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Economic performance evaluation of flexible centralised and decentralised blue hydrogen production systems design under uncertainty

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HIGHLIGHTS

- Techno-economic study of flexible blue H_2 production plants under uncertainty.
- Use cases of centralised/decentralised plants for transport around San Francisco.
- Fixed, phased, flexible designs analysed using NPV, capex, value-at-risk/gain.
- Flexible centralised designs yield better value, despite modularity cost-premium.
- Flexibility mitigates market & regulatory uncertainty around global H_2 economy.

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ABSTRACT

Blue hydrogen is viewed as an important energy vector in a decarbonised global economy, but its large-scale and capital-intensive production displays economic performance vulnerabilities in the face of increased market and regulatory uncertainty. This study analyses flexible (modular) blue hydrogen production plant designs and evaluates their effectiveness to enhance economic performance under uncertainty. The novelty of this work lies in the development of a comprehensive techno-economic evaluation framework that considers flexible centralised and decentralised blue hydrogen plant design alternatives in the presence of irreducible uncertainty, whilst explicitly considering the time value of money, economies of scale and learning effects. A case study of centralised and decentralised blue hydrogen production for the transport sector in the San Francisco area is developed to highlight the underlying value of flexibility. The proposed methodological framework considers various blue hydrogen plant designs (fixed, phased, and flexible) and compares them using relevant economic indicators (net present value (NPV), capex, value-at-risk/gain, etc.) through a detailed Monte Carlo simulation framework. Results indicate that flexible centralised hydrogen production yields greater economic value than alternative designs, despite the associated cost-premium of modularity. It is also shown that the value of flexibility increases under greater uncertainty, higher learning rates and weaker economies of scale. Moreover, sensitivity analysis reveals that flexible design remains the preferred investment option over a wide range of market and regulatory conditions except for high initial hydrogen demand. Finally, this study demonstrates that major regulatory and market uncertainties surrounding blue hydrogen production can be effectively managed through the application of flexible engineering system design that protects the investment from major downside risks whilst allowing access to favourable upside opportunities.

1. Introduction

In a quest to decarbonise the global economy and mitigate challenges from climate change, increased attention has been placed on reliable, affordable, and low-carbon energy vectors potentially deployed in versatile application fields. This necessity has generated renewed interest in hydrogen that has lately received significant public and private support [20] as evidenced by recent announcements involving 359 large-scale projects worth $500 billion [38]. Parts of these projects have been

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Nomenclature

a	Translation parameter, (–)
ATR	Autothermal reforming, (–)
b	Sharpness parameter, (–)
B	Slope of learning curve, (–)
Capex	Capital expenditure, (million $)
CCS	Carbon capture and storage, (–)
CDF	Cumulative density function, (%)
CF_t	Cash flow at year t, (million $)
$CTGR_t$	Expected growth rate of carbon price at year t, (–)
$D(t)$, $D(t)_{projected}$	Normal and projected demand of hydrogen at year t, (*tpa*)
ENPV	Expected (or average) NPV over n simulation runs, (million $)
EoS	Economies of Scale, (–)
FC	Fixed operating cost, (million $)
GBM	Greater Brownian Motion, (–)
LCOH	Levelised cost of hydrogen, ($/kg H_2)
LR	Learning rate, (%)
Max	Maximum value, (–)
M_t, M_{vol}, M_{nom}	Limit of demand at year t, volatility of demand limit and nominal value of demand limit, (tpa)
Min	Minimum value, (–)
NPV	Net Present Value, (million $)
OC	Variable operating cost, (million $)
Opex	Operational expenditure (or TPC), (million $)
P_t	Price of hydrogen at year t, ($/kg)
r	Discount rate, (%)
rand	Random number, (–)
ROA	Real Option Analysis, (–)
R_t	Revenue at year t, (million $)
STD	Standard Deviation, (million $)
SV	Salvage value, (million $)
TC_t	45Q tax credit, ($/t$CO_2$)
TCI	Total Capital Investment, (million $)
TDC	Total Direct Cost, (million $)
tpa	Tonnes per annum, (–)
TPC	Total production cost, (million $)
tpd	Tonnes per day, (–)
U_1, U_i	Capital cost of the first and i^{th} modules, (million $)
VaG	Value at Gain (90%percentile), (million $)
VaR	Value at Risk (10% percentile), (million $)
VoF	Value of flexibility, (million $)
X	Expansion threshold, (%)
α	Scale exponent, (–)
δ	Growth rate, (–)
ε	Wiener process variable, (–)
η_t	Plant downtime, (%)
θ_f, θ_s	Federal tax and State, (%)
μ_{demand}, μ_{CO2}	Drift rate for demand and CO_2 price modelling, (–)
ν	Annual CO_2 emissions, (*tpa*)
σ_{demand}, σ_{CO2}	Annual volatility for demand and CO_2 price, (–)
ψ_τ	Depreciated capital, (million $)

dedicated to blue hydrogen production which has been envisioned as an 'enabler' of the global hydrogen economy. The most widespread technology solution for blue hydrogen production at large-scale is steam methane reformation (SMR) [48]. In the near-term, SMR is likely to remain the preferred blue hydrogen alternative considering its strong economies of scale (EoS), technological maturity level and available infrastructure in place [30].

Despite the evident potential of blue hydrogen, multiple technical, financial and market challenges hinder its production at a global scale [32]. This inherent uncertainty is primarily driven by the dynamics of the energy industry, technological innovation, and geopolitics. The nature and interdependency of these key elements are highly complex and often unpredictable, thus emphasising the need to consider them explicitly in future decision-making on the hydrogen economy.

Flexible system design has emerged as a relevant, logical, and value-enhancing paradigm, aimed to manage the impact of irreducible uncertainty on the overall economic performance profile of a given system. The fundamental idea of this design framework is focused on constructing and operating an adaptable, changeable and reconfigurable system [12] [9]. It is termed a flexible system since by design it provides system operators with the 'right, but not the obligation' [39] to change cost-effectively a system subject to fluctuating market, regulatory or technological conditions. The latter concept is reminiscent of the real options theory which was inspired by the field of financial options to strategically manage uncertainty [42–44]. As such, flexible engineering system design leverages the conceptual and analytical appeal of real option analysis to manage uncertainty and enhance economic performance of the system through a novel methodological and analytical/computational framework.

Considering the above, the primary aim of this study is to develop a systematic and insightful economic performance assessment framework using engineering real options analysis and apply it to flexible blue hydrogen production system design. In the present study, centralised and decentralised blue hydrogen production systems have been investigated under market, regulatory and technological uncertainty with emphasis on finding optimal designs and capacity planning based on economic performance. A case study of hydrogen fuel production for on-road transport in the San Francisco area was formulated to investigate the potential value-enhancing characteristics of flexibility. The reason for this was two-fold. First, the use of hydrogen as a fuel for heavy duty transport was identified as a strategic use-case in the recent [31] study and likely would form the majority of hydrogen fuel demand in San Francisco. Second, California is one of the leading hydrogen-powered transport regions in the world with available refuelling infrastructure already in place and ambitious expansion plans in the coming decades [5]. Furthermore, California holds access to cheap and abundant US natural gas ($2–3/MMBtu) and high levels of CO_2 storage capacity that is crucial for cost-competitive blue hydrogen production [57]. To extend the analysis further, centralised and decentralised hydrogen production modes were comparatively assessed to elucidate the underlying trade-offs between EoS and production flexibility. Moreover, time value of money, cost uncertainty, EoS and learning effects were all explicitly considered in the proposed economic performance assessment and technology option valuation method to provide a more thorough and nuanced evaluation of flexible blue hydrogen production prospects. As such, this study introduces a novel approach in evaluating the techno-economic performance profile of blue hydrogen production under uncertainty and different production scales. A core objective of this study is to provide key-decision makers with the ability to characterise and assess (i) the value of flexibility, (ii) the impact of the inherent uncertainty on process economics and (iii) the viability prospects of decentralised blue hydrogen production.

The paper is structured as follows: Section 2 provides a literature review of conventional system design flexibility, engineering real options analysis and economic performance assessment of blue hydrogen production. Section 3 outlines the structure of the proposed conceptual, methodological and analytical framework inspired by the principles and methods of engineering systems flexibility and real options analysis [14,43,44]. Section 4 encompasses the main results of the study and a discussion on the derived insights within the context of the proposed uncertainty modelling, flexibility analysis and economic performance assessment framework. The final section offers concluding remarks on the value of flexible system design and operation in an inherently uncertain environment that accompanies centralised and decentralised blue hydrogen production, as well as policy-relevant recommendations and suggestions for further research.

2. Literature review

Engineering systems are complex systems that are subjected to a high degree of change throughout their life-cycle [43]. This inherent complexity has often prompted system architects and management to design and evaluate system performance based on average conditions [14]. Such practice stems from a focus on long-term planning assuming that the external environment remains fairly constant, and where trends can be readily anticipated [24]. This has largely led to robust, narrowly optimised, and non-adaptive systems deployed at a large scale. These systems have been typically evaluated using conventional valuation methods such as discounted cash flow analysis, which discounts future profits at a given rate and bring them to present day value. Of these, net present value (NPV) is the leading “risk-neutral” valuation method that informs senior management of the expected project value [56]. Neither NPV nor other methods (IRR or cost-benefit ratio) account for two crucial aspects [43]. First, these methods do not recognise changing market or system dynamics, and rely on fixed, average, and deterministic forecasts that often lead to the “flaw of averages” [54], i.e. the fallacy that system performance evaluated at average conditions represents average performance in an uncertain world. Second, they do not acknowledge the inherent optionality element in management decision-making that can proactively change or reconfigure a system and its operating mode in response to changing circumstances.

Considering the role and impact of uncertainty, flexible engineering system design is an emerging paradigm that attempts to provide enhanced system performance considering an inherently dynamic and uncertain world [16]. The overall goal of flexibility is to enhance economic performance by incorporating adaptive, changeable and responsive design which can respond to a range of possible internal or external eventualities. In practice, “flexible engineering design options” are divided into two groups: “on” and “in” systems [59] sometimes also referred to as ‘strategy’ and ‘enabler’ [12], respectively. The former category relates to managerial flexibility that system operators can exercise to provide flexibility. Common forms of ‘on’ system flexibility relates to (i) expansion, contraction or phasing of system capacity, (ii) deferral of investment in the system until favourable market conditions materialise or (iii) switching between various inputs and/or outputs in design (e.g., fuel type, produced commodity and its specifications) [14]. For instance, fluctuating fuel or raw material prices might prompt a system operator to change input fuel or materials to produce the same commodity by leveraging flexible design features that allow switching between different fuel and material types. Conversely, “in” design flexibility refers to technical features of the system that can enable adaption, change or reconfiguration [12]. One form of ‘in’ system design flexibility could be constructional flexibility whereby the system is designed to readily host integration of additional process units or ancillary equipment with the aim to improve the overall economic performance of the system [61]. For instance, the 25 de Abril bridge in Lisbon is a relevant example where the initial design in the 1960s considered additional build-out for additional driving lanes and a railway, under a future scenario of increased traffic levels, which the system operators rightfully exercised in the 1990s [59].

A key aspect for the system designer(−s) or operator(−s) is to recognise that various strategies and enablers have contrasting qualities and therefore can react differently to certain sources of uncertainty [12]. If the objective of system design is to access upside opportunities, then production capacity expansion and/or constructional flexibility could provide better options to deal with increased prices or demand levels, albeit ones that are uncertain at the initial stage of design and project planning. Conversely, if the focus is to minimise exposure to downside risks, then deferral/abandonment of investment in the desired project size or production capability could be more suitable. For instance, system managers could defer full investment in a large, capital-intensive project in its early phases, as they hold their options, monitor market developments and act when the desired conditions materialise.

Incorporating flexibility in system design provides multiple advantages over robust, narrowly optimised, and large-scale designs. It also comes with its own challenges and costs. First, flexibility protects the system against project downside risks such as poor market conditions (low demand and price of the produced commodity), unfavourable regulatory support (limited incentives) and technological breakthrough associated with a competing commodity or design. Second, it captures favourable market conditions that are often unexpected and thus further enhances overall system economic performance potential [10]. Despite the outlined advantages, flexible design comes at (i) a cost-premium, largely driven by possible loss of EoS, (ii) faces challenges in identifying key flexibility features in a complex design space and (iii) hinges on the intricate customer-designer relationship where advantages might be realised by less sophisticated design solutions [25].

Flexible engineering design and analysis insightfully draws from the theory of real options that attempts to manage uncertainty and reduce risk for physical systems. Indeed, pertinent research work in the real options analysis (ROA) field has enabled the quantification of the value of flexibility while informing decision-makers of its valuable insightfulness into the specific project’s economic performance under uncertainty [11]. Multiple ROA valuation methods exist that include partial differential equations (e.g., Black and Scholes equation), dynamic programming techniques, lattice-based and path-dependent simulation methods. All methods account for changing circumstances [33] and require forecasts of future values of key model input variables and appropriate uncertainty quantification [62]. In the present study a practical Monte-Carlo simulation technique is used to overcome some of the limitations of the Black-Scholes and multinomial lattice methods such as the ones associated with the determination/quantification of risk-adjusted discount rate or probabilities [44]. Furthermore, the approach gives rise to additional valuable information through a comprehensive statistical characterisation of the derived NPV distributions. As a result, multiple performance metrics can be evaluated and used to support decision making and comparison of alternatives. Such metrics include a probabilistically unbiased estimation of expected NPV (successfully addressing the “flaw of averages”), standard deviation, Capex, Value at Risk (VaR; for quantifying downside risk) and complementary Value at Gain (VaG; quantifying upside potential), thus establishing a direct link to the risk profile of the decision maker. In the context of engineering systems, decision rules such as IF-THEN statements are used as logic-based elements that enable system operators to exercise real options. Modelling real options using decision rules has been shown to quantify the value of flexibility very closely as compared to standard ROA methods, while providing intuitive and readily usable solutions for system operators [16]. A decision rule formulation aims at capturing the optionality element inherent to management’s decision-making process by offering a practical framework as to when and how they should deal with uncertainty and risks in operations i.e., like sign-posts or triggering criteria for adaptation [43]. Within such a flexibility option valuation context, [10] introduced also a taxonomy framework as well as a systematic five-step methodological procedure. This 5-step framework consists of: (1) the development and economic assessment of a baseline design, (2) the identification and modelling of key uncertainty sources, (3) a concept generation of a flexible system, (4) an evaluation and exploration of the design space through engineering options analysis and Monte Carlo simulation and (5) a holistic process operation management strategy recognizing irreducible uncertainty, technology risks and the interests of the stakeholders involved.

Considering the relevance of flexible system design to large-scale blue hydrogen production, only a handful of studies have been pursued to investigate the value-enhancing prospects of flexible design in the space of blue hydrogen production. In particular, ([34,61] investigated the effect of operational and constructional flexibility for coal derived blue hydrogen production using membrane technology and carbon capture options. The authors demonstrated that under moderate carbon pricing ($30/tCO$_2$) both forms of flexibility exhibited higher financial upside opportunities and reduced economic downside risks. Contrary to the latter study, however, most recent academic efforts have been devoted to deterministic techno-economic analysis of hydrogen production at various scales and modes. For instance, [52] modelled levelised hydrogen cost for centralised and decentralised hydrogen production using SMR and investigated the impact of adding CO_2 capture units. The authors used the NREL's H2A Production Model Version 2 resulting in a $2/kgH$_2$ difference in the levelised cost. [28] compared hydrogen production costs for fuel stations based on centrally produced and distributed hydrogen versus on-site production modes. Their work demonstrated that centralised hydrogen production was the more economic option, mostly attributed to high capital expenditure (Capex) levels for on-site SMR hydrogen production. Similarly, [41] conducted a techno-economic performance assessment of blue hydrogen production using SMR on large and small scales. Their results indicated that the cost of decentralised hydrogen production was double the cost of large-scale SMR with and without CO_2 capture. This cost disparity was linked to strong EoS.

All the aforementioned techno-economic performance assessment studies relied on a methodological framework that did not explicitly and sufficiently address the impact of irreducible uncertainty on the overall economic performance profile of blue hydrogen production. To provide a more complete, realistic and nuanced outlook on blue hydrogen production using SMR with an integrated carbon capture unit, an application of flexible engineering system design analysis is performed in the present study. The proposed design framework enables a comparative assessment of centralised and decentralised blue hydrogen production in greater details and the identification of various levels of potentially value-enhancing flexibility embedded in each production mode in the presence of uncertainty. Thus, additional insights could be derived to complement the existing strategy of advocating large-scale blue hydrogen production. As such, the primary aim of the study is to address the following research question: How significant is the potential economic value of flexible system design for blue hydrogen production plants (centralised/decentralised), considering uncertain market conditions (hydrogen demand and price), environmental regulations (carbon pricing) and techno-economic factors (learning rate, EoS and technology costs)? Additional research themes that are addressed include:

- How significant are the combined effects of the time value of money, economies of scale and technology learning on centralised and decentralised blue hydrogen production?
- What is the cost-premium associated with flexible blue hydrogen plant design and what conditions must be established to favour flexible design over a robust and fixed design alternative?

3. Methodology

3.1. Step 1 - baseline model development

Following the flexible design approach outlined by [10], economic value of fixed capacity centralised and decentralised blue hydrogen plant designs was estimated performing standard discounted cash flow analysis. The NPV baseline functional model enables the formulation of a benchmark case against which the results of flexible design strategies are compared. Eq. (1) presents the general formula for calculating *NPV:*

$$NPV = \sum_{t=0}^{n} \frac{CF_t}{(1+r)^t} \tag{1}$$

where CF denotes the cash flow at year t and r is the discount rate.

The annual cash flow CF is comprised of the annual hydrogen sales revenue R_t, total capital investment TCI in year t, total production costs TPC_t, depreciation D_t, and salvage value SV. In turn, the annual TPC_t (i.e., Opex) value was determined as the sum of annual fixed and variable operating costs, FC_t and OC_t as given by Eq. (2)

$$TPC_t = FC_t + OC_t \tag{2}$$

Under this cost category, FC_t included land lease, wages, administrative costs, overhead, and annual operating maintenance costs. OC_t included costs of natural gas, materials, transport costs, electricity, and CO_2 tax.

The generated annual revenue was linked to three main factors – retail price, demand, and plant downtime due to maintenance or modular expansion requirements. Eq. (3) is used for the calculation of annual revenues:

$$R_t = P_t \cdot D_t \cdot (1 - \eta_t) \tag{3}$$

where R_t is the generated revenue in year t, P_t is the annual merchant hydrogen price, D_t is the available demand and η_t is the assumed plant downtime for centralised and decentralised facilities due to required maintenance or expansion (modular requirement): 0.50 and 0.15, respectively.

Considering depreciation and tax, the California state law requires commercial projects to use the 150% declining balance Modified Accelerated Cost Recovery System (MACRS) deprecation method [4]. Supplementary to the depreciation, multiple tax rates in the United States had to be considered. Of these, the federal tax was set at 21% [51] and California state tax at −8.625% [8]. Furthermore the IRS 45Q tax credit - $50/tCO$_2$ [18] was applied to centralised production plants.

Considering the cost parameters/variables and tax data, the annual cash flow was determined using Eq. (4).

$$CF_t = (R_t - TCI_t - TPC_t)\cdot\left(1 - \theta_f - \theta_s\right) + \psi_t\cdot\left(\theta_f + \theta_s\right) + TC_t\cdot\nu \text{ where } t = 0, 1, \ldots, 24 \tag{4}$$

$$CF_t = (R_t - TCI_t - TPC_t)\cdot\left(1 - \theta_f - \theta_s\right) + \psi_t\cdot\left(\theta_f + \theta_s\right) + TC_t\cdot\nu + SV \text{ where } t = 25 \tag{5}$$

where θ_f is the federal tax rate, θ_s the California state tax rate, ψ_t the depreciated capital, TC_t the 45Q tax credit, ν the annual CO_2 emissions (tpa) and SV the salvage value (recoverable value of an asset at the end of its lifetime or once depreciation is complete). In this study, the salvage value was assumed to cover the costs of decommissioning all blue hydrogen production sites [17].

3.1.1. Plant techno-economics

A body of literature was reviewed to find recently published and relevant plant design data for blue hydrogen production through the SMR process. Recent techno-economic analysis by [17] included detailed plant design data which was representative of average hydrogen production facility in California [27] and hence chosen for this study. A 190,950 kg H_2/day hydrogen production plant with 90% capture rate was considered. The plant lifetime was specified to be 25 years with a start date of 2025 to account for construction time and a 0.95 annual production factor (efficiency).

Collodi et al. [17] specified the total capital investment (*TCI*) at €398.54 million with €98.85 million/year operating costs (TPC_t). These specified costs were converted to US dollars and adjusted to 2022 levels using the chemical engineering plant cost indices (CEPCI) as given in Eq.

(6)

$$Cost_{current\ year} = Cost_{given\ year} \cdot \left(\frac{CEPCI_{current\ year}}{CEPCI_{given\ year}} \right) \tag{6}$$

where CEPCI in was 797.6 and 567.5 in years 2022 and 2017, respectively [37].

To provide a more granular estimation of the associated capital costs that were not quantitatively specified in the [17] study, cost percentage estimates were used from [35]. A detailed breakdown of the associated capital costs is given in Appendix A (Table 9).

Given the limited accumulated operating experience and commercial status of decentralised blue hydrogen production [47], the current study modelled this production mode by considering on-site hydrogen production at currently existing hydrogen refuelling stations in San Francisco. This approach is similar to the one implemented in [58]. The latest comprehensive report H2A 2022 v.3 model from [46] provided reliable initial cost data, which until recently, was hardly available in the literature due to the relatively nascent nature of decentralised blue hydrogen production. Specifically, in the aforementioned [46] model, decentralised hydrogen production was modelled as on-site hydrogen production using SMR unit(s), which can be envisaged as modular units, situated next to a refuelling station. A modular production level of 1500 kgH_2/day was selected as a sensible production output level based on commercial on-site production capacity data presented in [1]. The associated capital cost of 1500 kgH_2/day module was determined to be \$1.57 million as the sum of direct materials and engineering service costs from the [46] model. Furthermore, an additional capital cost adder of 2.5 was considered for the decentralised production plants upon the recent circa two-fold increase in complex hydrogen plant cost estimation [36] and upon consultations with industry experts.

In this study, each refuelling station was set at a 6000 kg H_2/day production limit which represents the maximum threshold of decentralised hydrogen production, according to the information provided by the H2A model. Hence, each station could host 4 production modules (4 $\times$ 1500 kg H_2/day). Besides the cost of 4 production modules, each refuelling station was assumed to incur costs associated with site preparation, project contingency and upfront permitting. These latter costs were also determined using the H2A model by setting the production capacity at 6000 kgH_2/day. A detailed breakdown of the associated capital costs is given in Appendix B (Table 10).

To estimate the operational costs (Opex) for centralised and decentralised plants, available data from the ([17,46] reports were used and where required, additional data was added. The fixed operation costs for centralised and decentralised facilities were given at \$17.67 million and \$0.44 million, respectively. To determine the variable component of Opex (*OC*), price data for natural gas, electricity, CO_2 price, and H_2 delivery cost was identified in the pertinent literature. These costs are summarised in Table 1.

Emphasis was placed on selecting the average price data. This was done to emulate the conventional approach followed by key-decision makers. It is worth noting that hydrogen transport costs were applied only to centralised production plants with a 200 km delivery radius to cover sufficiently large delivery area. Transport costs for decentralised production at hydrogen refuelling stations were excluded, as the production was modelled as an on-site activity, and it was assumed that all hydrogen fuel sales would occur at these stations. Moreover, the space dimension of optimal centralised plant placement was not investigated within the context of this study, as it was assumed to be constructed at a greenfield site adjacent to a natural gas pipeline network in the outskirts of San Francisco. However, a current lack of comprehensive blue hydrogen plant placement and spatial distribution studies highlights a meaningful future research area. Furthermore, the specified CO_2 capture costs in Table 1 were considered only for decentralised production plants since these costs were already included in the overall Capex and Opex estimates for centralised plants [17]. Eq. (7) was used to adjust the given CO_2 capture costs for a 500 kgH_2/day plant to a 6000 kgH_2/day decentralised production plant (refuelling station)

Table 1
Operational costs for blue hydrogen production.

Cost Category	Value	Remarks	Source
Natural gas	\$4.16/ MMBtu	(1997–2021 average)	[22]
Electricity	\$0.061/ kWh	(1997–2022 average)	[23]
H_2 transport – centralised	\$1.07/ kgH_2*	trucked gas	[30]
H_2 transport – decentralised	\$0 /kgH_2	–	–
CO_2 price	\$22.43/ tCO_2	(average of 2021)	[29]
CO_2 capture**	\$50/tCO_2	for decentralised plants only; CO_2 capture costs in centralised plants considered throughout the entire operational cost section	[50]
CO_2 transport & storage	\$15/tCO_2	–	[26]

* Cost adjusted for inflation and represents delivery costs with a 200 km radius.
** Cost for a 500 kgH_2/day decentralised hydrogen production facility.

$$Cost_{plant\ B} = Cost_{plant\ A} \cdot \left(\frac{Capacity_{plant\ B}}{Capacity_{plant\ A}} \right)^{\alpha} \tag{7}$$

where the cost of plant A is known, and the cost of plant B is determined using the capacity ratio that is raised to a given scale exponent α (representing the economies of scale). In this study, the scale exponent for centralised SMR plants was specified at 0.68 [48] and 0.60 for decentralised plants [46].

Appendices C and D (Table 11, Table 12) provide a detailed breakdown of the fixed and variable Opex (*FC* and *OC*) at a full-scale plant capacity for centralised and decentralised plants respectively.

3.1.2. Deterministic blue hydrogen demand modelling

A S-curve hydrogen demand profile was modelled to capture the anticipated growth in hydrogen demand in California and thereafter in San Francisco. In general, the advantage of using a S-curve model is the ability to represent an underdeveloped market state of a given commodity with low demand level, but one that is expected to grow rapidly, eventually reaching saturation in the future [14]. Eq. (8) mathematically represents the S-curve model which was applied to model growing hydrogen demand:

$$D(t) = \frac{M}{1 + ae^{-bt}} \tag{8}$$

where $D(t)$ is demand in year t, M is the limit of demand at time ∞, a is the translation parameter, and b is the sharpness parameter. Herein, a can be approximated by equating it to the demand in year $t = 0$ as given by Eq. (9):

$$a = \frac{M}{D(0)} - 1 \tag{9}$$

To establish the demand trajectory of a S-curve, a hydrogen demand profile for transport in California was used from [58] by considering its low case scenario and from [5] for the projected demand in years in 2023 and 2024.

The S-curve fitting parameters were obtained using an S-curve prediction model from [19] library. The values of the fitting parameters are specified in Table 2. These parameters were specifically obtained by normalising the demand within the (0 to 1) interval to achieve better computational performance. Thereafter, demand was scaled back to absolute values.

Table 2
Normalised fitting parameters used in the S-curve modelling.

M	b	a
1.2043	0.2012	49.1298

To account for the share of hydrogen produced via SMR in California, a constant market-share of 40% was used based on the [5] study and applied across the investigated time-horizon from 2025 to 2049 in this study. The assumption of a constant market-share was based on the expected competitiveness of blue hydrogen in the United States given (i) its large reserves of cheap natural gas ($2–3/MMBtu) [57], (ii) abundant CO_2 storage capacity at levels close to 3000 gigatonnes [57] and (iii) the commercial interest of major US fossil fuel companies to produce blue hydrogen as an opportunity to remain competitive in the growing low carbon energy market [53]. Finally, the demand for blue hydrogen was narrowed down from California state level to expected demand in San Francisco by applying a constant market-share of 18%, as indicated by the [60] study. Fig. 1 summarises the modelled blue hydrogen demand in San Francisco as an S-curve where gradual demand increases up to the year 2030 can be observed, followed by a rapid growth period and subsequent approach to demand saturation around 2050.

3.1.3. Optimum centralised and decentralised production capacity

Determining an optimal production level of a centralised production facility is crucial for improved economic performance. In this study, multiple production rates were investigated (47.74 to 524.88 t per day (tpd)) with an incremental production level of 47.74 tpd under various EoS. The latter production specifications were chosen to represent reasonable minimum and maximum production rates that follow industry standards for centralised blue hydrogen production, as outlined by ([27,58]. Furthermore, an incremental production expansion of 47.74 tpd was chosen for two main reasons. First, it allowed to accommodate at least three-fold expansion for flexible and phased centralised production facilities, as shown in the following sections. To the best knowledge of the authors, no reliable information of modular centralised blue hydrogen plants was found in the pertinent literature as well as public sources which led to an assumption for a reasonable limit on the number of expansion instances. Given that the sample blue hydrogen plant design had a production capacity of 190.95 tpd [17], a 47.74 tpd expansion increment was used to enable a three-fold expansion of an initial production facility (47.74 tpd + 47.74 tpd * 3 ~ = 190.95 tpd). Therefore, the latter expansion increment formed the lower threshold of production capacity considered in the present study. Second, a 47.74 tpd production increment was representative of the production range of centralised plants [58] [27]; whereby if no expansion occurs, then the size of flexible (modular) plant is still representative of a centralised production facility.

Under the baseline (deterministic) market conditions (Table 1 and Table 5), the NPV of fixed centralised production plants with various production rates and levels of EoS (α) was evaluated and graphically illustrated in Fig. 2. Two major observations were made. First, under strong EoS (0.60) the optimal production capacity was 238.69 tpd with an NPV of $858 million. Second, under moderate to weak EoS (0.68–1.00) the optimal production capacity was 190.95 tpd which resulted from optimal Capex and Opex relative to the generated revenue from the available market demand for on-road hydrogen transport fuel. Considering both observations, the optimal production capacity was set at 190.95 tpd given that 0.68 appears to be a more realistic scale exponent for SMR systems with high CO_2 capture levels [48]. One should also note that a higher NPV for larger scale exponents (α) under 190.95 tpd was due to the sixth-tenth rule expression in Eq. (7). This was because a higher scale exponent value reduced the scaled Capex cost for production levels below the nominal value (190.95 tpd).

The production level associated with a decentralised pathway was matched with the centralised one (190.95 tpd) to establish a fair comparison between the two design alternatives. Given that one decentralised production facility (refuelling station) had a capacity of up to 6 tpd with an annual production efficiency of 0.86 (Table 10), then a total of 36 refuelling stations were required. As of 2022, there are at least 36 refuelling stations (in operational, constructional or permitting phases) in and around San Francisco as indicated by [7]. As such, the selected production level enabled a commercially realistic case-study whereby decentralised hydrogen production could occur at these 36 stations,

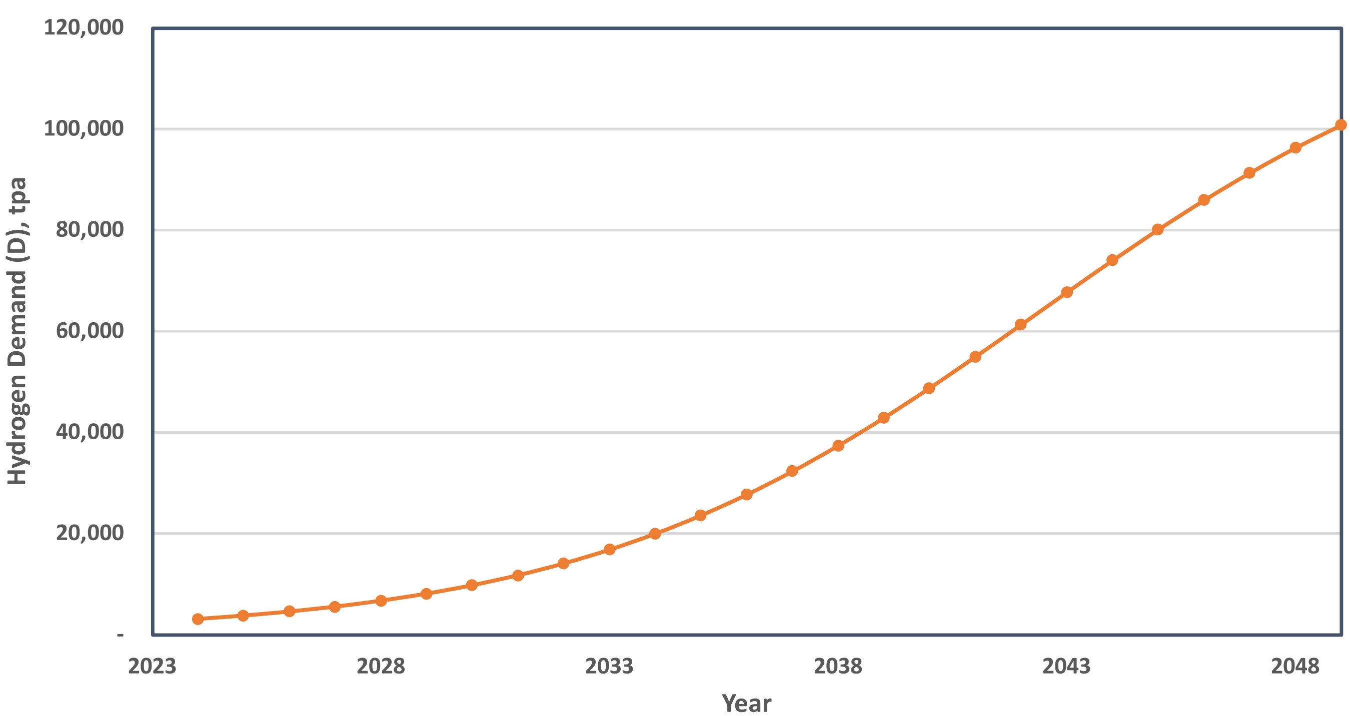

Fig. 1. Forecast of deterministic blue hydrogen demand for on-road transport in San Francisco. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

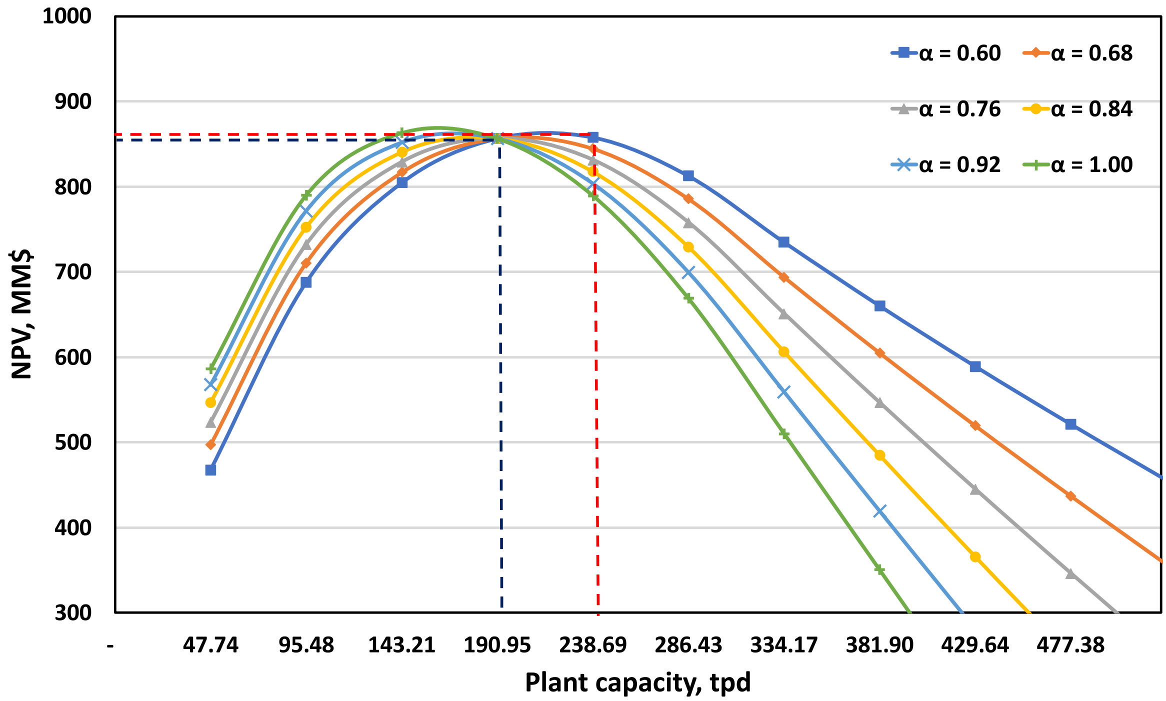

Fig. 2. Optimum plant design under various economies of scale. Stronger economies of scale (lower α) achieve higher NPV levels across various plant capacities.

whilst centralised production would be based at a greenfield site.

3.1.4. Modular (flexible) centralised plant design and costs

Theoretical cost estimation of modular centralised blue hydrogen plant was performed to account for flexibility cost-premium and loss of EoS. To the best knowledge of the authors, no reliable public information exists on modular commercial hydrogen plants or oil refineries and thus the dearth of pertinent industrial data motivated a theoretical analysis. The rigorous [55] study was considered to determine the total capital investment (TCI) for the modular centralised plants. Within this framework, costs for the initial backbone facility (i.e., plant together with the first modular production unit) and subsequently installed additional modules are determined based on empirical cost-correlations and literature data. In this study, the TCI of the backbone facility was determined by considering costs of a scaled 47.74 tpd plant based on Eq. (6) and the cost data of a 190.95 tpd plant [17]. The capital cost of additional modules was determined by applying appropriate capital cost reduction factors as indicated in the [55] study for various cost categories associated with a Total Direct Cost (TDC) calculation, given in Table 3 and Appendix A.

Using the aforementioned cost estimation methodology and also accounting for 15% working capital [49], the *TCI* of a 190.95 tpd modular plant (1 backbone facility +3 isolated modules) was estimated at $ 644 million. The latter TCI value presented a 8.4% cost-premium relative to the fixed capacity 190.95 tpd plant estimated at $ 594 million, as detailed in Appendix A. This was perceived as a sensible cost-premium given that modular design cannot fully capture the benefits of economies of scale as compared to a large, fixed design [12].

Table 3
Cost of modular centralised blue hydrogen plant (initial backbone facility + isolated module costs).

Capital cost category	Initial backbone facility* ($)	Capital Reduction Factors [55]	Isolated module** ($)
Direct Materials/ Equipment	106,327,372	0.00%	106,327,372
EPC Services	15,949,106	≤ 70.00%	4,784,732
Construction	26,581,843	45.00*** %	14,620,014
Contingency	17,721,229	50.74%	8,729,477
Other costs	10,632,737	70.60**** %	3,126,025
TDC	177,212,286	–	137,587,619
Owner's cost	12,404,860		
Spare parts	886,061	–	0*****
Start-up	4,949,500		
WC	35,858,282	–	
TCI	231,310,990	–	137,587,619

* Contains one 47.74tpd production module with underlying plant infrastructure.
** Production module with 47.74 tpd capacity.
*** Greenfield investment in the [55] study.
**** Average of auxiliary & buildings in the [55].
***** Owner's costs, spare parts, start-up costs and working capital costs assumed to be incurred only for the initial backbone facility.

3.2. Step 2 - uncertainty analysis

3.2.1. Blue hydrogen demand modelling under uncertainty

To forecast a wide range of future demand scenarios, the adopted S-curve model was stochastically simulated by assigning volatility values for each demand parameter in Eq. (8). In the absence of any publicly available data on hydrogen market data, volatility values were used from the [14] study which modelled a similar uptake of LNG as a transport fuel in an uncertain and underdeveloped market. Table 4 summarises the used volatility values for each fitting parameter, which were each assigned to a uniform statistical distribution for stochastic modelling.

Table 4
Volatility data for stochastic demand modelling.

Fitting parameter	Volatility	Statistical distribution
M	0.50	Uniform
b	0.70	
a	0.50	
δ_{demand}*	0.15	–

* Annual demand volatility – measure of dispersion around the mean demand value.

To model a stochastic demand parameter, Eq. (10) was used. In this case an example has been provided using the stochastic upper demand limit M_{stoch} but it was similarly applied to model stochastic values of b_{stoch} and a_{stoch}

$$M_{stoch} = (1 - M_{vol}) \cdot M + 2 \cdot M_{vol} \cdot M \cdot rand \tag{10}$$

where M_{vol} is the volatility of M, M is the nominal M value and $rand$ is a randomly drawn number between 0 and 1. Furthermore, to model the stochastic demand, a standard Geometric Brownian Motion (GBM) model was used with a projected demand $D(t)_{proj}$, a drift rate $\mu(t)_{demand}$, and a realised growth rate $\delta_{realised}$, calculated through Eqs. (11)–(13) as follows:

$$D(t)_{projected} = \frac{M_{stoch}}{1 + a_{stoch} e^{-b_{stoch}\ t}} \tag{11}$$

$$\mu(t)_{demand} = \frac{D(t)_{projected} - D(t-1)_{projected}}{D(t-1)_{projected}} \tag{12}$$

$$\delta(t)_{realised} = \mu(t)_{demand} + \sigma_{demand} {}^{*} \varepsilon_t \tag{13}$$

In the above Eq. (11), ε_t represents a typical Wiener process under a standard normal distribution [13].

Using the above stochastic demand modelling framework, 25 simulation runs were performed to generate a range of example demand profiles (Fig. 3). The derived results clearly demonstrated a wide range of variability driven by the uncertain market conditions, which can have positive/negative impacts on the project.

3.2.2. CO_2 price modelling

Like the uncertain hydrogen demand, the rising CO_2 price in California represents an uncertain regulatory compliance cost. To model the subsequent CO_2 price, two main inputs were specified: the initial CO_2 price and the stochastically determined growth rate. The initial CO_2 price considered was the closing market price in 2021. Eq. (14) was used to determine the expected growth rate $CTGR_t$ at year t [61]

$$CTGR_t = \mu_{CO2} + \sigma_{CO2} {}^{*} \varepsilon_t \tag{14}$$

where μ_{CO2} is the drift rate of the CO_2 price, and σ_{CO2} denotes the annual volatility in the above CO_2 price model.

The drift rate and annual volatility were determined by performing regression analysis on the historical California's Cap-and-Trade price [6] yielding values (data) of 0.234% and 38%, respectively. However, considering that the annual volatility was significantly high, an assumption was made that it would be half the calculated value: 19%. The latter value falls in line with the volatility range used for stochastic CO_2 price modelling in the [34] study: 0 to 20%, thus providing a reasonable estimate. Considering the above, the annual CO_2 price was modelled by forming the product of CO_2 price in the previous year (t-1) with the annual growth rate in year (t) as given by Eq. (14).

3.2.3. Cost estimation of natural gas and electricity

The price of natural gas was modelled using a bootstrap resampling method and the publicly available EIA historical price record (1997–2021) of the Henry Hub spot price [22]. An assumption was made that the resample draws would follow a normal distribution yielding a mean price around \$3.8/MMBtu with a standard deviation of \$1.94/MMBtu. A similar approach to the one outlined above was implemented by [34] to model the uncertain coal price in the US for blue hydrogen production.

Similarly, the electricity price for decentralised hydrogen production was modelled using the bootstrap resampling method and the publicly available historical electricity price (1997–2021) for industrial consumers [23]. The sample draws were assumed to follow a normal distribution giving a mean price around \$0.061/kWh with a standard deviation of \$0.01/kWh.

3.2.4. Cost estimation of hydrogen and CO_2 capture

For the remaining cost variables (merchant hydrogen price, hydrogen delivery costs, CO_2 transport and storage, and CO_2 capture costs for decentralised facilities), a triangular distribution range was used to account for price uncertainty. Herein, triangular distribution provides a meaningful and reliable distribution range whilst accounting for potential extremes. Table 5 summarises the nominal values found in the relevant literature and the assigned low and high values following

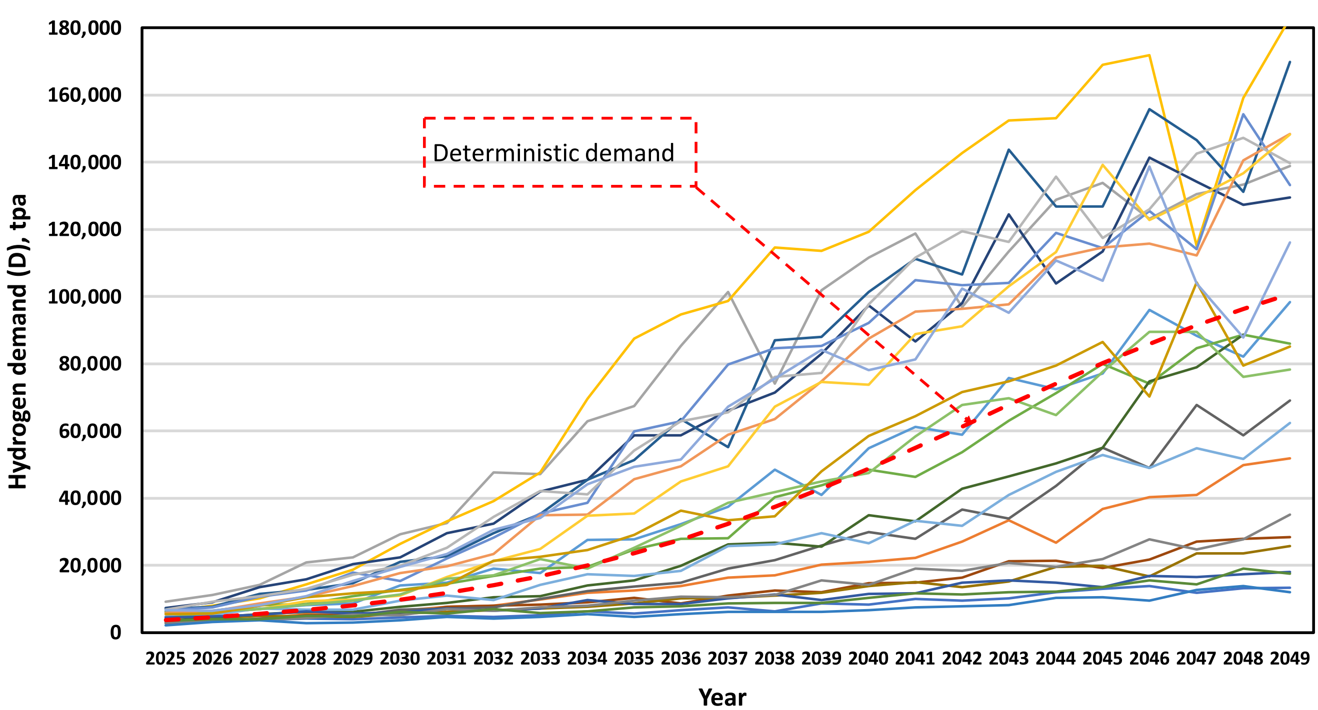

Fig. 3. Stochastically derived hydrogen demand projections for transport sector in San Francisco.

Table 5
Cost ranges for uncertain plant and market inputs.

Cost Category	Nominal cost	Low cost	High cost	Source
Hydrogen retail price	$11.5/ kg H_2	$8/kg H_2	$15/kg H_2	[2]
Hydrogen delivery costs*	$1.07 / kg H_2	$0.75/kg H_2**	$1.39/ kg$H_2$**	[30]
CO_2 transport and storage	$15/ t$CO_2$	$10/t$CO_2$	$30/ t$CO_2$	[26]
CO_2 capture and storage ***	$222/ t$CO_2$	$155/t$CO_2$	$289/ t$CO_2$	[50]

* Gaseous state – trucked; 200 km delivery radius.
** ± 30% cost uncertainty range.
*** For decentralised plant (6 tpd H_2) only.

the conventional ±30% uncertainty range in cases where a specific cost range is not given.

3.2.5. Monte Carlo simulation

In this study, Monte Carlo simulation techniques were used to perform uncertainty analysis. To provide a statistically reasonable analysis 2000 runs were performed with each run drawing a stochastic sample for the uncertain cost and demand parameters as specified in the previous sub-sections.

Using Monte Carlo simulation enables the generation of a distribution of potential outcomes. A conventional way of characterising the distribution range is to calculate the expected (average) value of NPV. This is given by Eq. (15)

$$ENPV = \frac{1}{N} \cdot \sum_{i=1}^{N=2,000} NPV_i \tag{15}$$

where *ENPV* is the average *NPV* over *N* simulation runs and NPV_i is a stochastically modelled *NPV*. It should be pointed out that a Monte Carlo method offers a probabilistically unbiased ENPV estimator derived from the sample, and thus, its employment effectively overcomes the "flaw of averages" [43].

It should be noted that *ENPV* is a risk neutral economic performance measure and might not be deemed sufficient as a single performance metric by decision makers who might be interested in a more comprehensive and nuanced economic performance assessment [14]. Complementary metrics to it can include the value at risk (*VaR*) and value at gain (*VaG*) which in this study were expressed as the 10th percentile (P10) and 90th percentile (P90), respectively. Finally, each simulation run was also summarised by plotting cumulative probability distribution profiles of the NPV values.

3.3. Step 3 - flexibility analysis

3.3.1. Flexible design alternatives

Two design alternatives were selected and contrasted against the baseline fixed design alternative for both centralised and decentralised production modes. The first alternative was a phased design that would incrementally increase the production capacity over 12 years with an expansion taking place after every 4 years. The second alternative was a flexible design alternative that would be triggered conditional upon the right market conditions being fulfilled, controlled by an IF-THEN decision rule formulation. Out of these 2 alternative designs, the latter could leverage flexibility better whilst the phased design represented a conceptually balanced "middle way" between fixed and flexible designs also capturing existing practice. Table 6 summarizes the characteristics of the six design alternatives considered in this study.

3.3.2. Optimal decision rule formulation

In this study, a practical approach was implemented by formulating the decision rule around the observed hydrogen demand given the high degree of uncertainty that it carries. An IF-THEN decision rule was used to control the expansion based on demand-supply balance:

Table 6
Summary of design characteristics for each plant type and production mode.

Criterion \Design	Centralised production			Decentralised production		
	Fixed	Phased	Flexible	Fixed	Phased	Flexible
Initial Capacity (tpd)	190.95	47.74	47.74	190.95	47.74	47.74
Final capacity (tpd)	190.95	190.95	Based on demand	190.95	190.95	Based on demand
Lifetime (*years*)	25	25	25	25	25	25

- **IF** the demand reaches expansion threshold X (%) of available supply over Y consecutive year(s):
  - o **THEN** expand the modular production capacity
  - o **ELSE** – do nothing

Various expansion thresholds were investigated over time to determine an optimal decision rule. For both facilities (centralised and decentralised) the optimum expansion threshold settled at 75% with a time dimension of 1 year (Fig. 4) giving the highest ENPV results.

Fig. 4 illustrated that considering expansion after each year was more advantageous rather than considering it over a two-year time-window. The implemented S-curve demand modelling likely led to such an outcome given that the accelerated expansion option enabled capturing the steeply rising demand in the middle of the S-curve region. Moreover, one should recognise that the optimal expansion thresholds might not necessarily represent the global optima, since only a small range of expansion thresholds (*X*) and required consecutive years above the threshold (*Y*) were explored. Despite this, the obtained results were deemed practical and logical when considering the expansion options of commercial plants, rather than theoretical thresholds.

In addition to the expansion threshold, the ENPV value is also dependent on the selected production capacity increment. In the case of centralised design, the capacity expansion was fixed to the size of a module (47.74 tpd) while in the decentralised design, the expansion increment was more flexible given that it was controlled by the number of H_2 refuelling stations brought in operations. Thus, the amount of capacity expansion for decentralised production was evaluated under four expansion threshold options (50%, 75%, 100% and 125%). Fig. 5 illustrates ENPV as a function of deployed production capacity based on the difference between demand and supply. Here values below 100% indicate that the increase in production capacity was X (%) of the demand & supply difference. In contrast, values above 100% indicate that an increase in production capacity was X (%) percent greater than the demand-supply difference.

As Fig. 5 indicated, increasing production capacity above the demand-supply difference increases the ENPV. This was likely driven by high demand scenarios where a greater expansion increment enabled capturing the rapidly growing demand. The highest ENPV value ($900 million) was observed when the decentralised production capacity was increased 250% above the demand and supply difference with an expansion threshold of 75%. Hence, both conditions will be used for optimal production capacity increase in the case of decentralised facilities. Similarly to Fig. 4, the results likely did not show the global optima but were nonetheless deemed practical under a commercial setting given the nascent state of decentralised hydrogen plants, and considering stakeholder unwillingness to over-commit to significant plant capacity expansion in one-go.

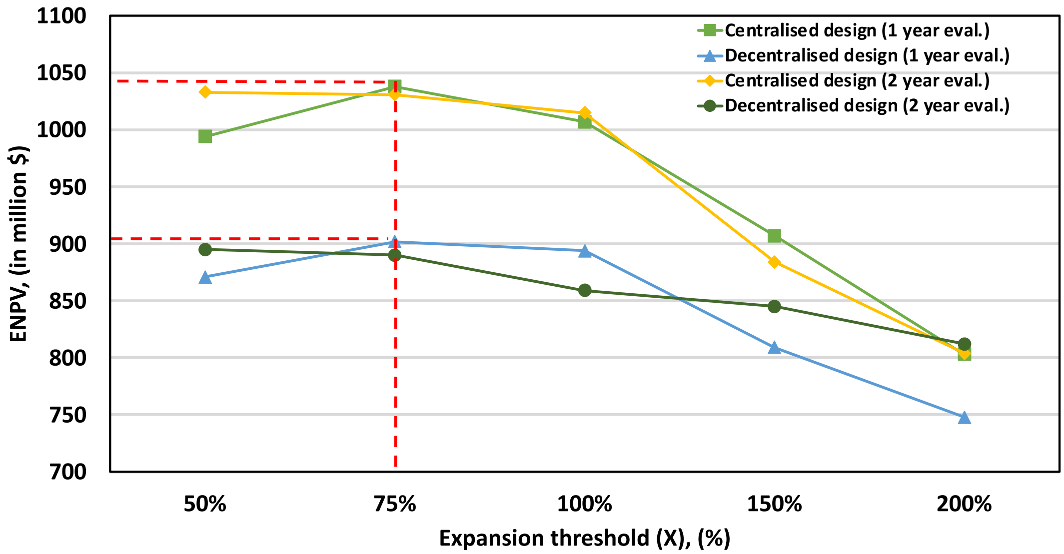

Fig. 4. ENPV as a function of the expansion threshold (demand to supply ratio) across 1 and 2 year evaluation. Optimal expansion threshold and time period is mutually shared between centralised and decentralised production.

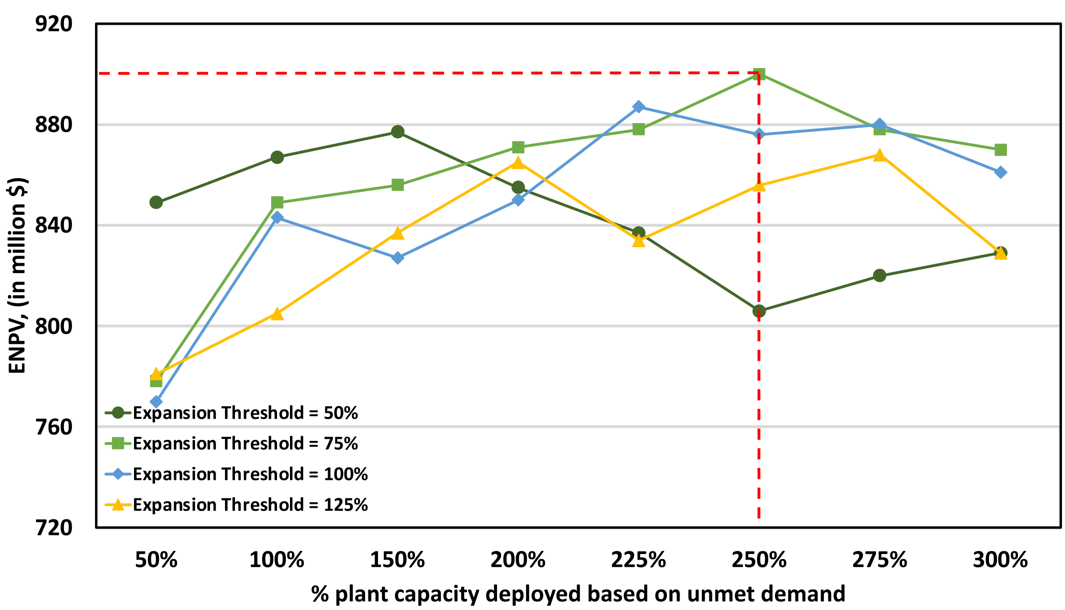

Fig. 5. ENPV as a function of the fraction of decentralised production facilities brought in operation. Results indicate linear relationship between ENPV and % deployed capacity.

3.3.3. Learning rates

One of the key advantages of a modular design is the ability to achieve cost-reduction through learning effects. In the context of blue hydrogen production, cost reduction is crucial since the common approach in the industry has historically focused on large-scale and capital-intensive production strategies. Eq. (16) represents the capital cost of a given module based on an empirical correlation [43]:

$$U_i = U_1 * i^B \tag{16}$$

where U_i is the capital cost of the i^{th} module, U_1 is the capital cost of the initial module and B is the slope of the learning curve. The latter value can be determined using Eq. (17) where a higher learning rate LR leads to a greater slope and hence lower cost [14]. In this study, the learning effect was investigated for centralised flexible production plants and only applied in specific cases as discussed in the following results section.

$$B = \frac{log_{10}(100\% - LR)}{log_{10}2} \tag{17}$$

3.3.4. Value of flexibility

The value of flexibility (*VoF*) is a useful key performance indicator that informs system designers of the upper bound on the expected value of flexibility. Often, designers know the cost-premium of flexibility but are unaware of its associated value given the lack of consideration of uncertainty. This leads to incomplete, often misguided decision making that undermines the upside that flexibility can typically provide, and reduced exposure to downside risks. In practice, the value of flexibility is calculated as the difference in *ENPV* between flexible and inflexible design alternatives, the latter often referred as "benchmark". Eq. (18) provides a general expression for *VoF:*

$$VoF = ENPV_{Flexible\ design} - ENPV_{Optimal\ fixed\ design} \tag{18}$$

Given the determined cost premium of centralised modular production (8.4%), *VoF* was used to indicate the value-enhancing potential of flexible design. Furthermore, *VoF* can reliably inform the calculation of the additional engineering and design cost ("premium") that decision makers can commit without undermining the project value [15].

3.4. Step 4 - sensitivity analysis

The conventional approach in most techno-economic performance assessment studies involves the use of classical sensitivity analysis to evaluate the effect of an uncertain model input on key system performance metrics. This approach provides a reasonable first insight but is limited to variations of only one variable while keeping all other input variables at their respective "average" baseline values. Within a flexible system design framework, sensitivity analysis is used to determine and evaluate the robustness of the recommended design(−s). Such a step is a crucial aspect in the overall decision-making, as it enables to determine range(−s) of conditions over which the recommended design remains viable and whether another design option might be more preferable. [14]. In this study, the economic performance impact of all three S-curve demand parameters (*M, a, b*), the discount rate and hydrogen price were evaluated during the sensitivity analysis. These parameters/variables were chosen, as they proved to be the most impactful factors on the net present value of centralised and decentralised flexible plant design.

4. Results and discussion

4.1. Baseline model (deterministic) results

Baseline model conditions enabled an economic performance assessment of centralised and decentralised blue hydrogen production under average conditions and in the absence of uncertainty. Flexible and phased design in centralised and decentralised production pathways already led to a higher NPV value as indicated by Fig. 6. In the centralised production case, NPV of all three designs (fixed, phased, and flexible) was similar but with a higher value for the alternative designs: $ 857 million, $940 million and $972 million. Similarly, under the decentralised production pathway, flexible and phased designs offered higher economic value relative to the fixed design strategy: $858 million and $764 million versus $424 million. It should be noted that the NPV values of decentralised plants are representative of the sum of NPV and LCOH for all 36 refuelling stations.

The reason for the difference in NPV values was a combination of two factors. First, the fixed design led to a higher cumulative Opex under both production pathways, as indicated in Table 7. Building a greater capacity at first required to incur high Opex which accumulated over time and reduced the NPV. Second, the time value of money caused the initial capital investment for fixed centralised and decentralised facilities to have a greater effect on the NPV value. Concurrently, the flexibility cost-premium for centralised production was reduced in present value terms, since these capital costs were incurred later.

The centralised production pathway was a more economically attractive alternative for cost-competitive blue hydrogen production relative to each design option, as indicated in Fig. 6 and supported by commercial analysis [3]. Under the best design option (flexible design strategy) the LCOH for centralised production was \$3.73/ kg H_2 compared to \$5.13/ kg H_2 under a decentralised production mode. This was driven by weaker *EoS* for flexible decentralised plants, even at the expense of \$907.5 million required for hydrogen transportation from the centralised production site to the end-users (\$1.07/kg delivered H_2). Moreover, higher production costs in the decentralised case outlined the importance of achieving lower Opex levels to achieve cost competitiveness with centralised production. This was largely driven by the high CO_2 capture costs (\$222/tCO_2) with a cumulative cost of \$1276 million across all 36 stations which could have been readily underestimated given the nascent level of CO_2 capture at the refuelling station level. Although the industry has yet to develop a considerable decentralised blue hydrogen market, the need to reduce high CO_2 capture costs was evident. Finally, it is likely that the true costs of decentralised production (no matter the design alternative) would be higher under commercial project conditions, given the lack of decentralised production infrastructure in place and its nascent market state.

4.2. Uncertainty (stochastic) results

The observed stochastic results under the base modelling conditions (economies of scale – 0.68; learning rate = 0%) highlighted the inherent limitations of a baseline deterministic analysis. The ENPV for all 6 design options (Table 7, Fig. 7) was different than the initially calculated NPV under deterministic conditions. As discussed in Section 2, the expected value of NPV calculated using Monte Carlo simulations represents a non-biased, reliable estimate that overcomes the "flaw of averages". In this case, one observes that the ENPV is higher than the deterministic NPV which is contrary to the results observed in similar flexible design studies under uncertainty such as in ([14,21]. This is because the benefits of upside opportunities (high demand, above average hydrogen price, low delivery costs) overcompensate for downside/adverse conditions (poor demand, low hydrogen price). The underlying phenomena are captured in the cumulative density function plots for both production modes (Fig. 7). All the negative or break-even NPV simulation runs lie in the 20th percentile whilst most simulations yield a positive NPV (above the 20th percentile). Moreover, in both production pathways the deterministic NPV coincides with the 40th and 60th percentile indicating that half of the simulation runs produce an above average NPV. Considering both factors, the ENPV value seems more attractive than the baseline NPV value.

The flexible design strategy was more favourable under uncertain market conditions for both production pathways. For the centralised

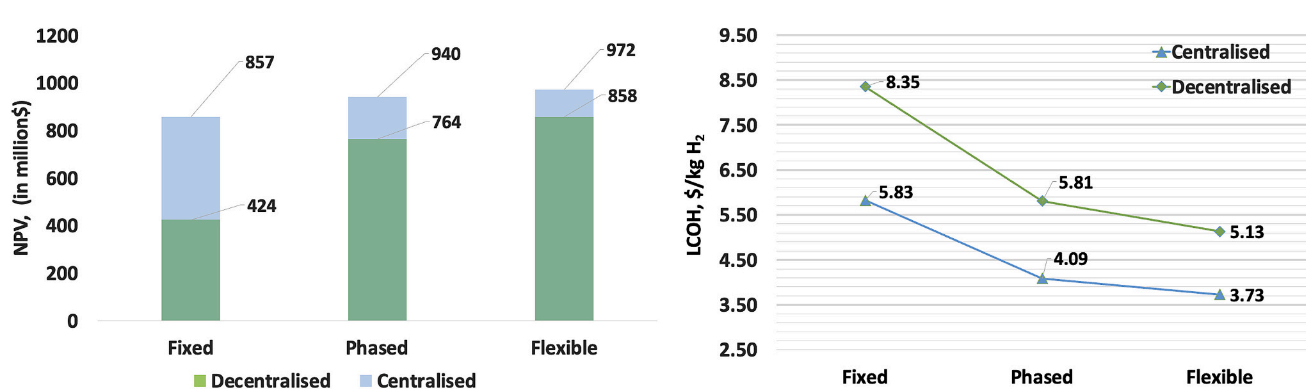

Fig. 6. NPV and LCOH under deterministic conditions for centralised and decentralised production.

Table 7
Multi-criteria evaluation of centralised and decentralised hydrogen production under various designs and stochastic conditions (α = 0.68, learning rate = 0%, figures in million $).

Criterion	Centralised production			Decentralised production			Best design
	Fixed	Phased	Flexible	Fixed	Phased	Flexible	
NPV (deterministic)	857	940	**972**	424	764	858	Central – flexible
ENPV	893	958	**1038**	474	781	893	Central – flexible
VoF (wrt. fixed)	–	65	145	–	298	**419**	Decentral – flexible
Improvement (wrt. fixed design)*, %	–	7%	17%	–	65%	**88%**	Decentral - flexible
*Capex***	594	644	644	**820**	**820**	**820**	Central - fixed
*Opex***	2458	2296	**2221**	2451	2340	2301	Central-flexible

* *Improvement defined as VoF / ENPV (fixed design).*
** *Indicates Capex and Opex costs under baseline model (deterministic) conditions;*

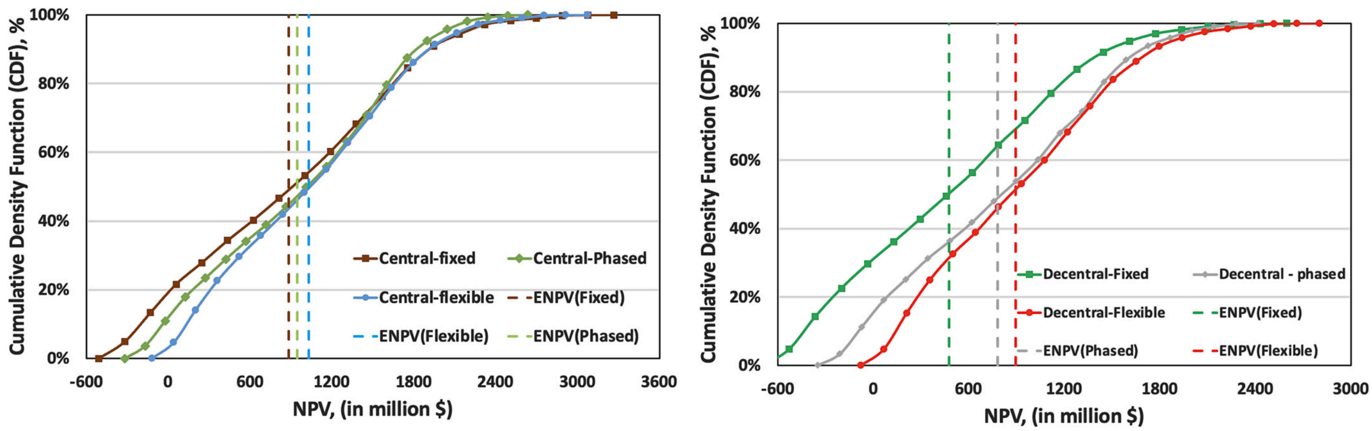

Fig. 7. Cumulative probabilistic NPV distribution of various centralised and decentralised hydrogen plant designs.

pathway, a flexible design strategy yielded the highest ENPV at $1038 million which indicated the benefits of flexibility. Compared to the fixed and phased centralised designs, the difference in ENPV was $65 million and $145 million, respectively. These results supported the argument that deploying all the production capacity at first can lead to sub-optimal results especially in the context of an underdeveloped hydrogen market and its uncertain future. Moreover, the cost-premium of flexible design (Capex: $644 million - $594 million = $50 million as given in Table 7) proved not to be substantial in the overall economic performance. This is because the ability to phase capacity as the demand unfolds enables to strategically incur Capex, flexibility cost premium, and fixed Opex costs. For instance, under poor market conditions, a flexible design avoids a high, one-off capital investment and fixed Opex by not reaching its full production capacity while still meeting the required demand. A fixed design, however, is highly dependent on the expected demand level being reached and therefore under poor market conditions may suffer from irreversible Capex and Opex costs. This is evident in Fig. 7 where the CDF curve of a fixed design lags behind (i.e., to the left of) the phased and flexible CDF curves in the 20th percentile region (poor market conditions) indicating that phased and flexible plants have higher NPVs than in the fixed design case at the same probability level, hence providing better protection against downside conditions.

Nevertheless, decentralised production did offer a greater value of flexibility compared to the centralised design. As indicated in Table 7, the value of flexibility and the associated improvement (expressed as *VoF/ENPV*) was around twice as high for a flexible decentralised design compared to a flexible centralised one: $419 million vs. $145 million; 88% vs. 17% improvement over their fixed counterparts, respectively. This demonstrated that flexibility is a clear value-driver for decentralised production strategy and, hence, should not be ignored by decision makers and planners. To the contrary, centralised production is driven by strong *EoS* which limits the value of flexibility. Moreover, similar results were observed when comparing *VoF* between phased and fixed designs: $298 million vs. $65 million; 65% vs. 7% (Table 7). In both decentralised design instances (phased and flexible), the associated improvement (*VoF/ENPV*) was >10% which indicated that the derived results were above the statistical noise (≤ 10%) with higher confidence.

Another key insight of this study was the observed value at risk (*VaR*) and at gain (*VaG*) results. As indicated in Table 8, the highest *VaR* was observed for decentralised flexible design option ($155 million), followed by $136 million for a flexible centralised design. The results indicated that a flexible design provides 'insurance' against uncertain market and regulatory uncertainty, thus yielding a better economic performance profile relative to both fixed and phased designs. Moreover, both flexible designs offered the lowest standard deviation (*STD*) further strengthening the *VaR* and *VaG* results.

VaR findings are important because blue hydrogen has been mostly envisioned as an important enabler of a global hydrogen economy, with green hydrogen overtaking it in terms of LCOH by 2028 in the United States and 2030 globally ([3,31]. On one hand, if decision makers are willing to use blue hydrogen as only an enabler of the hydrogen economy and are convinced of the cost-competitiveness of green hydrogen, then flexible decentralised production offers the highest protection against adverse market conditions. On the other hand, if centralised production is preferred over the decentralised mode due to its maturity level, then a flexible centralised design is the best alternative for hedging against inherent market risks relative to fixed or phased designs. Either way, both flexible designs perform better under tight market conditions and provide meaningful 'insurance' to key-decision makers who are keen to accelerate the emergence of a global hydrogen economy.

One should also note that *VaG* under a centralised production mode was higher for a fixed design rather than phased or flexible designs: $1922 million vs. $1811 million and $1900 million. In simulation runs with high initial demand and favourable market conditions (i.e., high hydrogen price), fixed capacity design could operate at a higher

Table 8
Value at risk (P10) and gain (P90) for centralised and decentralised production designs.

Criterion	Centralised production			Decentralised production			Best design
	Fixed	Phased	Flexible	Fixed	Phased	Flexible	
VaR (10%)	−217	−43	136	−441	−97	**155**	Decentral – flexible
VaG (90%)	**1922**	1811	1900	1388	1619	1680	Central – fixed
STD	809	699	676	695	646	**592**	Decentral – flexible

production level from the start and, hence, generate higher revenues. In comparison, the phased and flexible plants had to gradually increase their output and lose additional revenue on plant downtime due to capacity expansion (50% reduction in the annual output). *VaG* should however be viewed with caution since it only represents the 90th percentile of simulated outcomes (Fig. 7). Hence, the possibility of having these market conditions in-place is rather low. Only one market scenario will materialise in the real world, which puts a lot of risk on relying on the fixed centralised strategy.

Contrary to a centralised mode of production, a different insight emerged when considering the *VaG* for decentralised plants. Herein, a flexible design provided the highest *VaG* ($1680 million) which was $61 million greater than the *VaG* for phased design (Table 8). Furthermore, *VaG* for the fixed decentralised design was lower than for both alternative designs ($1388 million) exhibiting a different trend relative to the centralised production case. The reason for this was likely two-fold. First, phased and flexible decentralised plants were already endowed with considerable flexibility that enabled them to swiftly adjust to favourable market conditions and limit the upside that fixed decentralised production could capture by having all the production capacity in place from the start. Second, phased and flexible decentralised designs did not incur a flexibility cost-premium and were not driven by strong EoS that allowed them to minimise the expenditure levels and benefit more from the upside opportunities.

Considering the previous findings, a considerable dilemma arises for key-decision makers regarding an optimal strategy for blue hydrogen production:

i. Select the industry's preferred centralised blue hydrogen production strategy to achieve lower LCOH and combine it with a flexible system design to hedge against market risks, whilst hoping that green hydrogen does not become cost competitive in a relatively short period of time (by 2028)
ii. Select the flexible decentralised production strategy to scale up the hydrogen economy at a higher cost but under the privilege of greater production flexibility, thus hedging against the risk of cost-competitive green hydrogen by 2028

4.2.1. *Effect of learning rates and economies of scale*

Sensitivity analysis of joint economies of scale and learning rates further indicated that the value of flexibility increases with weaker EoS and higher learning effects. Despite the extra cost of a flexible design, uncertain market conditions proved to offset the 8.4% flexibility cost-premium whilst generating additional value (*VoF* in Table 7). Fig. 8 summarises the impact of various learning rates and economies of scale for centralised flexible design relative to the fixed design option.

The underlying analysis was extended further by also considering various EoS. Herein, as *EoS* got weaker (the α factor increased in Eq. (7)), the value of flexibility increased. This was due to the reduced cost premium between flexible and fixed centralised plants in terms of monetary value. As such, two notable conclusions emerged: (i) the cost of a flexible system design decreases with greater installation rates (i.e., deployment rate) and (ii) a flexible blue hydrogen plant design becomes more appealing when EoS weakens.

4.3. *Effect of the time value of money on VoF*

Blue hydrogen production involves a moderate to high investment-risk considering the underdeveloped hydrogen market world-wide and the long operational time horizon. Given that higher discount rates decrease the time value of money more and are commonly used to represent higher risk-premium projects, the effect of the chosen discount rate was investigated on the value of flexibility. Fig. 9 illustrates the *VoF* profile for flexible centralised and decentralised blue hydrogen production with varying rates (i.e., increasing risk-premium of the investment) relative to their respective fixed designs.

As indicated by Fig. 9, a greater risk-premium could incentivise a flexible design strategy for large- and small-scale blue hydrogen production. A higher discount rate results in a reduction of the present value

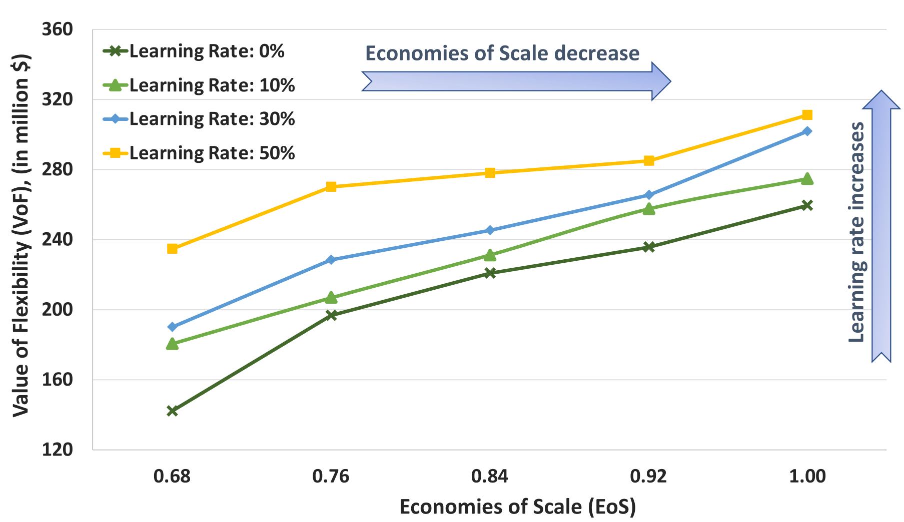

Fig. 8. Impact of learning effect and economies of scale on the value of flexibility (centralised production).

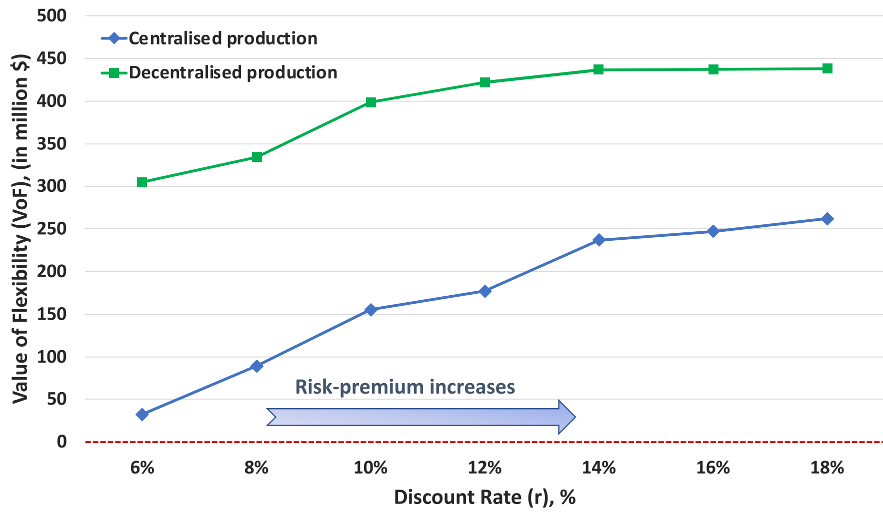

Fig. 9. Value of flexibility as a function of time value of money.

of the flexibility cost premium and, hence, increases *VoF*. Moreover, the effect of an increasing discount rate is less significant for decentralised production compared to centralised production. The reason is that decentralised production was already endowed with a greater degree of flexibility compared to the centralised production case.

4.4. Sensitivity analysis

As outlined in Section 3.4, the role of the sensitivity analysis in flexible system design is to determine the robustness of the recommended design solutions. For the preferred designs (flexible centralised and decentralised plants), a pre-defined range of the most sensitive parameters was used to capture the possible variation of these parameters with a higher certainty. This is contrary to the conventional ± X% approach because it provides a more realistic outlook on how much a given parameter could vary [14]. Fig. 10 illustrates the obtained results under deterministic conditions with 0.68 EoS, 0% learning rate and the associated parameter range as specified throughout Section 3. Furthermore, baseline model (deterministic) conditions were used to avoid statistical interference with the varied input parameter(s).

For both production pathways, the most sensitive parameter is the sharpness factor (b) which led to a $1773 million and $1500 million spread (max-min values) under centralised and decentralised production. Herein, if the rate of demand increase is slow (i.e., −70% reduction in b which leads to a shallow S-curve) then demand does not exceed the initial production capacity of the flexible plant and, hence, leads to a low NPV. In contrast, if the demand for hydrogen accelerates fast (+70% increase in b), then maximum production capacity is brought into operation faster, yielding the maximum revenue for a longer production time. Besides sharpness factor, initial demand (a) and its limit (M) also proved to be significant value-determining factors. It should be noted here that a lower initial demand (a) led to a higher NPV under both production pathways since in mathematical terms decreasing a in Eq. (8) leads to a greater demand at year t, whereas increasing a, reduces the demand. Further analysis on the S-curve demand modelling could be performed to yield a more complete outlook on various demand implications and their impact on the overall plant performance.

Moreover, the importance of using an accurate discount rate and reliable hydrogen price also proved to be crucial for a realistic project evaluation. An argument could be made that both parameters are closely linked. For instance, a lower discount rate represents a lower risk-premium that likely indicates a higher certainty in a stable and profitable hydrogen price. Contrary, a higher discount rate represents a greater risk-premium that emphasises greater uncertainty and volatility of a profitable hydrogen price. As such, further analysis could also be performed to investigate the combined effect of discount rate and hydrogen price under various market scenarios.

To extend the sensitivity analysis further, the impact of key demand parameters was investigated under various EoS and learning rates. In most of the low demand scenarios, the fundamental conclusion was the same – centralised and decentralised flexible design performed better given their ability to defer capacity expansion and limit the cumulative investment compared to the fixed or phased designs (Table 13 in Appendix E and Table 14 in Appendix F). The only exception was under

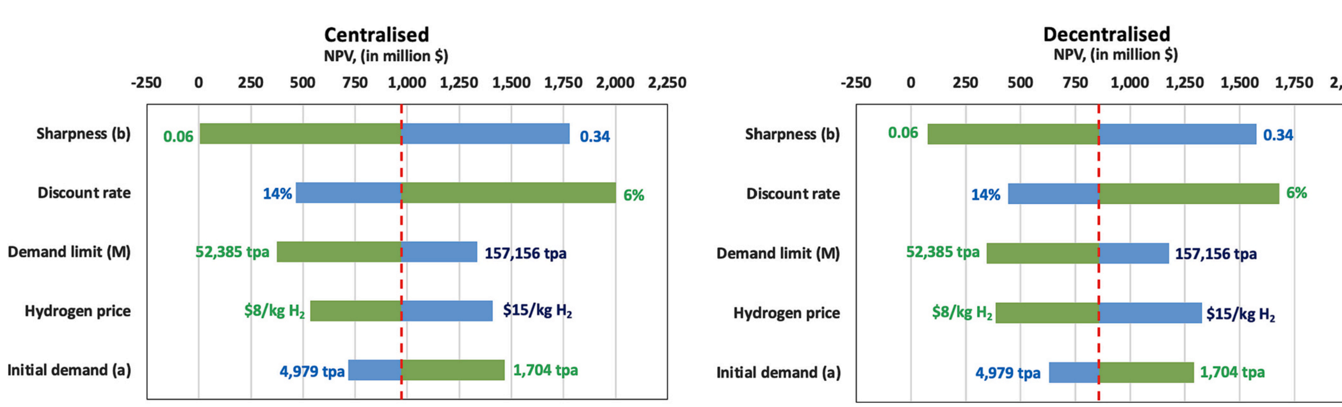

Fig. 10. Sensitivity analysis of flexible centralised and decentralised design under deterministic conditions (α = 0.68; learning rate = 0%).

centralised production with low initial market demand (a) where the phased design was preferred over the flexible design. This was because the expansion timing for a flexible design almost exclusively coincided with the expansion schedule for phased design (years 4, 8 and 11 for flexible & 4, 8, and 12 for phased design). The slight edge for a phased design could be because of the time value of money, as the difference between flexible and phased NPVs under low initial market demand is negligible (approximately $1 million). One should also note that low initial market demand (a) leads to greater NPV than under high initial market demand levels because of the rationale underlying Eq. (8) where lower initial demand a leads to higher overall demand levels in the following years.

One notes that high demand conditions presented a slightly different outlook on the preferred design alternatives. Under a centralised production mode and high sharpness factor (b), a fixed design emerged as a better solution relative to phased and flexible alternatives. This arose due to a combination of two main factors. First, high levels of early demand enabled fixed capacity plants to generate higher revenue than initially expected. Second, phased and flexible plants had to undergo expansion to match the rapidly rising demand, which limited their generated revenue due to plant downtime. Preference for a fixed design under a high sharpness factor was, however, only true for strong economies of scale and low learning rates. As economies of scale got weaker (0.68 to 0.84) and the learning rate increased (0% to 20%), a flexible design once again emerged as the preferred solution. This occurred due to a decreasing flexibility cost-premium, as discussed in previous sections. Moreover, one should note that under a decentralised production mode, a flexible design was expected to remain the preferred design given that (i) economies of scale hardly play any role in small-scale hydrogen production and (ii) increasing learning rates for phased/flexible plants would disadvantage fixed design plants even more.

The preference for a fixed design in an underestimated demand scenario provided another dilemma for key-decision makers. A fixed design can be a justified investment option only if current H_2 demand models indicated a high chance of underestimating the realised outcomes. It is also worth pointing out that increasing uncertainty about global and US-wide hydrogen economy conditions and the role of blue hydrogen suggest that a flexible system design provides greater investment security and better risk mitigation strategies.

5. Concluding remarks

A systematic and comprehensive economic performance evaluation of blue hydrogen production was presented using flexible system design and engineering real-options to deal with growing H_2 demand uncertainty. The presented analysis contrasts with conventional techno-economic performance assessment framework(s) where little to no consideration is given to a range of irreducible uncertain market, regulatory, and technological risk factors that often lead to erroneous conclusions. To recognise the inherent uncertainty and maximise economic performance of blue hydrogen production, flexible system designs were considered by implementing a modular production approach. This design strategy was examined across centralised and decentralised blue hydrogen production scales using the San Francisco area as a case study for transport fuel production. Such a problem formulation allowed identification and evaluation of the trade-offs between reduced production costs, benefits of on-site production and greater levels of production flexibility in this important market. Furthermore, the value of modular (flexible) design was investigated under various key uncertainty parameters, EoS, learning rates and the time value of money.

The proposed methodological framework provides multiple insights that could reliably inform and support a more nuanced decision-making on blue hydrogen production at different scales in the presence of uncertainty. First, it showed that a conventional deterministic techno-economic evaluation of blue hydrogen production most likely underestimates economic performance considering market, regulatory and technological uncertainty. Second, centralised flexible production achieved the highest economic performance among alternative designs despite the associated flexibility cost premium. Further analysis revealed that the value of flexibility increased with greater learning effects and weaker EoS relative to a fixed centralised design. Third, decentralised blue hydrogen production failed to compete with large-scale (centralised) production due to strong EoS and relatively nascent decentralised SMR & CCS technology that substantially increase production costs. Despite the lower market competitiveness, flexible decentralised production offered the highest value of flexibility and value at risk that was driven by highly responsive production expansion. Finally, a sensitivity analysis indicated that key demand parameters (sharpness factor, initial demand, and saturation point) along with discount rate and hydrogen price were the most impactful parameters in the proposed economic performance assessment framework.

Considering these results, decision makers are presented with the following dilemma:

i. Choose centralised hydrogen production and endow it with flexible system design to maximise system performance, but at the expense of a 25-year investment commitment and the inherent risk of green hydrogen emerging as a more cost-competitive energy vector
ii. Choose decentralised blue hydrogen production that comes at a higher production cost, but enables greater production flexibility and decreased investment risk while contributing to the scale up of CCS capacity and a hydrogen economy in the US

Despite the novel analysis presented here on the role of flexibility in blue hydrogen production system design, further analysis can be pursued to provide a more complete outlook. First, the proposed form of flexibility was solely focused on modular expansion, but alternative operational and constructional forms could be explored. For instance, operational and constructional flexibility could be investigated by considering a dual plant with SMR and autothermal reforming (ATR) production with the aim of reduced production costs. Herein, if technological breakthrough(−s) or increased learning effect applies to ATR, then this form of flexibility analysis would also provide an opportunity to address technological uncertainty. This would further strengthen the overall methodology used here and reinforce some of the arguments accompanying the key results and insights. Second, constructional flexibility could be considered by investigating the expansion of CCS capacity to achieve the intended capture rate that industry has often failed to attain in the past [40]. Third, centralised and decentralised production could be investigated in locations beyond San Francisco to evaluate the attractiveness of flexible plant design regionally or even globally. Although blue hydrogen production is currently preferred in locations with abundant and cheap natural gas supply, as well as favourable production subsidies (both relevant to the United States), a thorough flexibility analysis could provide a compelling investigation in emerging hydrogen markets such as in Europe and the Middle East region. Herein, demand and price uncertainty would have a greater impact on the economic performance of production plants given the nascent state of the hydrogen industry, which could either reinforce or limit the attractiveness of flexibility. Finally, all the above suggestions could involve and benefit from a spatial dimension being integrated into holistic energy systems models. This would provide a more realistic outlook of flexible system design applications in blue hydrogen production and its overall role in the global energy system as it transitions to a low-carbon economy.

CRediT authorship contribution statement

Davis Bigestans: Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Michel-Alexandre Cardin:** Validation, Supervision, Resources, Project administration, Methodology, Investigation, Conceptualization, Writing – review & editing. **Nikolaos Kazantzis:** Validation, Supervision, Resources, Investigation, Conceptualization, Writing – review & editing.

Declaration of Competing Interest

None.

Data availability

Data will be made available on request.

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Appendix A

Table 9
Capital costs of centralised production plant.

Plant Specifications		Centralised Plant	
Production rate, kg H_2/day		190,950	
Plant capacity factor, hrs./year		0.95	
Annual H_2 production, tonnes/yr.		66,212	
CO_2 Capture Rate		90%	
CO_2 emission rate (v), tonnes/yr.		63,247	
Annual CO_2 capture rate, tonnes/yr.		569,225	
Plant lifetime, years		25	
		Capital Investment	
Direct Costs	***Costs, $2022 basis***	***Cost Estimate***	***Reference***
Direct Materials/ Equipment	272,926,605	TDC – (Construction+EPC services, Other costs + Contigency) Collodi et al. [17] did not provide direct estimate apart from TDC which was kept as the baseline direct cost estimate and sub-cateogry costs were estimated as presented herein	Collodi et al. [17]
Construction	68,231,651	15% * TDC	Ma et al. [35] -Construction
EPC Services	40,938,991	15% * Direct Materials/Equipment	Ma et al. [35] -Engineering and Supervision
Other Costs	27,292,660	10% * Direct Materials/Equipment	Ma et al. [35] - Buildings, process, and auxiliary
Contingency	45,487,767	10% * TDC	Ma et al. [35] -Contingency
Total Direct Costs (TDC)	454,877,675		Collodi et al. [17]
Indirect Costs			
Owner's cost	31,841,437	7% * TDC	Collodi et al. [17]
Spare parts costs	2,274,388	0.5% * TDC	Collodi et al. [17]
Start-up costs	12,125,631	2%*TDC + 25% * (1 month fuel) + 3 months*(maintenance + labour) +1 month*(chemicals +catalysts). • 1 month fuel = 5466.17 t • 3 months of Maintenance + labour = $960,915 + $1,705,791 • 1 month of Chemicals + catalysts = $52,413 /Annual maintenance, labour, chemicals & catalysts costs are listed in Appendix C/	Collodi et al. [17]
Working capital	92,621,898	TCI – (TDC + Owner's + Spare parts + Start-up costs). Working capital represents 15.6% share of TCI (industry standard)	Collodi et al. [17], [35]
Total Capital Investment (TCI)	**593,741,029**	$2022 value	Collodi et al. [17]

Appendix B

Table 10
Capital costs of decentralised production plant.

Plant Specifications	Decentralised Plant
Production rate, kg H_2/day	6000
Plant capacity factor, hrs./year	0.86
Annual H_2 production, tonnes/yr.	1883
CO_2 Capture Rate	90%
CO_2 emission rate, tonnes/yr.	1590
Annual CO_2 capture rate, tonnes/yr.	14,313

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Table 10 (*continued*)

Plant Specifications		Decentralised Plant	
Plant lifetime, years		20	
		Capital Investment	
Direct Costs	***Costs, $2022 basis***	***Cost Estimate***	***Reference***
Direct Materials/Equipment	8,595,293	$2005 cost * installation cost* inflation factor * scale ratio * cost adder: • $2005 costs for 1500 kg H_2/day module = $869,827.38 • Installation costs = 1.1 • CEPCI (2005 – Jan 2010) = 1.176 • US CPI (Jan 2010 -April 2022) = 1.33 • Inflation factor = CEPCI * CPI • Scale ratio = $(6000\ kg\ H_2/day\ /\ 1500\ kg\ H_2/day)^{0.6}$ • Cost adder = 2.5	H2A v3 model. [46] CEPCI factors: [37] Cost adder: [36]
Construction	1,782,235	18.85% share of direct materials/equipment cost * installation cost factor (=1.1) * cost adder (=2.5)	H2A v3 model [46] Cost adder: [36]
EPC Services	449,165	$2005 cost * scale ratio * inflation factor*cost adder: • $2005 cost for 1500 kg H_2/day module = $50,000 • Scale ratio = $(6000\ kg\ H_2/day\ /\ 1500\ kg\ H_2/day)^{0.6}$ • CEPCI (2005 – Jan 2010) = 1.176 • US CPI (Jan 2010 -April 2022) = 1.33 • Inflation factor = CEPCI * CPI • Cost adder = 2.5	H2A v3 model. [46] Cost adder: [36]
Other Costs	269,498	$2005 cost * scale ratio * inflation factor * cost adder: • $2005 cost for 1500 kg H_2/day module = $30,000 • Scale ratio = $(6000\ kg\ H_2/day\ /\ 1500\ kg\ H_2/day)^{0.6}$ • CEPCI (2005 – Jan 2010) = 1.176 • US CPI (Jan 2010 -April 2022) = 1.33 • Inflation factor = CEPCI * CPI • Cost adder = 2.5 (Taken as the Upfront Permitting Costs in the H2A model.)	H2A v3 model. [46] Cost adder: [36]
Contingency	1,289,295	15.00% share of direct materials/equipment cost *cost adder (=2.5)	H2A v3 model. [46] Cost adder: [36]
Total Direct Costs (TDC)	**12,385,485**		
Indirect Costs			
Owner's cost	**866,985**	No information provided by H2A v3model. Assumed the cost to be similar to the centralised case for equal comparison – 7% of TDC * cost adder (=2.5)	Collodi et al. [17] Cost adder: [36]
Spare parts costs	**61,928**	No information provided by H2A v3model. Assumed the cost to be similar to the centralised case for equal comparison – 0.5% of TDC * cost adder (=2.5)	Collodi et al. [17] Cost adder: [36]
Start-up costs	**247,710**	No information provided by H2A v3model. Assumed the cost to be similar to the centralised case for equal comparison – 2% of TDC* cost adder (=2.5) Fuel, maintenance, labour, and chemical costs were neglected due to the relatively small size of production units compared to the centralised plants.	Collodi et al. [17] Cost adder: [36]
Working capital	2,390,848	15% of TCI (solved iteratively) * cost adder (=2.5)	H2A v3 model. [46] Cost adder: [36]
Total Capital Investment (TCI)	**15,952,955**	All capital costs solely considered following H2A v3 model. [46]; thus, no interest, owner's cost, working capital, spare parts cost and start-up costs considered	H2A v3 model. [46]

Appendix C

Table 11
Operating costs of centralised production plant.

Annual Operating Costs			
Fixed costs (FC)	*Costs, $2022 basis*	*Cost Estimate*	*Reference*
Direct labour	3,266,921	€60, 000/employee.annum * 43 personnel staff * (1 + ECI) • €1 = $1.06 (May-2022) • Employment Cost Index (Apr-2017 to Apr-2022) = 19.46%	Collodi et al. [17]
Administrative and general overhead cost	3,027,026	30% * (Labour + Maintenance). • Includes costs of management, administration, R&D, personnel services, clerical staff, technical services.	Collodi et al. [17],
Insurance	2,274,388	0.5% * TPC	Collodi et al. [17]
Local Taxes and Fees	2,274,388	0.5% * TPC	Collodi et al. [17]

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Table 11 (*continued*)

Annual Operating Costs			
Fixed costs (FC)	*Costs, $2022 basis*	*Cost Estimate*	*Reference*
Annual Operating and Maintenance	6,823,165	1.5% * TPC	Collodi et al. [17]
Land Rent	–	Land included under owner's cost	Collodi et al. [17]
Total FC	17,665,888		
Operating Costs (OC)			
Feedstock + Fuel	67,837,342	Natural Gas (feedstock) - 26.231 t/h Natural Gas (fuel) - 7.347 t/h.; Natural Gas Price = $4.16/MMBtu	Consumption rate and natural gas chemical specifications (Table 1): Collodi et al. [17] Natural gas price: EIA [22]
Water Makeup	104,434	• 2017 water cost: €70,100 • CEPCI 2022/ CEPCI 2017 = 797.6/567.5 • €1 = $1.06 (May-2022)	Cost: Collodi et al. [17] CEPCI factors: Maxwell [37]
Chemicals and Catalysts	625,712	• 2017 chemicals cost: €100,000(• 2017 catalyst cost: €320,000 • CEPCI 2022/ CEPCI 2017 = 797.6/567.5 • €1 = $1.06 (May-2022)	Cost: Collodi et al. [17] CEPCI factors: Maxwell [37]
CO_2 Tax	1,418,630	Tax rate = $22.43/tCO2	ICAP [29]
CO_2 Capture and Compression	–	Costs considered throughout all other fixed and operating cost categories	–
CO_2 transport & storage	8,538,375	Transport and storage rate: $15/tCO2	Global CCS Institute [26]
H_2 Delivery cost	70,846,746	$1.07/kg; gaseous hydrogen transport via tube trailers (delivery radius < 200 km)	IEA [30]
Other variable Operating costs	–	Costs considered throughout all other fixed and operating cost categories	–
Total OC	**149,371,239**		
Total Production Costs TPC (FC + OC)	**167,037,127**		

Appendix D

Table 12
Operating costs of decentralised production plant.

Annual Operating Costs			
Fixed costs (FC)	*Costs, $2022 basis*	*Cost Estimate*	*Reference*
Direct labour	61,886	Operating + Maintenance + Administrative labor • Operating labour = 0.80% of Direct Material/Equipment Cost • Maintenance labour = 0.80% of Direct Material/Equipment Cost • Administrative labour = 0.20% of Direct Material/Equipment Cost	Ma et al. [35]
Administrative and general overhead cost	12,377	• 20% of Direct Labour	H2A v3 model [46]
Insurance	68,762	2% of Direct Material/Equipment Cost	H2A v3 model. [46]
Local Taxes and Fees	24,771	0.5% of Total Direct Cost • Assumed that taxes and fees are similar to the centralised facility given limited data availability	Collodi et al. [17]
Annual Operating and Maintenance	171,906	5% of Direct Material/Equipment Cost	H2A v3 model. [46]
Land Rent	101,243	Land area*scale ratio * lease cost ($2005) * US CPI • Land area = 748 m^2 (1500 kg H_2/day facility) • Scale ratio = (6000 kg H_2/day / 1500 kg H_2/day)$^{0.6}$ • Lease cost: $38.76/$m^2$.year (2005 cost cost) • US CPI (Jan 2005 -April 2022) = 1.52	H2A v3 model. [46]
Total FC	440,945		
Variable Costs			
Feedstock + Fuel	1,349,490	Natural Gas (0.156 MMBtu/kg H_2; $4.16/MMBtu) + Electricity (1.11 kWh/kg H_2; $0.061/kWh)	Consumption: [46] Price: EIA [22], EIA [23]
Water Makeup	31,481	Hydrogen production * water usage * cost rate * US CPI • Hydrogen production = 1883,000 kgH2.annum • Water usage = 5.77 gal/kg H_2 • Cost rate = $0.002375/gal (H2A default: 2016 cost) • US CPI (Jan 2016 -April 2022) = 1.22	H2A v3 model. [46]
Chemicals and Catalysts	–		
CO_2 Tax	35,664	CO_2 emissions * tax rate • CO_2 emissions (6000 kg H_2/day) = 1590 CO_2/annum	ICAP [29]

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Table 12 (*continued*)

Annual Operating Costs			
Fixed costs (FC)	*Costs, $2022 basis*	*Cost Estimate*	*Reference*
		• Tax rate = $22.43/tCO_2$	
CO$_2$ Capture and Compression	3,178,406	capture cost * scale ratio * captured CO$_2$ • Capture cost (500 kg H$_2$/day station) = $50/t CO$_2$ • Scale ratio = (6000 kg H$_2$/day / 500 kg H$_2$/day)$^{0.6}$ • Captured CO$_2$ (6000 kg H$_2$/day station) = 14,313 CO$_2$/annum	Psarras et al. [50]
CO$_2$ transport & storage	214,695	Captured emissions * cost rate • captured emissions (6000 kg H$_2$/day) = 14,313 CO$_2$/annum • Cost rate = $15/t CO$_2$	Global CCS Institute [26]
H$_2$ Delivery cost		None due to on-site production	
Other variable Operating costs	11,261	Nominal cost * Scale Factor * Inflation factor • Nominal cost ($2005 level) = $1800/annum • Scale Factor = (6000 kg H$_2$/day / 1500 kg H$_2$/day) = 4 • CEPCI (2005 – Jan 2010) = 1.176 • US CPI (Jan 2010 -April 2022) = 1.33 • Inflation factor = CEPCI * CPI	H2A v3 model. [46]
Total Production Costs TPC (FC + OC)	**5,261,942**		

Appendix E

Table 13
Deterministic results of sensitivity analysis for centralised production mode under various learning rates and economies of scale (bolded values represent the best NPV result under respective low or high conditions in sensitivity analysis).

Condition	Demand parameter	Low Estimate	Low NPV (million $)			Base NPV (million $)	High Estimate	High NPV (million $)		
			Fixed	*Phased*	*Flexible*	*Flexible*		*Fixed*	*Phased*	*Flexible*
	Sharpness (b)	−70%	−348	−204	**6**	972	70%	**1822**	1667	1779
EoS = 0.68; LR = 0%	*Demand limit (M)*	−50%	170	293	**375**	972	50%	1283	1325	**1337**
	Initial demand (a)	−50%	1444	**1469**	1467	972	50%	562	668	**716**
	Sharpness (b)	−70%	−348	−182	**6**	988	70%	**1822**	1689	1805
EoS = 0.68; LR = 10%	*Demand limit (M)*	−50%	170	315	**385**	988	50%	1283	1347	**1357**
	Initial demand (a)	−50%	1444	**1491**	1490	988	50%	562	690	**730**
	Sharpness (b)	−70%	−348	−121	**61**	1048	70%	1822	1751	**1866**
EoS = 0.84; LR = 0%	*Demand limit (M)*	−50%	170	377	**443**	1048	50%	1283	1409	**1417**
	Initial demand (a)	−50%	1444	**1553**	1552	1048	50%	562	752	**789**
	Sharpness (b)	−70%	−348	−86	**61**	1073	70%	1822	1785	**1906**
EoS = 0.84; LR = 20%	*Demand limit (M)*	−50%	170	411	**459**	1073	50%	1283	1443	**1449**
	Initial demand (a)	−50%	1444	**1587**	1587	1073	50%	562	786	**810**
	Sharpness (b)	−70%	−348	−53	**104**	1109	70%	1822	1818	**1936**
EoS = 1.00; LR = 0%	*Demand limit (M)*	−50%	170	444	**498**	1109	50%	1283	1476	**1482**
	Initial demand (a)	−50%	1444	**1620**	1619	1109	50%	562	819	**847**
	Sharpness (b)	−70%	−348	−13	**104**	1138	70%	1822	1858	**1982**
EoS = 1.00; LR = 30%	*Demand limit (M)*	−50%	170	484	**517**	1138	50%	1283	1516	**1518**
	Initial demand (a)	−50%	1444	1660	**1660**	1138	50%	562	859	**871**

Appendix F

Table 14
Deterministic results of sensitivity analysis for decentralised production (bolded values represent the best NPV result).

Condition	Demand parameter	Low Estimate	Low NPV (million $)			Base NPV (million $)	High Estimate	High NPV (million $)		
			Fixed	*Phased*	*Flexible*	*Flexible*		*Fixed*	*Phased*	*Flexible*
	Sharpness (b)	−70%	−538	−195	**76**	858	70%	1273	1486	**1576**
EoS = 0.68; LR = 0%	*Demand limit (M)*	−50%	−149	193	**346**	858	50%	796	1134	**1178**
	Initial demand (a)	−50%	941	1279	**1290**	858	50%	169	510	**630**

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