgrading fuels and 6% for a range of applications in the electronics industry. Currently, hydrogen production technology pathways involve the direct chemical conversion of fossil fuel resources, i.e. steam reforming of natural gas (methane) or coal gasification and electro-chemical conversion through water electrolysis using electricity, nuclear or renewables [2,5]. Please notice that almost 95% of the total hydrogen generated in the U.S. is currently produced from fossil fuels via steam reforming of natural gas, partial oxidation of hydrocarbons and coal gasification [6]. Focusing on the U.S. market in particular, coal gasification represents a quite economically attractive, reliable and mature hydrogen production technology option given that the U.S. geologically possesses over one fourth of the global coal reserves (Figure 2) [7].

Figure 1 Distribution of the global hydrogen market. Data adapted from Linde Engineering [8].

Figure 2 Share of global recoverable coal resources in 2011. Data adapted from U.S. EIA [9].

Coal gasification technology produces H_2 by generating syngas from pulverized coal and O_2 at $677^\circ C$ and 5.6 MPa. Syngas is composed mainly by CO , CO_2 , H_2 and H_2O along with other particulate impurities which are treated with water wash in a scrubber. Conventionally, syngas is sent to Water-Gas-Shift (WGS[†]) reactors to convert CO to CO_2 and simultaneously generate H_2 as shown in Equation 1-1. The H_2 -rich gas is then cleaned from NH_3 , SO_2 , Hg and H_2S followed by the H_2 purification step performed by pressure swing adsorption (PSA) units [2].

As mentioned earlier, hydrogen production will mainly rely on fossil fuels in the near/medium-term and inevitably continue to be a source of significant greenhouse gas (GHG) emissions. It is expected that the use of Carbon Capture and Sequestration (CCS) systems in hydrogen production facilities will receive increasing attention due to future regulatory action on CO_2 emissions, such as the introduction of a carbon tax or market-inspired emission permit trading mechanisms. Indeed, carbon taxation levels, currently considered as appropriate to generate the “right” market price signals and thus facilitate their internalization by the pertinent markets, display variability thereby affecting the realization prospects of demonstration plants and the final adoption of new advanced clean energy technology options. Examples of various carbon tax levels include the \$12 per tonne of CO_2 in Boulder Colorado [10], \$30 per tonne of CO_2 in Finland [11] and the \$23 per tonne CO_2 in Sweden [11]. Furthermore, carbon tax changes over time have been observed, such as in the Norwegian offshore which in 1991 was U.S.\$50/t, but was reduced to U.S.\$38/t in 2000.

However, from an economic view point, the implementation of CCS systems requires substantial capital investment while incurring additional Operation and Maintenance (O&M) costs. In particular, the CO_2 capture process component is the most expensive one representing approximately 75% of the overall cost.

[†] Please notice that a list of acronyms is included at the end of the document.

Consequently, various CCS options have been investigated throughout the literature [12] relying on adsorption, absorption, chemical looping and membrane separation. While amine-based sorption methods for CO₂ capture are well known and considered mature technology options, their thermal and oxidative degradation characteristics could generate potentially hazardous and toxic substances and carcinogens [13]. Moreover, due to demonstrated enhanced capture efficiency levels and additional benefits, the use of membrane-based separation methods is now recognized as a potentially meritorious technology option [13].

In light of the above considerations, the production of hydrogen via the WGS reaction of coal-derived syngas in integrated catalytic membrane reactors (CMRs) represents an appealing technology option (HP-CMR) due to its great potential for CO₂ capture, H₂ purification, as well as process intensification. As shown throughout the pertinent literature [14,15,16] the constant removal of the product leads to higher conversion levels of the WGS reaction than the ones attainable under conventional conditions. Moreover, CMRs used in WGS process systems make possible the generation of pure H₂ and clean pressurized CO₂ realized in a single unit, and display higher product recovery and energy-efficiency potential than pressure swing adsorbers of traditional H₂ separation units [17]. In particular, Pd- and Pd/Alloy-based membranes with stainless steel, Hastelloy or Inconel supports also exhibit significant advantages including the capacity of yielding ultra-pure H₂ at a stable high flux under high temperatures (400-600 °C) and pressures (20-50 bar). Supplementary advantages include their long term durability, improved thermal, chemical and mechanical stability, cost-effective fabrication and maintenance, as well as easiness in scale up and practical assembly/disassembly capabilities for both small and large scale industrial applications [14,15,16,18,19,20,21,22]. Given the appealing performance characteristics that HP-CMR exhibits, it is expected that the HP-CMR technology option integrated into coal-fired hydrogen production plants could potentially lead to:

- i) enhanced environmental performance through a cost-effective design accommodation of a CCS system while maintaining competitive efficiency performance levels compared to the conventional technology option.
- ii) attractive economic performance prospects, particularly in light of the anticipated future regulatory action on CO₂ emissions.

It should be pointed out that increasingly stringent environmental performance requirements on CO₂ emissions in coal-fired hydrogen production plants provide ample motivation for the possibility of integrating CCS systems into their design [2,23,24]. However, despite advancements in our conceptual understanding of many potential design integration options of CCS systems into conventional hydrogen production plants, the lack of any accumulated operating experience even on the technology demonstration front poses significant challenges for HP-CMR plants. Within such a context, any preliminary research attempt to assess the economic viability and performance prospects of the new technology option is certainly justified, thus contributing to recently intensified efforts to provide the appropriate incentives and stimulate the realization of advanced technology demonstration projects at the commercial scale worldwide. Indeed, the use of advanced technology options such as the proposed one offer reasonable prospects of inducing appealing economic performance and valuation profiles in a carbon-constrained world [25]. Muller-Langer et al. [2] offered a comprehensive evaluation of the techno-economic performance characteristics associated with conventional hydrogen production options (based

on methane steam reforming, coal and biomass gasification as well as water electrolysis) within the European Union (EU) context, and also pointed out the prospects of enhanced environmental and economic performance through the adoption of more advanced options such as HP-CMR with CCS capabilities. Based also on attainable process efficiency levels, CO₂ emissions and H₂ production costs, it was concluded that natural gas and coal-based HP-CMR options could represent important viable routes for clean H₂ generation. Further economic studies for H₂ production plants include those reported by Kreutz et al. [26,27] who evaluated the co-production of H₂ and electricity from coal using conventional technologies via the EPRI TAG methodology. Low operating costs were found to be the most important factor contributing to the overall economic competitiveness of this option, while H₂ distribution and storage technologies acted as the biggest constraints. Van Vuuren et al. [28], developed interesting projected economic performance profiles of the deployment of CCS technologies taking into account various techno-economic parameter uncertainties, concluding that uncertainty in techno-economic parameters could have a severe impact on model-based process economics projections. Additionally, Saboohi et al. [29] developed a stochastic model for an energy supply system with uncertain fuel prices and applied it to a case where gas fired engines were competitive with renewable energy sources. The results were discussed in terms of expected value of perfect information and the value of a stochastic analytical framework.

In the absence of any accumulated operating experience and associated data, an economic performance evaluation framework for a new technology option such as HP-CMR would be inevitably based on reasonable theoretical estimates (by drawing on the most comprehensive studies and expert opinion) while explicitly acknowledging irreducible uncertainty sources (market, regulatory, etc.) [30]. In the present study such a methodological and analytical perspective is followed. First, a detailed comprehensive baseline Net Present Value (NPV) model is structured in order to assess the economic performance characteristics of HP-CMR plants. Then various sources of uncertainty are identified and integrated into the proposed framework, while their impact on the HP-CMR plant's valuation profile is explicitly taken into account through Monte-Carlo simulation methods by which the above uncertainty "drivers" (model inputs) are propagated through the above NPV-model [30,31]. As a result, the proposed economic performance evaluation framework for the HP-CMR plant allows the derivation of more realistic distribution profiles of economic performance outcomes rather than single-point value estimates that often lead to unsatisfactory valuation assessments by overlooking significant uncertainty effects over the plant's lifetime [30,31]. Furthermore, a comparative economic performance assessment in the presence of uncertainty is conducted between the HP-CMR and the conventional hydrogen production options, demonstrating that appealing economic performance outcome distribution profiles of HP-CMR plants could emerge as regulatory action on CO₂ emissions is introduced.

The paper is organized as follows: A description of the structure and the associated tools of the proposed economic performance assessment framework for HP-CMR plants are presented in Section 2. Section 3 encompasses the study's main results as well as a detailed discussion on its key findings. Finally, some concluding remarks are provided in Section 4.

2. Economic Performance Assessment and Analysis Framework

2.1 Technology options integrated into coal-fired H₂ production plants for CO₂ capture: Absorption versus Membrane Technology

Several approaches for CO₂ capture applicable to fossil fuel-based electricity and H₂ co-production process systems have been thoroughly studied in the relevant body of literature [25,32,33,34], primarily falling into four categories: absorption, adsorption, chemical looping and membrane-based separation. The most common approach for CO₂ capture is physical absorption which uses solvents such as Selexol, Rectisol, Purisol, Sepasolv MPE and Fluor Solvent [35,36]. Specifically, the integration of a Selexol unit into conventional HP plants for CO₂ capture has been recommended in the DOE/NETL report [24,36] as shown in Figure 3. Therefore, a conventional coal-fired HP plant with CO₂ capture consists of five basic processes:

- (1) Gasification. In this process pulverized coal reacts with O₂ (supplied by an air separation unit (ASU)) in the gasifier at elevated pressure and temperature (56 bar and 677 °C) to produce syngas, primarily composed of CO, CO₂, H₂, H₂O and other particulate impurities.
- (2) Particulate removal. Syngas is treated with water in a scrubber to remove chlorides, alkali, and particulate matter.
- (3) WGS reaction. The CO present in syngas reacts with steam in a series of WGS reactors (high temperature and low temperature reactors) to convert CO and H₂O into H₂ and CO₂.
- (4) Gas clean up. This step involves three process units: the sour water stripper, the mercury removal, and the Selexol unit. First, the syngas passes through the sour water stripper to remove NH₃, SO₂, and other impurities from the scrubber. Then, 95% of mercury is removed through a carbon bed. Finally, both H₂S and CO₂ removal is performed in the Selexol unit. The Selexol unit used in this study is a dual stage one and the attainable efficiency of CO₂ capture can reach a level as high as 90% [37].
- (5) H₂ Purification. Solid adsorbents, such as 5A zeolite, alumina, and activated carbon, in the pressure swing adsorption (PSA) unit adsorb all gas species contained in the syngas, except for H₂. Typically, the PSA unit is operated at 51 bar to yield 99.99% pure H₂ with a recovery efficiency of 80% [24,38].

The integration of Pd-based membrane technology in power plants is recognized as a quite promising technology option [39,40,41,42]. Indeed, CMR modules for the simultaneous CO₂ capture and high purity H₂ production embedded in Integrated Gasification Combined Cycle (IGCC) with CCS systems have been shown to generate rather good prospects for enhanced environmental and economic performance especially under future CO₂ emissions regulations [40,42]. In the present research work, motivated by the above considerations, preliminary studies and pertinent recommendations found in [2] whereby the HP-CMR technology option for future clean hydrogen production is supported, the integration of industrial scale Pd-based CMR modules into coal-fired H₂ production plants is economically evaluated under uncertainty within a systematic and comprehensive framework. The process block flow diagram of HP-CMR plant with CO₂ capture, based on the design of the DOE/NETL report [24], is presented in Figure 4.

Figure 3 Process block flow diagram of the conventional coal-based H_2 production plant with CO_2 capture, based on the design of the DOE/NETL report [24].

Figure 4 Process block flow diagram of the coal-based H_2 production plant integrated with membrane technology.

Compared to the conventional HP process system, the higher attainable CO conversion levels in an industrial scale CMR module allows for lower operating temperatures. Thereby, potential gains in terms of prolonged catalyst lifetime, lower production costs and reduced material costs can be realized [15,43]. Furthermore, combined with higher H₂ recovery levels, production of high-pressure CO₂ readily available for sequestration purposes takes place [39,40]. Therefore, the HP-CMR technology option exhibits great potential in enhancing the productivity of HP plants as well as the associated environmental performance in a cost-effective manner. It is important to mention that the main disadvantage of HP-CMR technology lays in the lack of accumulated operating experience and the absence of plant data at the commercial scale. Other technical disadvantages of the CMR technology include the membranes' sensitivity to sulfur poisoning as well as challenges in the membrane preparation and process scale up stages [14,22,44,57].

2.2 Technical performance evaluation framework

The technical performance of industrial scale Pd-based CMR modules potentially integrated into HP plants is evaluated with the aid of a model accompanied by the following simplifying assumptions:

- All gas species follow the ideal gas law.
- Isothermal conditions apply to the module's operation.
- Isobaric conditions apply to both retentate and permeate sides.
- The membrane exhibits theoretically infinite selectivity of H₂ while the H₂ permeation flux of the membrane follows Sieverts' law as shown in Equation 2-1.
- Plug flow conditions apply to both retentate and permeate streams. Note that radial and axial dispersions are neglected.
- There are no mass transfer limitations or concentration polarization.
- No poisoning of the catalyst occurs during the WGS reaction.

The structural configuration, depicted in Figure 5, as well as the modeling and simulation framework of the above CMRs is presented in previously reported work [44]. Please notice that our model based on steady state mass balance equations is in very good agreement with the experimental results reported by Augustine et al. [20]. The membranes used in the CMRs are Pd/Au alloy (12 wt% Au) composite membranes for the purpose of retaining high permeance levels in the presence of trace amounts of H₂S, as well as ensuring permeance recoverability whenever feed conditions with high sulfur concentration levels occur. The permeance of the membranes is affected by the presence of Au. Therefore, a quite standard Equation 2-1 is used to describe the temperature-dependent H₂ flux (J_{H₂}) in m³/m²-h-bar^{0.5}:

$$J_{H_2} = \phi_{H_2S \text{ poisoning}} \cdot \phi_{Au \text{ alloying}} \frac{Q \cdot (\sqrt{P_{H_2}^{ret}} - \sqrt{P_{H_2}^{per}})}{\delta} \quad (2-1)$$

where $Q = Q_0 \cdot \exp\left(\frac{-E_Q}{R \cdot T}\right)$

In Equation 2-1, $\phi_{H_2S \text{ poisoning}}$ is the permeance decline coefficient due to exposure to 2 ppm H₂S at 400°C assumed in the present study, $\phi_{Au \text{ alloying}}$ is the permeance decline coefficient due to the alloying of 12 wt% Au, δ is the Pd/Au membrane thickness in μm , Q is the H₂ permeability of pure Pd foils in m³- $\mu\text{m}/(\text{m}^2\text{-h-bar}^{0.5})$, Q_0 is the H₂ permeability constant in m³- $\mu\text{m}/(\text{m}^2\text{-h-bar}^{0.5})$, E_Q represents the activation energy for H₂ permeation in kJ/mol, R is the gas constant in J/(mol-K), T is the operating temperature in

K, and $P_{H_2}^{ret}$ and $P_{H_2}^{per}$ represent the H_2 partial pressure (bar) in the retentate side and permeate side respectively. Please notice that, membranes with thickness values ranging from 5 μm to 10 μm have been synthesized at WPI's Center for Inorganic Membrane Studies and their satisfactory performance levels have also been experimentally confirmed [14,21,22,56,57]. The parameters of the membrane and high-temperature shift catalysts used in the aforementioned modeling framework are summarized in Table 1. Within this context, the CMR model was simulated for industrial conditions under the feed specifications [42], reaction conditions, and H_2 permeance of membranes listed in Table 2. Furthermore, the process system dimensions and the required inlet stream for CMR modules are based on the H_2 production target of 616.5 tonnes per day in conventional coal-fired H_2 production plants for comparison purposes [24]. The CMR system consists of 10 bundles of CMRs in a parallel configuration with 4313 membrane tubes. This process system is capable of achieving 99% CO conversion and 96% H_2 recovery, and its specifications used for cost analysis are summarized in Table 3. A conservative 98% CO_2 capture efficiency is assumed to avoid overestimating the associated economic performance of HP-CMR plants, even though in practical use, higher efficiencies can be currently achieved by membrane technology [42].

Table 1 Parameters of Pd/Au alloy composite membranes and high-temperature shift catalysts used in the process modeling framework.

Pd/Au alloy membrane thickness, δ [μm]	6
H_2 permeability constant, Q_0 [$m^3 \cdot \mu m / (m^2 \cdot h \cdot bar^{0.5})$]	6281.2
Activation energy for H_2 permeation, E_Q [J/mol]	15630
Permeance decline coefficient due to exposure to 2 ppm H_2S at 400°C, $\phi_{H_2S \text{ poisoning}}$	0.6
Permeance decline coefficient due to the alloying of 12 wt% Au, $\phi_{Au \text{ alloying}}$	0.58
Solid catalyst density, d_{cat} [kg/m^3]	2628
Porosity of catalyst, θ [%]	50
Void fraction of catalytic bed, ε [%]	20

Table 2 Feed specifications, reaction conditions, and H_2 permeance of membranes.

Retentate pressure [bar]	50
Permeate pressure [bar]	1
Reaction temperature, T [°C]	400
Inlet stream [mol/s]	8270
Inlet composition [%]	CO: 23.0 – CO_2 : 8.8 – H_2 : 22.1 – H_2O : 46.1
Retentate outlet stream [mol/s]	4702
Retentate outlet composition [%]	CO: 0.4 – CO_2 : 55.6 – H_2 : 3.1 – H_2O : 40.9
H_2 permeance [$m^3 / (m^2 \cdot h \cdot bar^{0.5})$]	22.3

Table 3 Industrial scale CMR module specifications used for cost analysis.

Single membrane tube		Industrial scale CMR module	
Pd thickness [μm]	6	Total Pd weight [kg]	1260.6
Au thickness [μm]	0.51	Total Au weight [kg]	171.9
Outer radius of the membrane, r_1 [cm]	2.54	Number of bundle CMRs in the module	10
Inner radius of the shell casing, r_2 [cm]	3.81	Number of membrane tubes in each CMR	4313
Membrane tube length, L [m]	2.54	Total V_{shell} [m^3]	499
Membrane area [cm^2]	4052	Total membrane area [m^2]	17474
V_{annulus} [cm^3]	6432	Total V_{annulus} [m^3]	277
W_{catalyst} [kg]	6.76	Total W_{catalyst} [tonne]	291.6
F_{inlet} [mol/s]	0.192	Total F_{inlet} [mol/s]	8270
$F_{\text{per_H2}}$ [mol/s]	0.083	Total $F_{\text{per_H2}}$ [TPD]	616.5
$F_{\text{ret_CO2}}$ [mol/s]	0.061	Total $F_{\text{ret_CO2}}$ [TPD]	9935.8

TPD = Tonne Per Day

Figure 5 Schematic of a catalytic membrane reactor (CMR) containing three Pd/Au membranes for Water Gas Shift reaction

277 2.3 Economic performance assessment and cost analysis framework

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279 2.3.1 Capital Investment Baseline Estimation

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Conforming to standard practice in engineering system economic analysis, the calculation of the fixed capital investment (FCI) is performed through the sum of direct and indirect costs, followed by the calculation of the total capital investment TCI as the sum of FCI and working capital (WC) [45]. In the TCI estimation, cost figures associated with the assorted process units/equipment such as the GE energy

gasifier, the syngas scrubber, and the single stage Selexol unit are adopted from the DOE/NETL report [36]. Furthermore, the six-tenths factor rule [45] (Equation 2-2) is used to calculate equipment costs since pertinent cost data are not available for the commercial scale HP-CMR plant under consideration (685 tonnes H₂ per day). The six-tenths factor rule represents a standard and widely used empirical set of practical guidelines used for designing chemical plants (sizing industrial process system units) on the commercial scale that has been proven quite satisfactory in practice while maintaining sound robustness margins [68]. The Chemical Engineering Plant Cost Indexes shown in Table 4 (available for year 2012) [46] are used to update all pertinent cost estimates by taking into account the time-value of money. It should be pointed out that cost indexes are used only to provide general, rather conservative estimates without incorporating the reasonable cost-reducing possibility of future technological advances mathematically represented by “learning curves”. The TCI for the HP-CMR technology option includes various components as shown in Table 5. Furthermore, the key cost components of the FCI, such as installation and engineering & supervision, depend on purchased equipment costs.

$$\text{Cost of Equipment A} = \text{Cost of Equipment B} \times \left(\frac{\text{Capacity of Equipment A}}{\text{Capacity of Equipment B}} \right)^{0.6} \quad (2-2)$$

Table 4 Economic parameters used in the cost analysis.

Chemical engineering plant cost indexes	In 2007	525.4
	In 2012	584.6

Table 5 Estimation of the capital investment for an industrial scale Pd-based CMR module*.

I. Direct Costs	
<i>A. Equipment + installation + instrumentation + piping + electrical + insulation + painting</i>	
1. Purchased equipment	
a. WGS reactor	
b. HTS catalyst	
c. Pd/Au alloy composite membrane	
2. Installation (25-55% of purchased equipment)	
3. Instrumentation and controls, installed (8-50% of purchased equipment)	
4. Piping, installed (10-80% of purchased equipment)	
5. Electrical, installed (10-40% of purchased equipment)	
<i>B. Buildings, process and auxiliary (10-70% of purchased equipment)</i>	
<i>C. Service facilities and yard improvements (40-100% of purchased equipment)</i>	
<i>D. Land (4-8% of purchased equipment)</i>	
II. Indirect Costs	
<i>A. Engineering and supervision (5-30% of direct cost)</i>	
<i>B. Legal expenses (1-3% of fixed capital investment)</i>	
<i>C. Construction expense and contractor's fee (10-20% of fixed capital investment)</i>	
<i>D. Contingency (5-15% of fixed capital investment)</i>	
III. Fixed capital investment (= I + II)	
IV. Working capital (10-20% of V)	
V. Total capital investment (= III + IV)	

* Please notice that the cost proportions/ranges shown in this Table are commonly used for the estimation of capital investment [42, 45]

2.3.2 Total Product Cost Baseline Estimation

Motivated by the fact that the total product cost (TPC) represents another major indicator broadly used in the economic performance analysis of chemical plants, a detailed TPC model for coal-fired HP-CMR plants is proposed as shown in Table 6. Within the TPC model, the production cost consists of several components including operating costs, CO₂ transportation and storage, H₂ delivery, carbon tax, insurance, patents and royalties, as well as plant overhead-relevant costs. In particular, the overall operating cost is comprised of three key components: (1) fuel, (2) fixed O&M costs, and (3) variable O&M costs. In this study, bituminous coal is considered as fuel (Illinois No. 6), and pertinent costs were obtained from the United States Energy Information Administration (US EIA) [47]. The fixed and variable O&M costs were obtained from relevant DOE/NETL reports [24, 36] and also updated utilizing the 2012 Chemical Engineering Plant Cost Indexes [46].

Table 6 Total product cost estimation for the HP-CMR plant.

I. Production cost	
<i>A. Operating costs</i>	
1. Fuel	
2. Fixed O&M costs	
a. Operating labor cost (0.8% of fixed capital investment)	
b. Maintenance labor cost (0.8% of fixed capital investment)	
c. Administrative & Support labor (25% of operating labor cost)	
d. Property taxes (2% of fixed capital investment)	
3. Variable O&M costs	
a. Maintenance material cost (2% of fixed capital investment)	
b. Water	
c. Chemical	
(1) COS catalyst	
(2) WGS catalyst	
(3) Selexol solution	
(4) Waste disposal	
(5) PSA adsorbent	
d. Membrane replacement (= membrane cost/membrane lifetime)	
<i>B. CO₂ transport & storage</i>	
<i>C. H₂ delivery</i>	
<i>D. Carbon tax levied in 2015</i>	
<i>E. Insurance (0.4-1% of fixed capital investment)</i>	
<i>F. Patents and royalties (0-6% of total product cost)</i>	
<i>G. Plant overhead costs (5-15% of total product cost)</i>	
II. General expenses	
<i>A. Administrative costs (2-5% of total product cost)</i>	
<i>B. Marketing costs (2-6% of total product cost)</i>	
<i>C. R&D costs (5% of total product cost)</i>	
<i>D. Financing interest (6-10% of total capital investment)</i>	
III. Total product cost (=Production cost + General expenses)	

* Please notice that the cost proportions/ranges shown in this Table are commonly used for the estimation of total product cost [42, 45]

The annual operating labor costs for the CMR module are estimated by multiplying the annual working hours (h/yr) by the labor cost rate (\$/h). A working hour is calculated based on the assumption of a unit operation under 53 employee hours/day/processing step, with two major steps involved in the CMR module's operating mode (heat transfer and reaction/separation) [45]. The operating labor requirement for large equipment was estimated based on the plant's capacity as specified by Peters et al. [45]. Furthermore, membrane replacement costs are taken into account in the variable O&M costs and calculated by dividing the membrane cost by the membrane lifetime. CO₂ transport and storage (T&S) costs are also included in the production cost. The estimation for CO₂ T&S costs is based on the cost assessment study in the DOE/NETL report [48]. The H₂ delivery costs include the transport and

distribution expenses for compressed H₂ (350 bar). Please notice that the H₂ delivery costs vary depending on the dispensing pathways; for instance, the H₂ delivery costs in 2013 by pipeline, pipeline-tube trailer, and tube trailer are \$4.44, \$3.16, and \$3.00 per kg, respectively [49]. Additionally, a carbon price (tax) is explicitly taken into account within this framework. Finally, for the incorporation of all other production cost components and general expenses in the TPC model, the standard procedure presented in the book by Peters et al. [45] has been followed in Table 6.

2.3.3 Economic Performance Assessment: Baseline Net Present Value Model

The net present value (NPV) represents a measure of the increase or decrease in wealth associated with an investment in an engineering project/plant [50]. Moreover, the NPV metric (in particular the expected NPV (ENPV) in the proposed stochastic evaluation framework) represents a risk neutral valuation metric to assess lifecycle economic performance and a rather helpful one for ranking valuation outcomes of competing technology options [50]. As it will be seen in sub-section 3.3, the proposed economic performance assessment framework under uncertainty incorporates additional/complementary economic lifecycle performance metrics such as the “value at risk” and “value at opportunity” that are used from the perspective of risk-averse and risk-seeker analysts/decision makers respectively.

In this study, the baseline NPV-model relies on the standard calculation by forming the difference of the gross present value (GPV) of future net cash flows and the initial TCI [50] (Equation 2-3).

$$NPV = GPV - TCI \quad (2-3)$$

It should be pointed out that the primary objective of the present study is the development and presentation of the structural characteristics of a methodologically sound economic performance assessment framework in the presence of irreducible uncertainty (rather than a detailed investment valuation method that would require data derived from accumulated plant operating experience). This assessment can potentially inform decision making regarding the realization of demonstration plants for a new, yet untested, technology option such as HP-CMR at the commercial scale. In light of the above objective, and given the fact that the latest Chemical Engineering Plant Cost Index needed to update all pertinent cost estimates of HP plants is available for the year 2012, in the present study all HP plants considered are assumed to start operations in the year 2013, the lifetime of each plant is 30 years, and regulatory action on carbon is introduced in the year 2015. Within this context, the GPV is defined as the sum of the discounted stream of net cash flows over 30 years [50]:

$$GPV = \sum_{t=1}^{30} \frac{CF_t}{(1+r)^t} = \frac{CF_1}{1+r} + \frac{CF_2}{(1+r)^2} + \dots + \frac{CF_{30}}{(1+r)^{30}} \quad (2-4)$$

where CF_t is the nominal net cash flow in year t encompassing annual revenue generated by hydrogen sales and TPC, depreciation as well as the plant’s savage value. In the above equation r represents the nominal discount rate that is used in this assessment. In particular, the reportable net income in year t (I_t) was estimated using Equation 2-5, where R is the revenue generated through hydrogen sales in the pertinent market:

$$I_t = R_t - TPC_t \quad (2-5)$$

Please notice that the levelized cost of hydrogen production (the minimum required hydrogen selling price to achieve a 10% annual rate of return over the life of the HP plant) changes since the selling price varies broadly within the pertinent market [51]. Therefore, to avoid a possible overestimation of the revenue stream, the H₂ selling price was conservatively based on a figure of \$10 per kg. In addition, the inflation rate (λ) used in the calculation of the above discounted cash flows was estimated using Equation 2-6, where CPI is the consumer price index [52].

$$\lambda_t = \frac{CPI_t}{CPI_{t-1}} - 1 \quad (2-6)$$

The depreciation cost is deducted as a business expense, practically acting as a tax shield (β) and calculated as follows:

$$\beta_t = FCI \cdot D_t \cdot (\Phi_{State} + \Phi_{Federal}) \quad (2-7)$$

In Equation 2-7, D_t represents the depreciation rate in year t [53], and Φ_{State} and $\Phi_{Federal}$ are the combined state and local sales tax rate and federal corporate tax rate respectively. Please notice that the value of $\Phi_{Federal}$ follows the federal corporate tax schedule defined by the Internal Revenue Service (IRS), U.S. Department of the Treasury that depends on the taxable income level [54], while the value of Φ_{State} is determined by the plant location. The salvage value (S) of HP plants [50] was computed using Equation 2-8, where M denotes the market value of the HP plants considered and B is their book value:

$$S = M - (M - B) \cdot (\Phi_{State} + \Phi_{Federal}) \quad (2-8)$$

In this study, since the recovery period is 20 years, the book value of the plant after 30 years is zero. The term $(M-B)$, in Equation 2-8, is used to represent the taxable gain at the time the plant is sold.

2.3.4 Economic Performance Analysis and Evaluation under Uncertainty: Integration of a Monte Carlo Simulator

Our starting point is the recognition that the TCI, TPC and NPV models are inherently uncertain and driven by various irreducible market, regulatory and other uncertainties. Therefore, an economic performance evaluation framework of a technology option based on expected/average/baseline values for all the above uncertainty sources (the uncertain TCI/TPC/NPV model inputs) leads to single-point estimates and quite often to unsatisfactory economic appraisals [30,31]. This is known as the “flaw of averages” according to which the economic performance evaluated at average/baseline conditions does not necessarily represent the average economic performance [30]. Furthermore, a Monte Carlo simulator integrated into the proposed framework can simultaneously take into account multiple uncertain model inputs associated with the future state of the economic, regulatory and process operating environment as

opposed to the conventional sensitivity analysis where one input variable is allowed to vary while keeping all others fixed [30]. In light of the above, the present study's key objective is the development of a methodologically sound economic performance evaluation framework for HP plants by explicitly taking into account various sources of uncertainty. Consequently, the derivation of TCI, TPC and NPV distribution profiles is sought that allows the statistical characterization of "risks and opportunities/rewards" in the presence of uncertainty [30,31]. For the attainment of such a goal the following methodological path is pursued (Figure 5):

- 1) Step 1: Comprehensive baseline functional TCI/TPC/NPV-models are developed first (please see previous sub-sections)
- 2) Step 2: Key uncertain model input variables are identified admitting reasonable probabilistic representations through appropriately selected distribution profiles. Using Monte Carlo techniques and random sampling from the above distributions, model input uncertainties are propagated through the TCI/TPC/NPV-model, generating distribution profiles for TCI/TPC/NPV that can be characterized in a statistical/probabilistic sense. Please notice that the expected value of the above sample of TCI/TPC/NPV values generated by Monte Carlo simulations represents an unbiased estimator of the expected value of TCI/TPC/NPV, and thus the aforementioned "flaw of averages" can be effectively overcome [30].

As mentioned above, integrating standard Monte Carlo simulation methods into the proposed framework allows the inherent uncertainty of key model inputs to be explicitly recognized. Indeed, the Monte Carlo simulator generates a broad range of economic performance outcomes, and therefore allows the statistical/probabilistic characterization of the impact of uncertain future states on the economic performance of the CMR module as well as the entire HP plant. In the present study, the software package XLSim was used for conducting the Monte Carlo simulation runs [30]. All 33 uncertain model inputs considered are listed along with the corresponding probability distributions in Table 7. Please notice that the lack of accumulated operating experience and the dearth of plant data at the commercial scale pose significant challenges to any economic performance evaluation of HP-CMR plants. In this study, we considered three different types of probability distributions for the uncertain model input variables (please see Table 7):

- i) In the presence of available historical data the associated distributions were developed using standard re-sampling techniques [30].
- ii) In the absence of any reliable data at the commercial scale, simple uniform and triangular distribution forms were considered (minimum, maximum and most likely values; [30]) that span the range of estimates reported in recent comprehensive studies/reports (cited in the list of bibliographical references).

Figure 6 Methodological steps in the Monte Carlo simulation procedure

Table 7 Probability distributions associated with various uncertain model inputs

Uncertainty driver	Minimum	Most likely	Maximum
Pd unit price [\$/g], RH	Historical data from 2010-2014, www.kitco.com		
Au unit price [\$/g], RH	Historical data from 2010-2014, www.kitco.com		
Labor cost per hour [\$/h], RH	Historical data from 2010-2014, www.bls.gov		
Coal price [\$/tonne], RH	Historical data from 2010-2014, www.eia.gov		
Inflation rate, RH	Historical data from 2010-2014, U.S. Dept. of Lab. [2014]		
H ₂ delivery cost [\$/kg], RH	350 bar H ₂ dispensing pathways, www.hydrogen.energy.gov [2013]		
	Pipeline	Pipeline-tube trailer	Tube trailer
	4.44	3.16	3.00
316L PSS support price [\$/cm ² for a 24 cm ² support area], TD	10.2	11.3	12.4
Pd/Au membrane lifetime, TD ^a	1	3	5
Nominal discount rate for HP-CMR plant, TD ^b	14.4%	16.0%	17.6%
CO ₂ transport & storage cost [\$/tonne], TD	9	10	11
CO ₂ tax rate (start at 2015) [\$/tonne], TD	27	30	33
Annual growth rate of CO ₂ tax, TD	5.4%	6.0%	6.6%
H ₂ selling price [\$/kg], TD	9	10	11
Combined state and local sales tax rates, TD	0.0%	6.4%	9.5%
Ratio for market value of plant after 30 years, TD ^c	13.5%	15.0%	16.5%
Ratio for Installation, UD ^d	25.0%		55.0%
Ratio for instrumentation and controls, installed, UD ^d	8.0%		50.0%
Ratio for piping, installed, UD ^d	10.0%		80.0%
Ratio for electrical, installed, UD ^d	10.0%		40.0%
Ratio for buildings, process and auxiliary, UD ^d	10.0%		70.0%
Ratio for service facilities and yard improvements, UD ^d	40.0%		100.0%
Ratio for land, UD ^d	4.0%		8.0%
Ratio for engineering and supervision, UD ^e	5.0%		30.0%
Ratio for legal expenses, UD ^c	1.0%		3.0%
Ratio for construction expense and contractor's fee, UD ^c	10.0%		20.0%
Ratio for contingency, UD ^c	5.0%		15.0%
Ratio for insurance, UD ^c	0.4%		1.0%
Ratio for working capital, UD ^f	10.0%		20.0%
Ratio for financing interest, UD ^f	6.0%		10.0%
Ratio for plant overhead costs, UD ^g	5.0%		15.0%
Ratio for patents and royalties, UD ^g	0.0%		6.0%
Ratio for administrative costs, UD ^g	2.0%		5.0%
Ratio for marketing costs, UD ^g	2.0%		6.0%

RH = Resample historical data, TD = Triangular distribution, UD = Uniform distribution

^a Based on available lab-scale data and estimates reported in the literature [21], ^b Notice that the nominal discount rate used for the conventional plants was 12.95% [24], ^c Based on fixed capital investment, ^d Based on purchased equipment cost, ^e Based on direct cost, ^f Based on total capital

investment, ^g Based on total product cost.

3. Main Results and Discussion

3.1 Capital investment cost estimation under uncertainty: The CMR module case

A CMR module cost analysis in the presence of uncertainty is conducted with the integration of standard Monte Carlo simulation methods into the FCI/TCI model presented earlier. The cumulative probability distribution FCI and TCI profiles as well as the associated expected values for industrial scale CMR modules are presented in Figure 7. These profiles and the corresponding statistical characterization possibilities provide valuable pieces of information with respect to potential economic performance outcomes [55]. For example, it is possible to observe that there is a 10% probability for the FCI to be lower than 225 M\$ and a 90% probability for the TCI to be higher than 400 M\$. The “value at risk” and the “value at opportunity” are quantified at pre-specified probabilistic levels of 95% and 5% (P_{95} and P_5) respectively. A threshold-value of P_{95} represents that there is a 5% probability of incurring a cost higher than this value, while there is a 5% probability of incurring a cost lower than a P_5 threshold-value. P_{95} , P_5 , and expected values of FCI/TCI for the CMR module are summarized in Table 8.

Figure 7 Cost distribution of an industrial scale CMR module.

Table 8 Industrial scale CMR module cost summary.

	Fixed capital investment		Total capital investment	
	[M\$]	[\$/m ²]	[M\$]	[\$/m ²]
P ₉₅	354.3	20,275	419.7	24,018
Expected value	279.1	15,969	328.6	18,805
P ₅	212.5	12,161	249.6	14,284

3.2 Economic Assessment of HP Technology Options

The technical performance of HP-CMR plants is first comparatively evaluated in terms of coal feed requirements and CO₂ production and emission levels against conventional HP plants that utilize PSA as a purification unit (HP-PSA plants). Pertinent results are graphically shown in Figure 8. Correspondingly, plant specifications and capital investment costs associated with all technology options considered in this study are tabulated in Table 9. These results show that the higher efficiency displayed by the HP-CMR plant reduces the coal feed requirements to achieve the same H₂ production levels by 16% compared to the conventional HP-PSA plants. The reduction in the coal feed requirements is attributed to process intensification-relevant benefits attributed to CMRs in which the WGS reaction and separation are simultaneously carried out [58]. Furthermore, the lower CO₂ production level is directly reflected on the lower carbon feed requirements in the HP-CMR case, as shown in Figure 8. Please also notice that HP plants with integrated CCS systems lead to a substantial reduction of the amount of CO₂ emissions, but their degree of efficiency varies. The HP-PSA plant has an efficiency of 90% while the HP-CMR plant displays an efficiency of 98%. Considering both the lower CO₂ production levels and the higher CO₂ capture efficiency achieved by the HP-CMR technology option, the HP-CMR plant emits 0.07 Mtonnes of CO₂ per Mtonnes of coal feed compared to a value of 0.23 for the conventional HP plant, leading to an overall reduction in CO₂ emissions of 70%. Other than higher levels of technical performance displayed by the HP-CMR plant, lower capital investment costs for the same H₂ production target level can be also achieved using the HP-CMR technology option as seen in Table 9. Notice that the benefits of the HP-CMR technology option lead to a reduction of the TCI costs for HP by 26%. Indeed, process intensification opportunities combined with the simultaneous CO₂ capture and extra purity H₂ production enabled by CMRs allow a significant reduction in the pertinent TCI costs by reducing the size of the process equipment needed and replacing the traditional WGS reactors, PSA as well as Selexol units.

Figure 8 Coal feed, CO₂ production, and CO₂ emissions of hydrogen production plants for various technology options

Table 9 Hydrogen production plant specifications and capital investment costs for various technology options.

	TCI [B\$]	Plant size [TPD]	H ₂ production [TPD]	Coal feed [TPD]	CO ₂ production [TPD]	CO ₂ captured [TPD]	CO ₂ emissions [TPD]
HP-PSA plant w/o CCS sys.*	1.82	685	616.5	5,302	12,137	0	12,137
HP-PSA plant w CCS sys.*	2.14	685	616.5	5,302	12,137	10,954	1,183
HP-CMR plant w CCS sys.	1.58	685	616.5	4,384	9,936	9,737	199

TPD = Tonne Per Day

*For the pertinent data sources of the HP-PSA plants, please see DOE/NETL report [24]

Considering all uncertain model inputs listed in Table 7, the economic performance of HP plants and range of potential outcomes are comparatively evaluated amongst the various technology options by conducting detailed simulation studies. As it will be demonstrated below, the inclusion of regulatory action on carbon has a significant effect on the NPV distribution profiles of all technology options considered in the present study, generating comparative economic performance advantages and noticeably promising prospects in the HP-CMR case. Indeed, it is shown that HP-CMR could become an economically appealing technology option under a certain set of regulatory conditions, thus deserving attention as a potentially meritorious option whose realization prospects of an initial fleet of demonstration plants at the commercial scale ought to be seriously considered.

The simulation results of NPV distribution profiles in the absence and presence of regulatory action on carbon are presented in Figure 9(a) and Figure 9(b), respectively. It should be pointed out that the initial CO₂ tax rate of \$30 per tonne of CO₂ considered represents a reasonable first estimate based on current market conditions and average “best” estimates provided by experts [66]. Furthermore, \$30 per tonne of CO₂ indicates an initial tax level higher than the CO₂ abatement cost, thus providing an incentive for HP plant owners/operators to invest in CCS systems. At this point, it should be pointed out that a price on emissions (of any type) conforming to a simple stochastic model that makes use of an initial emissions price and an annual growth rate (such as the one presented) could have been considered within the context of the present research study. We chose the “carbon tax” term since such a type of emissions price is now widely acknowledged of generating the appropriate price signals that can be internalized by the pertinent markets in the most direct and seamless manner [10,28]. In Figure 9(a), notice that in the absence of CO₂ tax, the conventional HP-PSA plant without any CCS system installed has the most attractive NPV distribution profile, and therefore, the graphically depicted results naturally reproduce the current state of affairs in the field of hydrogen production. Moreover, it also confirms the fact that the capital investment and O&M costs associated with the installation and operation of a CCS system would result in less attractive economic outcome profiles in all cases in the absence of a CO₂ tax. However, under the conditions considered and in the presence of regulatory action on carbon the NPV distribution profile of HP-CMR emerges as a comparatively appealing one. Indeed, one observes that key performance assessment metrics deduced from the above NPV-distribution profiles such as ENPV, P₉₅ and P₅ - threshold values (“value at opportunity”, “value at risk”) are improved compared to the ones associated with the NPV distribution profiles of the traditional technology option with CCS. This outcome can be jointly attributed to the fact that superior efficiency gains in the HP-CMR case coupled with higher regulatory cost savings (versus CCS-operating costs) realized when compared to the traditional option result in enhanced economic performance in an uncertain carbon-constrained world over the plant’s lifetime. In light of these findings, a stronger justification basis could be built for the provision of the right incentives aiming at the realization of technology demonstration projects at the commercial scale for a technology option such as HP-CMR, thus supporting broader energy and environmental policy goals briefly presented in the Introduction section.

Finally, it would be worth noticing that the conventional HP-PSA plant without a CCS system appears to be the most sensitive to future regulatory action, while the HP-CMR plant appears to be less sensitive due to the fact that the degree of change of the NPV distribution profiles is mainly determined by the “carbon tax penalty” which is computed through the amount of CO₂ emissions and the CO₂ tax rate (thus allowing

536 the HP-CMR plant to exhibit more appealing economic performance outcomes under the stated regulatory
537 conditions).
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(a)

(b)

Figure 9 Cumulative probability distribution profiles of the Net Present Value for various technology options in (a) the absence of CO₂ tax and their ENPV rates with displayed rate changes and (b) under an initial tax rate of \$30 per tonne of CO₂

The effects of uncertainty on the expected NPV-value (ENPV) for the various technology options integrated with CCS systems are also analyzed through Tornado diagrams and presented in Figure 10. A Tornado diagram summarizes graphically the relative impact of variations of the numerous uncertain NPV-model inputs over their respective ranges (from the lowest to the highest value) under the assumption that all other model inputs remain at their baseline values (fixed at their expected values). In a Tornado diagram each model input is represented by a bar as it varies over its prescribed range depicting its impact on the above performance indexes, and all bars are sorted from the long ones at the top to the shorter ones at the bottom in a decreasing impact order [59]. In this manner, a Tornado diagram prioritizes the most consequential inputs (sources of uncertainty) in terms of bar length and facilitates the visualization of their impact on economic performance, primarily in cases of large-scale multi-input models. Figures 10(a) and 10(b) provide representative ENPV-Tornado diagrams for the case of the traditional HP as well as the HP-CMR option. The uncertain model inputs considered and their respective prescribed ranges used include the following: Pd unit price: 16.9-25.9 \$/g, Au unit price: 39.4-53.7 \$/g, coal price: 61.0-48.5 \$/tonne, inflation rate: 1.46-3.16%, H₂ delivery cost: 3.0-4.4 \$/kg, Pd/Au membrane lifetime: 1-5 years, CO₂ transport & storage cost: 9-11 \$/tonne, annual growth rate of CO₂ tax: 5.4-6.6%, H₂ selling price: 9-11 \$/kg, combined state and local sales tax rates: 0-9.5%, financing interest to total capital investment ratio range: 6-10%, and plant overhead costs to total product cost ratio range: 5-15%. Please notice that hydrogen selling price, hydrogen delivery cost, plant overhead costs, financing interest costs, taxation levels and inflation rate constitute the set of model inputs with the highest impact on ENPV.

As shown in Figure 10, hydrogen selling price has the most significant impact on NPV in both cases, suggesting that economic performance of HP plants greatly depends on the revenue generated through hydrogen sales. Additionally, since the H₂ selling price is mainly determined by production costs [51], production cost disruption (referring to situations where production costs undergo significant departures from their expected values used to design the coordination scheme which aligns the plans and objectives of the project undertaken [60]) can significantly influence the H₂ economy by shifting selling prices. However, in the short and medium term, production cost disruptions in the H₂ economy are unlikely to happen unless alternative energy prices become increasingly competitive, H₂ demand grows rapidly and/or a breakthrough in H₂ production technology occurs. Finally, when comparing the two cases, it is found that HP-PSA plants appear to be more sensitive to the selling price than HP-CMR plants, implying that the effect of the selling price on NPV-based performance evaluation is jointly determined by production costs and the nominal discount rate of the various HP options.

H₂ delivery cost is another uncertainty driver that exerts a significant effect on the NPV of HP plants. The delivery cost is determined by the geographic and market characteristics, such as transport distance, delivery chain, density demand, etc. Yang and Ogden [61] reported that compressed gas truck delivery is ideal for small stations with low demand, while cryogenic liquid trucks of liquefied H₂ is preferred for long distances and robust, healthy demand patterns. Within such a context, any geographic and market characteristics should be considered and carefully evaluated for customization of H₂ delivery in order to enhance the economic performance of HP plants. Furthermore, it should be pointed out that considerably high costs for H₂ delivery would drive the ENPV value of HP-PSA plants to become negative, while HP-CMR plants can withstand the effect of delivery costs to maintain a positive ENPV due to their production cost.

The lifetime of Pd/Au membranes is an uncertain model input that affects the ENPV of HP-CMR plants. A long lifetime would reduce the total product cost by lowering the membrane replacement cost, thus increasing the plant's ENPV. Since the replacement cost is jointly determined by the membrane cost and lifetime, the effect of lifetime is also correlated with the Pd unit price as well as the membrane thickness. When the membrane cost is relative low by using thinner membranes, the impact of the membranes' lifetime on the ENPV could be higher than the Pd unit price (see Figure 10 (b)); in contrast, when the membrane cost dominates the membrane replacement cost in cases of thicker membranes use, the Pd unit price could have a greater effect on ENPV than membrane lifetime [55]. It should be pointed out that currently the fabrication of thin membranes with high durability characteristics is attainable and has been demonstrated by Augustine et al. [21]. Moreover, lifetime extension can be also achieved by repairing defects on the membranes and/or through post-treatment for reactivation of contaminated membranes [62,63,64]. Given the current pace of advancements in membrane science and technology, it is reasonably expected that the effect of membrane lifetime could be further minimized in the future. Please notice that this feature was not included in the present evaluation framework.

Comparing the Tornado ENPV diagrams of the traditional HP-PSA plant to an HP-CMR plant, one infers that the HP-PSA plant appears to be more sensitive to financing interest costs, while HP-CMR plants appear to be more susceptible to combined state and local sales tax rates. Please notice that federal corporate tax rates, as mentioned before, depend on the reportable income and therefore are not shown as uncertainty drivers in the Tornado diagrams; however, they are expected to have a high impact on the ENPV of the plants. Indeed, higher capital investment costs for HP-PSA plants (Table 9) generate higher financing interest costs. In contrast relatively lower capital investment costs for HP-CMR plants could mitigate the effect of corresponding financing interest costs on ENPV. Please also notice that combined with a relatively low total product cost, tax rates become critical in the calculation of net cash flows. As a result, tax rates can have a more substantial impact on the ENPV than financing interest costs under low capital investment and total product costs. Focusing on the effect of taxation levels, tax incentives have been occasionally introduced by states to influence business relocation, expansion, or start-up formation-relevant decision-making [65]. However, tax incentives in isolation could not determine "optimal" technology choices and plant locations since they do not represent the only criterion in an inherently complex decision-making process (other factors include developments in hydrogen markets and distribution challenges, macroeconomic conditions, state of regulatory framework and geopolitical stability).

(a) HP-PSA plant w CCS sys.

(b) HP-CMR plant w CCS sys.

Figure 10 Tornado diagrams for the NPV of various technology options in the presence of CO₂ tax.

The effect of regulatory action (with an initial CO₂ tax rate starting on 2015) on ENPV is further examined in the following three technology option cases: i) Case A refers to an HP-PSA plant without any CCS system installed; ii) Case B corresponds to an HP-PSA plant with a CCS system installed, and iii) Case C corresponds to an HP-CMR plant with a CCS system installed.

The ENPV in the three cases considered is computed and tabulated at different initial CO₂ tax rates as shown in Table 10. From this table, it can be inferred that the ENPV of conventional HP plants without CCS varies significantly as the initial CO₂ tax rate increases, becoming economically problematic when the rate reaches \$65 per tonne of CO₂ and the associated regulatory compliance costs become quite significant. However, conventional HP plants with CCS systems do not display negative ENPVs within the range of CO₂ tax rates considered since the regulatory compliance cost savings exceed the costs associated with the operation of the CCS system.

The technology options considered were then evaluated under a set of different tax rates in order to visualize their impact on the associated ENPVs as shown in Table 11. First an economic performance comparison involving Cases A and B was performed and labeled as the “Traditional technology option.” This case demonstrates the economic effect of having a CCS system installed in a traditional HP plant under future regulatory action on CO₂ emissions. As shown in Table 11, the ENPV difference favors the use of CCS systems when the tax rate is higher than \$25 per tonne of CO₂. Lower tax rates do not seem to incentivize the integration of CO₂ capture technologies in HP plants. Similar conclusions have been previously drawn and discussed in the context of coal-fired power plants with CCS units installed [42,66,67].

The second economic comparison, performed in this study, was between Case C and A, which was labeled as “Membrane technology option.” This option shows the economic effect of integrating membrane technology into HP plants in the presence of future CO₂ emission regulations. Based on the proposed NPV-based assessment framework, the analysis indicates that Case C, i.e. the HP-CMR option becomes comparatively economically appealing when the regulatory tax rate reaches \$15/tonne of CO₂. Therefore, it is possible to conclude that, depending on the course of action of future regulatory policies on carbon, there is a window of opportunity for HP-CMR to be perceived as an economically robust, if not superior, competitor to the incumbent technology option exhibiting also enhanced environmental performance in a carbon-constrained world. However, in the absence of regulatory action, the conventional HP options would remain uncontested when economic metrics dominate decision making in selecting the best technology options. It would be also worth noting that the HP-CMR option, when compared to the traditional HP with CCS, attains a positive ENPV at lower regulatory tax rates.

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Table 10 ENPV performance (B\$) of technology options under various CO₂ tax scenarios.

Case	Case Explanation	Initial CO ₂ tax rate [\$/tonne CO ₂]														
		0	5	10	15	20	25	30	35	40	45	50	55	60	65	70
Case A	HP-PSA plant w/o CCS sys.	2.17	2.01	1.84	1.67	1.50	1.34	1.16	0.99	0.81	0.63	0.45	0.26	0.07	-0.13	-0.33
Case B	HP-PSA plant w CCS sys.	1.32	1.31	1.29	1.27	1.26	1.24	1.23	1.21	1.19	1.18	1.16	1.14	1.13	1.11	1.09
Case C	HP-CMR plant w CCS sys.	1.62	1.61	1.61	1.61	1.61	1.61	1.60	1.60	1.60	1.60	1.60	1.59	1.59	1.59	1.59

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Table 11 ENPV difference (B\$) between two technology options under various CO₂ tax scenarios.

ENPV difference	Initial CO ₂ tax rate [\$/tonne CO ₂]														
	0	5	10	15	20	25	30	35	40	45	50	55	60	65	70
Traditional technology option (Case B – Case A)	-0.85	-0.70	-0.55	-0.40	-0.25	-0.09	0.06	0.22	0.38	0.54	0.71	0.88	1.06	1.24	1.43
Membrane technology option (Case C – Case A)	-0.56	-0.39	-0.23	-0.06	0.10	0.27	0.44	0.61	0.79	0.96	1.15	1.33	1.52	1.72	1.92

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The rate under which the ENPV changes as a function of the initial carbon tax (shown in Equation 3-1) is considered in all cases as a measure of sensitivity or robustness of economic performance to future regulatory action on CO₂ emissions

$$r = - \frac{\Delta ENPV}{\Delta \text{Initial CO}_2 \text{ tax rate}} \quad (3-1)$$

Notice that the above ratio captures the degree of sensitivity of economic performance of an HP-relevant technology option (when evaluated through the ENPV-metric) with respect to a future carbon price. The calculated values of the rate r are: 0.035, 0.003 and 0.0004 [B\$] per \$/tonne of CO₂ for cases A, B and C, respectively. In Figure 11, NPV distribution profiles for all HP technology options considered are depicted in the absence of any regulatory action along with their respective rates. Furthermore, since the magnitude of the rate r is smaller in the HP-CMR case than in the traditional HP (Cases A and B), the NPV-profile of the HP-CMR finds itself located to the right of the NPV-profiles of Cases A and B (as also previously depicted in Figure 9(b) under an initial CO₂ tax rate of \$30 per tonne CO₂), thus starting to become comparatively more appealing under regulatory taxes greater than \$15/tonne of CO₂. It is important to mention that the NPV profile of the HP-CMR plants undergoes a smaller shift compared to the traditional technology option in response to the introduction of a carbon tax, thus demonstrating the relative robustness of its economic performance under regulatory uncertainties. Please notice that the arrows shown in Figure 11 represent the rate under which the NPV-curve of each technology option is displaced towards less attractive valuation zones when a carbon price is imposed.

Figure 11 Net present value cumulative probability distribution profiles for various technology options in the absence of CO₂ tax and their ENPV rates.

3.3 The role of discount-rate in the valuation of HP-CMRs: Sensitivity analysis

The discount rate at which future cash flows are discounted represents a key determinant of any technology investment project valuation approach, particularly in cases involving capital intensive projects where their respective NPV distribution profiles depend crucially on the choice of the discount rate. It should be pointed out that the aforementioned discount rate depends essentially on two factors: (i) the perceived risk of the specific project (ii) as well as its financing mechanism [31,50, 59]. Indeed, investment in advanced energy-relevant technology projects encompasses a diverse set of risks such as: macro-economic ones related to global economic growth and demand for hydrogen as well as availability of labor and capital, regulatory risks, technology reliability risks, price and volume risks in the hydrogen markets and fuel price (coal, natural gas) risks. Please notice that these project risks could affect different technology options in different ways. Focusing solely on capturing project risk, 100% equity financing is usually assumed, and the most common practice is to add a project specific risk premium to the risk free rate of return when estimating the discount rate (the risk free rate of return is generally determined by the long-term rates of return of government bonds in the United States) [31,50,59]. It should be pointed out that the estimation of the risk premium could become quite complex. If the risk of the project under consideration is similar to other ones undertaken by the firm, and if the firm's common stock is traded on open markets then in principle the risk premium can be estimated using published historical stock price

data [31,50,59]. As mentioned earlier, the nominal discount rate used by the DOE for evaluating investments in conventional hydrogen production is 12.95% [24]. When the financing structure of the project is also taken into account, the risk-adjusted nominal discount rate is a weighted average of the cost of funds obtained from shareholders (“cost of equity”) and borrowed from debt-holders (“cost of debt”) with relative amounts of equity and debt being the respective weights (known as the Weighted Average Cost of Capital) [31,50]. In competitive hydrogen markets, what matters to the investor is the profitability of the investment against the risk to the capital employed. In particular, the level of risk anticipated by an investor in a hydrogen production plant will be reflected on the level of return expected on that investment. Moreover, the greater the business and financial risks, the higher the overall return that will be demanded. Since it is quite difficult for the traditional levelised cost-based methodology to incorporate risks and uncertainty effectively, the proposed approach using a detailed NPV model coupled with a Monte Carlo simulator represents a methodologically appropriate and sound approach to effectively cope with multiple risk and uncertainty sources by generating a range of economic performance assessment outcomes for a new technology option such as HP-CMR [31,50,59]. Within the above context, we complemented the valuation assessment with a sensitivity analysis conducted for different representative values of the discount rate that span a reasonable range (between 10 and 20% in nominal terms) associated with business and financing risks. Lower values of the discount rate could correspond to a more stable environment of the producing firm (low macro-economic risks, acceptable technology reliability levels, an available captive market and long-term contracts, availability of capital, low financing risks) whereas higher values of the discount rate could correspond to conditions of elevated risks in the firm’s (macroeconomic, operating, financing, market) environment. The simulation results derived are tabulated in Table 12. Please notice the expected adverse impact of a higher discount rate on the economic performance and valuation profile of HP-CMR reflected on all indicators: a deteriorating ENPV, an increasing probability of loss, a decreasing range of upside opportunities and a deteriorating “value at risk” pattern (downside risk). It becomes therefore apparent that creatively structured financing mechanisms leading to a reduction of the cost of capital/discount rate could induce more appealing economic performance outcomes and valuation profiles, thus unlocking the investment potential of a clean hydrogen production project that utilizes the HP-CMR technology option.

Table 12 Sensitivity analysis results of the NPV-based economic performance assessment for HP-CMR plants with various discount rates.

	Discount rate [%]										
	10	11	12	13	14	15	16	17	18	19	20
P ₅ [B\$]	0.73	0.52	0.35	0.21	0.08	-0.04	-0.14	-0.24	-0.31	-0.38	-0.46
ENPV [B\$]	3.56	3.11	2.72	2.39	2.10	1.84	1.60	1.42	1.24	1.08	0.94
P ₉₅ [B\$]	5.87	5.22	4.64	4.16	3.75	3.35	3.04	2.77	2.51	2.27	2.06
Standard deviation [B\$]	1.61	1.47	1.35	1.24	1.15	1.07	1.00	0.94	0.88	0.83	0.79
Probability of loss	2%	2%	3%	4%	5%	6%	8%	10%	12%	14%	17%

4. Concluding Remarks

Membrane reactor technology integrated into hydrogen production plants (HP-CMR) generates promising prospects of advancing energy and environmental policy goals. Technical advantages of HP-CMR include a reduction in coal-feed requirements and consequently CO₂ emission levels by means of process intensification and higher carbon capture efficiency. Indeed, the overall reduction of carbon emissions is 70% lower compared to the conventional technology option. Another technical and environmental performance-relevant advantage is the simultaneous CO₂ capture and generation of extra pure H₂ through the use of CMRs. This new technology option enables the elimination of traditional WGS reactors, PSA and Selexol units in conventional H₂ production plants, thus potentially enhancing the economic performance of an HP-CMR plant. Indeed, HP-CMR plants showed a 26% reduction in total capital investment costs and good valuation prospects even under higher nominal discount rates reflecting the added risks associated with a new technology option and the lack of relevant accumulated operating experience. Motivated by these preliminary realizations, a comprehensive economic performance assessment framework was developed in the presence of irreducible uncertainties through the integration of a detailed NPV-model with a Monte Carlo simulator. Within the proposed economic performance evaluation framework for a HP-CMR plant more realistic NPV-distribution profiles were derived rather than single-point value estimates that often lead to unsatisfactory valuation assessments by overlooking significant uncertainty effects over the plant's lifetime. Furthermore, the economic performance of a HP-CMR plant was comparatively assessed against the conventional coal gasification-based hydrogen production plant. The analysis conducted also suggested that in the absence of any regulatory action on CO₂ emissions HP-CMR could not be perceived as an economically viable option. However, better prospects for HP-CMR arise if future regulatory action on CO₂ emissions is introduced, and therefore, initiatives to stimulate the realization of demonstration projects of this innovative technology at the commercial scale might be warranted. Finally, it was found that the degree of sensitivity of economic performance (when evaluated through the ENPV-metric) with respect to a future carbon price conforms to the following inequality (in descending order amongst the technology options considered): HP-PSA without CCS system > HP-PSA with CCS system > HP-CMR.

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List of Acronyms

ASU	Air Separation Unit
CCS	Carbon Capture and Sequestration
CPI	Consumer Price Index
CMR	Catalytic Membrane Reactor
ENPV	Expected Net Present Value
FCI	Fixed Capital Investment
GPV	Gross Present Value
HTS	High Temperature Shift
HP	Hydrogen Plant
HP-CMR	Hydrogen Plant – Catalytic Membrane Reactor
HP-PSA	Hydrogen Plant – Pressure Swing Adsorption
IGCC	Integrated Gasification Combined Cycle
NPV	Net Present Value
O&M	Operation and Maintenance
PSA	Pressure Swing Adsorption
TPC	Total Product Cost
T&S	Transport and Storage
TCI	Total Capital Investment
WC	Working Capital
WGS	Water Gas Shift Reaction

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