Economic value of flexible hydrogen-based polygeneration energy systems

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Highlights

- Assess the economic value of fossil-fuel polygeneration energy systems (PES).
- Analyze the cost competitiveness of static and flexible PES.
- Derive and quantify PES levelized cost of hydrogen and unit profit-margin.
- Derive and quantify PES real-option values of diversification and flexibility.
- Assess the economic competitiveness of Hydrogen Energy California (HECA).

Abstract

Polygeneration energy systems (PES) have the potential to provide a flexible, high-efficiency, and low-emissions alternative for power generation and chemical synthesis from fossil fuels. This study aims to assess the economic value of fossil-fuel PES which rely on hydrogen as an intermediate product. Our analysis focuses on a representative PES configuration that uses coal as the primary energy input and produces electricity and fertilizer as end-products. We derive a series of propositions that assess the cost competitiveness of the modeled PES under both static and flexible operation modes. The result is a set of metrics that quantify the levelized cost of hydrogen, the unit profit-margin of PES, and the real-option values of ‘diversification’ and ‘flexibility’ embedded in PES. These metrics are subsequently applied to assess the economics of Hydrogen Energy California (HECA), a PES currently under development in California. Under our technical and economic assumptions, HECA’s levelized cost of hydrogen is estimated at 1.373 $/kg. The profitability of HECA as a static PES increases in the share of hydrogen converted to fertilizer rather than electricity. However, when configured as a flexible PES, HECA almost breaks even on a pre-tax basis. Diversification and flexibility are valuable for HECA when polygeneration is compared to static monogeneration of electricity, but these two real options have no value when comparing polygeneration to static monogeneration of fertilizers.

1. Introduction

Fossil fuels meet 87% of today’s global energy demand [1] and are used to generate 68% of the global electricity supply [2]. Concerns over climate change, growing energy consumption, and energy security compel fossil-fuel plants to meet increasing regulatory and market challenges: lower emissions, higher efficiency, and more flexible operations to complement intermittent renewables and hedge against fluctuations in energy prices. Polygeneration energy systems (PES) have the potential to meet all these challenges.

While polygeneration generally describes a wide range of multi-input multi-output industrial processes [3], this study focuses on polygeneration energy systems that use fossil fuels as inputs and produce hydrogen as an intermediate product [4]. PES offers multiple advantages over conventional single-output or ‘monogeneration’ systems. Technically, polygeneration allows better process- and heat-integration among various production and ancillary units, which reduces energy losses and thus results in higher energy-conversion efficiency. This higher efficiency, combined with the utilization of carbon in chemical synthesis,
results in lower carbon dioxide (CO₂) emissions [5,6]. In addition, the production rates of PES can be either fixed or adjusted over time. We refer to a system with fixed production rates as ‘static’ or ‘steady-state’ polygeneration and a system with variable production rates as ‘flexible’ or ‘dispatchable’ polygeneration [7]. Flexible polygeneration can exploit frequent variations in commodity prices; while fuel switching and mixing capabilities help attenuate the risks of fuel-price shocks, production diversification and dispatchability help capture the benefits of product-price peaks [9–11], which renders merchant hydrogen prices an imperfect indicator of cost and value. By converting hydrogen to valuable commodities, polygeneration offers an incentive to expand investments in hydrogen infrastructure.

The advantages of polygeneration systems merit a rigorous analysis of their economic competitiveness within the broader energy landscape. In this study, we develop a set of generalizable metrics that can be used to evaluate fossil-fuel polygeneration energy systems. These economic metrics achieve three goals. First, they calculate the levelized cost and profitability of both static and flexible polygeneration, irrespective of the type of used fossil fuels or generated end-products. Second, they facilitate a consistent comparison of the economics of polygeneration relative to that of monogeneration, with special emphasis on electricity monogeneration alternatives (e.g. natural gas or wind). Finally, they quantify the value of two real options enabled by polygeneration: the value of diversifying end-products and the value of flexibly varying the production rates of end-products over time.

The main motivation for our analysis stems from the fact that different methodologies have been used to evaluate polygeneration economics, including net present value [7,8,12,13], profit index [12], payout time [14], cost of energy [15,16], and others [17–19]. While each methodology has its own merits, the lack of methodological consistency prevents accurate comparison of polygeneration economics under different technical assumptions and operational settings. The economic metrics we propose offer one methodological consistency prevents accurate comparison of polygeneration economics under different technical assumptions and operational settings. The economic metrics we propose offer one
approach faces the following challenges. First, polygeneration may not necessarily generate electricity as an end-product, in which case the use of COE becomes impractical. Second, it is problematic to calculate COE as the cost of polygeneration less the cost of other non-electricity products from equivalent monogeneration [15,16]; this method assigns all cost-savings from polygeneration system-integration to the power unit and therefore might underestimate the actual cost of electricity. Our approach addresses this issue by converting the cost per unit of hydrogen to a cost per unit of any end-product, assuming that all hydrogen is converted to that single end-product. This methodology facilitates an economic comparison between polygeneration and monogeneration systems, including traditional power plants.

In addition, an assessment of the economic competitiveness of flexible polygeneration systems should include a quantification of the economic trade-offs associated with operational flexibility. Greater flexibility typically implies not only higher revenues but also higher cost of capacity due to larger equipment size [7,8]. We address this topic by deriving metrics that capture the economic impacts of flexible polygeneration, illustrating that production diversification and flexibility need not always result in economic gains [7].

On the technical side, there is an extensive literature on optimizing the design and operation of PES by combining several technologies and processes [6,13], incorporating investment planning procedures [20], or investigating the trade-offs associated with operational flexibility [7]. Other studies also performed detailed techno-economic analyses on specific polygeneration systems under various input- and output- portfolios [5,8,14,18,19] and process configurations [16,17]. Given the breadth of the available technical analysis, our work presumes that polygeneration is techni-
cally feasible and focuses predominantly on assessing its economic value. To that end, we use a simple yet generalizable PES configuration that can operate as both a static and a flexible system. Building specifically on the work by Chen et al. [7], which optimizes PES operations under uniform levels of flexibility, we impose different flexibility limits on different production units to explore the effect of real-life operational constraints on PES economics.

In the following sections, we first introduce the economic concepts and technical configuration used in assessing PES. Next, we present a detailed economic analysis for the modeled PES in three scenarios; Scenario 1 evaluates static operations while Scenarios 2a and 2b evaluate two modes of flexible operations. As the main focus of this paper, we explore the economic impacts of flexible polygeneration, illustrating that production diversification and flexibility need not always result in economic gains [7].

2. Research methodology

This section describes the economic concepts and technical specifications used in deriving the valuation metrics for PES. We first introduce the levelized cost of hydrogen concept, which is the foundational tool for economic assessment. Then, we explain the process configuration, fuel-inputs, and product-outputs of the adopted fossil-fuel polygeneration system.

2.1. Levelized cost of hydrogen

Similar to the concept of ‘levelized cost of electricity’ (LCOE) as cost per unit of energy generation ($/kWh), the metric of ‘levelized cost of hydrogen’ (LCOH) refers to the cost per unit of hydrogen production ($/kgH) [21,22]. Consistent with MIT’s The Future of Coal definition of LCBOE [23], this study defines LCOH as: “the constant dollar hydrogen price that would be required over the life of a hydrogen plant to cover all operating expenses, payment of debt and accrued interest on initial project expenses, and the payment of an acceptable return to investors”. In other words, the LCOH is a break-even metric that calculates the ratio of ‘lifetime cost’ to ‘lifetime hydrogen production’ of a facility.

The LCOH formulation adopted in this study is similar to the LCOE model in Reichelstein and Yorston [24]. As shown in (1), the LCOH ($/kgH) is the sum of three terms: cost of capacity per unit output \(c_c\), time-averaged fixed operating cost per unit output \(J_h\), and time-averaged variable cost per unit output \(w_h\) [24,25].

\[
LCOH = c_c + J_h + w_h
\]  
(1)

Assuming constant returns-to-scale, the cost of capacity per one kilogram of hydrogen can be expressed as:

\[
c_c(\$/kgH) = \frac{SP}{m \cdot CF \cdot \sum_{i=1}^{m}X_i \cdot \gamma^i}
\]  
(2)

\(SP \ (\$/[kgH/hr])\) in (2) denotes the system price of acquiring one unit of capacity to produce one kilogram of hydrogen per hour. It includes the cost of engineering procurement and construction, contingencies, and land purchase. The initial investment yields a stream of hydrogen output over \(T\) years, with \(m \cdot x_i \cdot CF\) kilograms delivered in year \(i\). While \(m = 8760\) refers to the total number of hours in a given year, the system degradation factor, \(\gamma\), accounts for potential losses in generation capacity over time and is technology-specific. In addition, since the facility may not be online at all times, the practical capacity is only a fraction of the theoretical capacity. This fraction is represented by the capacity factor, \(CF\). Furthermore, since the LCOH is a break-even formula, it is essential to specify an appropriate discount rate. We denote this discount rate by \(\tau\) and the corresponding discount factor by \(\gamma = (1 + \tau)^{-1}\).

Fixed operating costs can vary over time. Costs in this category include labor, administration and overhead, maintenance, and insurance. While fixed operating costs are assumed to scale proportionally with the capacity of the facility, they are independent of the actual amount of hydrogen generated by the facility.

\[
J_h = \frac{\sum_{i=n}^{T}SJ_i \cdot \gamma^{T-i}}{m \cdot CF \cdot \sum_{i=1}^{m}X_i \cdot \gamma^i}
\]  
(3)

Finally, variable costs can vary over time. Costs in this category include fuel consumption, raw-material inputs, auxiliary loads, and cash-conversion expenses. We use \(w_h(t) \ (\$/kgH)\) to denote the time-dependent variable cost per one kilogram of hydrogen in year \(i\), and we derive \(w_h \ (\$/kgH)\) in (4) as the yearly-averaged variable cost.

\[
w_h = \frac{1}{m} \int_0^m w_h(t) dt
\]  
(4)

Over the life cycle of the facility, the time-averaged variable cost per one kilogram of hydrogen \(w_h \ (\$/kgH)\) becomes as expressed in (5).
of polygeneration.\(^{(6)}\) needs to be expanded to assess the economic value of commodities with well-defined market prices. Therefore, the following benchmark result:

\[
\begin{align*}
\text{PH} &= \frac{\sum_{t=1}^{T} w_t \cdot m \cdot CF \cdot x_t \cdot \gamma_t^d}{\sum_{t=1}^{T} w_t \cdot x_t \cdot \gamma_t^d} \\
\text{wh} &= \frac{\sum_{t=1}^{T} w_t \cdot x_t \cdot \gamma_t^d}{\sum_{t=1}^{T} x_t \cdot \gamma_t^d}
\end{align*}
\]

Similar notation is used to characterize the time-dependency of all economic metrics in this study, including prices. For instance, \(P_h(t), P_m,\) and \(P_e\) refer to the time-dependent price of hydrogen in year \(i,\) the yearly-averaged price of hydrogen in year \(i,\) and the time-averaged price of hydrogen, respectively. Referring back to the definition of \(\text{LCOH}\) as a break-even value, we can obtain the following benchmark result:

A hydrogen production facility is cost-competitive if and only if:

\[P_h > \text{LCOH}\]

Cost-competitiveness is defined as the ability of the facility to achieve a positive NPV. Since a PES produces hydrogen as an intermediate product only, the price of hydrogen \(P_h\) must be substituted with revenue from the hydrogen-enabled end-products, which are commodities with well-defined market prices. Therefore, the formulation in (6) needs to be expanded to assess the economic value of polygeneration.

### 2.2. Technical configuration of PES

This study analyzes a simple yet generalizable fossil-fuel PES configuration, which can operate as either a static or a flexible system. Specifically, we consider a PES that uses coal as fuel, produces hydrogen then ammonia as intermediate products, and produces electricity and fertilizer (e.g. urea) as final end-products. In the assumed configuration, coal can be also mixed with biomass or petcoke as fuel inputs.

In a static PES, all units run at steady-state with fixed output flow-rates. In a flexible PES, however, some units can vary their output flow-rates over time while other units should run at steady-state with fixed flow-rates in order to maintain acceptable energy- and chemical-conversation efficiencies \(\text{[26]}\). To account for these real-life operational constraints, and to allow for a generalizable economic assessment, the adopted PES can be conceptually divided into four ‘subsystems’: hydrogen, electricity, ammonia, and fertilizer. While the electricity and ammonia subsystems can be either flexible or static, the hydrogen and fertilizer subsystems are always static.

Fig. 1 presents a simplified depiction of the process flow sheet for the polygeneration facility. As shown, coal is first fed into a gasifier where it is mixed with an oxygen (\(O_2\)) stream from the air separation unit (ASU) to produce hydrogen-rich syngas. In addition to the gasifier and the ASU, the hydrogen production subsystem includes: syngas clean-up units such as particulate removal unit (PRU), mercury removal unit (MRU), and acid-gas removal unit (AGRU); shift-reaction unit (SRU); and hydrogen separation unit (HSU). All these units should run at steady-state \(\text{[26]}\), resulting in a fixed output of hydrogen (\(H_2\)) and carbon dioxide (\(CO_2\)).

Hydrogen is either fed into a combined-cycle turbine unit for electricity generation or mixed with nitrogen (\(N_2\)) from the ASU to produce ammonia (\(NH_3\)), the precursor material for making fertilizers. Both electricity generation \(\text{[27,28]}\) and ammonia synthesis \(\text{[26]}\) units can operate flexibly, producing variable power and ammonia flows. Ammonia is then mixed with a fraction of the \(CO_2\) stream to produce fertilizer (e.g. urea). The fertilizer synthesis unit must run at steady-state \(\text{[26]}\), resulting in a fixed flow of the end-product. The remaining \(CO_2\) stream is either vented or compressed and transported for geologic sequestration. Finally, since the steady-state production of fertilizer is dependent on the variable production of ammonia, intermediate ammonia storage is necessary to buffer the variations in the ammonia output and secure a fixed ammonia input into the fertilizer subsystem.

Focusing specifically on the ammonia and electricity subsystems, their ranges of flexibility are constrained by system-integration and efficiency-related standards. For example, part of the generated electricity is used for auxiliary load within the facility \(\text{[26]}\), and power turbines must operate above minimum-capacity limits to avoid severe losses in energy efficiency \(\text{[28]}\). In addition, bounding the range of ammonia production is necessary to cap the size ammonia storage; the needed intermediate storage becomes increasingly larger as the range of variable production rates becomes wider. We account for these practical flexibility
constraints by imposing a lower bound on the production rates of both electricity and ammonia. The upper bound on production rates is imposed by the name-plate capacity of each production unit.

3. Economic analysis

Based on the preceding technical configuration, we investigate two scenarios, illustrated in Fig. 2. Scenario 1 analyzes a static PES whereas Scenario 2a and Scenario 2b analyze a flexible PES. In all scenarios, the PES can still be characterized as a combination of the four operational subsystems introduced above, with the rate of total hydrogen production fixed at \( N_h \) (kg/h). For simplicity, we set \( N_h = 1 \) in Fig. 2. For each unit of hydrogen produced, \( \lambda \) fraction is allocated to electricity production, and the remaining \( (1 - \lambda) \) is allocated to ammonia production. While \( \lambda \) is constant in Scenario 1, \( \lambda(t) \) may vary with time in Scenarios 2a and 2b. By definition, one kilogram of hydrogen can be converted to either \( X_e \) kilowatt hours of electricity or \( X_a \) kilograms of ammonia. The subsequent reaction of \( X_a \) kilograms of ammonia with CO2 results in \( X_f \) kilograms of fertilizer; thus, \( X_e / X_f \) units of ammonia are needed to produce one unit of fertilizer.

To account for flexibility constraints, we limit the feasible range of \( \lambda \), such that \( \lambda \in [\lambda_{\text{min}}, \lambda_{\text{max}}] \). \( \lambda_{\text{min}} \) is dictated by the minimum allowable rate of electricity generation, which necessitates that \( \lambda > \lambda_{\text{min}} > 0 \). On the other hand, \( \lambda_{\text{max}} \) is dictated by the minimum allowable rate of fertilizer generation, which necessitates that \( 1 - \lambda \leq (1 - \lambda_{\text{max}}) > 0 \), or equivalently, \( \lambda < \lambda_{\text{max}} < 1 \). Finally, \( K \) is a constant parameter related to buffering ammonia production for fertilizer synthesis, to be formally introduced in Scenario 2b.

To reflect current market conditions, the analysis in all scenarios assumes that the price of electricity changes on an hourly basis [29] whereas the price of fertilizer changes on a yearly basis [30]. The underlying assumption is that electricity is typically sold in competitive wholesale markets, but fertilizers can be sold through long-term contracts because they can be stored relatively easily. Also, to simplify the economic modeling, all fixed and variable costs are assumed to remain constant in a given year, but they may change across years. Section 5.2 discusses the implications of this assumption in more detail.

3.1. Scenario 1: Static PES with fixed production rates

If the polygeneration system is static, all subsystems run at steady-state with constant production rates. The ammonia stream is directly and completely converted to fertilizer without the need for an intermediate storage. For every kilogram of hydrogen, the PES outputs \( X_e \) kilowatt hours of electricity, \((1 - \lambda) \cdot X_a\) kilograms of ammonia, and \((1 - \lambda) \cdot X_f\) kilograms of fertilizer. We refer to \( X_e, (1 - \lambda) \cdot X_a\), and \((1 - \lambda) \cdot X_f\) as ‘production coefficients.’

The economic value of this static PES must account for the generation of electricity and fertilizer at each point in time. Therefore, the expression in (6) is modified by substituting the revenue from direct sales of merchant hydrogen with the net revenue from converting hydrogen to both end-products.

For each unit of produced electricity, the net revenue is the difference between the time-averaged price \( P_e \) ($/kWh) and the ‘levelized incremental cost’ of installing and operating the electricity subsystem, defined as \( \text{LIC}_e \) ($/kWh). \( \text{LIC}_e \) is distinguished from \( \text{LCOE} \). \( \text{LIC}_e \) captures the cost of the electricity subsystem only (e.g., combined-cycle turbine). In contrast, \( \text{LCOE} \) accounts for the full cost of electricity generation, which includes the cost of hydrogen. Therefore, if \( \lambda = 1 \), we obtain \( \text{LCOE} = \text{LCOH}/X_e + \text{LIC}_e \).

Similarly, for each unit of produced fertilizer, the net revenue is the difference between the time-averaged price \( P_f \) ($/kgf) and the levelized incremental cost of both the ammonia and fertilizer subsystems, defined as \( \text{LIC}_a \) ($/kgf) and \( \text{LIC}_f \) ($/kgf), respectively. Referring to Section 2.1, Definition 1 presents each \( \text{LIC} \) metric as the sum of three levelized cost components: a cost of capacity \( c \), a time-averaged fixed operating cost \( j \), and a time-averaged variable cost \( w \).

Definition 1.

\[
\text{LIC}_e = c_e + j_e + w_e \tag{7}
\]

\[
\text{LIC}_a = c_a + j_a + w_a \tag{8}
\]

\[
\text{LIC}_f = c_f + j_f + w_f \tag{9}
\]
As a result, it is now possible to assess the economic feasibility of this static PES by formulating Proposition 1.

**Proposition 1.** A static polygeneration facility is cost-competitive if and only if:

\[
\lambda \cdot X_e \cdot (P_e - LIC_e) + (1 - \lambda) \cdot (X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a) > LCOH
\]

(10)

As proven in the derivation of Proposition 1 in Appendix A, the unit revenue for hydrogen in (6), \( P_h \), is replaced with two net-revenue terms, one for each end-product: \((X_e \cdot P_e - X_e \cdot LIC_e)\) corresponding to the net revenue from hydrogen conversion to electricity and \((X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a)\) corresponding to the net revenue from hydrogen conversion to ammonia then fertilizer. The net revenue from each end-product is weighted by the fraction of hydrogen capacity allocated to it: \( \lambda \) for electricity and \((1 - \lambda)\) for fertilizer.

Proposition 1 provides several insights. For the static PES to break even, the prices of end-products must be high enough to compensate not only for their incremental cost but also for the cost of hydrogen. Furthermore, optimizing the economic value of the static PES requires maximizing hydrogen allocation to the end-product contributing the highest net revenue. Ultimately, this incentivizes setting \( \lambda = 1 \) when \((X_e \cdot P_e - X_e \cdot LIC_e) \geq (X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a)\) and setting \( \lambda = 0 \) otherwise; in both cases, static PES reduces to static monogeneration of either end-product. Therefore, Proposition 1 shows that the profitability of a static PES with multiple end-products is bounded by the profitability of the static monogeneration of its individual end-products.

To elaborate further on the economics of polygeneration, we introduce the ‘levelized cost of polygeneration’, or \( LCOP \) (\$/kg$_\text{hydrogen}$). Consistent with the earlier definition of \( LCOH \), we define \( LCOP \) in (11) as a weighted-average price of polygeneration end-products that would set the NPV of the PES to exactly zero.

**Definition 2.**

\[
LCOP = LCOH + \lambda \cdot X_e \cdot LIC_e + (1 - \lambda) \cdot [X_f \cdot LIC_f + X_a \cdot LIC_a]
\]

(11)

Proposition 1 can then be re-arranged into Proposition 1 in order to incorporate the mathematical form of \( LCOP \) in Definition 2.

**Proposition 1.** A static polygeneration facility is cost-competitive if and only if:

\[
\lambda \cdot X_e \cdot P_e + (1 - \lambda) \cdot X_f \cdot P_f > LCOP
\]

(12)

The \( LCOP \) formulation in (11) shows that the levelized cost of a static PES can be expressed as the sum of the levelized cost of its operational subsystems weighted by their respective production coefficients. While the levelized costs of individual subsystems can be calculated using multiple units, (e.g. \$/kWh for \( LIC_e \)), the conversion rates \( X_e, X_a \), and \( X_f \) ensure that the overall PES cost is expressed as a monetary value per unit of hydrogen. Clearly, this approach facilitates comparing the cost of different polygeneration systems with different configurations, all of which produce hydrogen as an intermediate product.

Furthermore, while (6) shows that the revenue from monogeneration is dictated by only one price, Proposition 1 in (12) shows that the revenue from polygeneration is determined by a sum of end-product prices weighted by their respective production coefficients. Consequently, for a fixed operation mode and thus fixed set of production coefficients, multiple combinations of end-product prices may achieve break-even. In imperfectly competitive markets, the PES firm can negotiate multiple portfolios of end-product prices with potential buyers. For instance, the firm may sell electricity at a competitive market price while having pricing power in selling fertilizers due to constrained regional supply.

Alternatively, in perfectly competitive markets with preset prices, break-even may be achieved by adjusting production coefficients on both sides of (12) because \( \lambda \) is a controllable design parameter. In short, a polygeneration facility can break even via multiple portfolios of end-product prices and production capacities.

### 3.2. Scenario 2: Flexible PES with variable production rates

For a PES in flexible mode, both electricity and ammonia generation rates can vary on an hourly basis; decreasing the power output results in increasing the ammonia output, and vice versa. While a constant hydrogen generation capacity \( N_h \) is maintained, the fraction of hydrogen converted to electricity and ammonia may vary with time. We use the notation \( \lambda(t) \) in Fig. 2 to highlight this fact. Still, due to flexibility constraints, the condition that \( \lambda_{\text{min}} < \lambda(t) < \lambda_{\text{max}} \) remains in place. When \( \lambda(t) = \lambda_{\text{max}} \), electricity production is maximized while fertilizer production is minimized. Conversely, when \( \lambda(t) = \lambda_{\text{min}} \), electricity production is minimized while fertilizer production is maximized.

The flexible PES is analyzed sequentially in Scenarios 2a and 2b below. Scenario 2a makes the simplifying assumption that the fertilizer subsystem can run flexibly, so the variable fertilizer output is perfectly synchronized with the variable ammonia output. In Scenario 2b, we acknowledge the real-world need for a static fertilizer subsystem. In other words, Scenario 2a presents a hypothetical operational configuration that aims to benchmark the performance of the more realistic Scenario 2b. Comparing these two scenarios provides insight into the role of technical constraints in controlling the economic value of flexible polygeneration.

#### 3.2.1. Scenario 2a: Flexible PES with a flexible fertilizer subsystem

As illustrated in Fig. 2, a variable fertilizer output results from the direct conversion of the variable ammonia output at each time interval \( t \), so no intermediate ammonia storage is needed in this case. Nonetheless, to accommodate the maximum possible flowrates, the production capacity of the flexible units should be set at \( \lambda_{\text{max}} \cdot X_e \) (kW) for electricity, \((1 - \lambda_{\text{min}}) \cdot X_a \) (kg$_\text{ammonia}$/h) for ammonia, and \((1 - \lambda_{\text{min}}) \cdot X_f \) (kg$_\text{fertilizer}$/h) for fertilizer.\(^3\) Similar to Scenario 1, the incurred capacity and fixed operating costs are scaled by these constant production capacities, independent of the variable production rates.

Since both capacity and fixed operating costs are constant in a given year \( i \), maximizing the profitability of the flexible PES requires maximizing the ‘contribution margin’ of hydrogen conversion at every point in time \( t \) of that year.\(^4\) Definition 3 introduces \( CM_e \) (\$/kg$_\text{hydrogen}$) and \( CM_f \) (\$/kg$_\text{fertilizer}$) as the contribution margins associated with converting one kilogram of hydrogen to \( X_e \) kilowatt hours of electricity and \( X_f \) kilograms of fertilizer, respectively.

**Definition 3.**

\[
CM_e(t) = [X_e \cdot P_e(t) - X_e \cdot w_e(t)]
\]

(13)

\[
CM_f(t) = [X_f \cdot P_f(t) - X_f \cdot w_f(t) - X_a \cdot w_a(t)]
\]

(14)

\(^3\) Our analysis speaks to the cost competitiveness of a flexible PES whose capacity is chosen to accommodate the maximum possible flowrate of ammonia. In future work, it would be desirable to explore under what conditions a flexible PES, accommodating a lower flowrate but requiring correspondingly smaller capacity investments, could be more economical.

\(^4\) Contribution margin refers to the difference between sales and variable costs. The analysis in Reichelstein and Sahoo [45] explains a related idea on quantifying the temporal co-variation between prices and generation capacity of an intermittent power source.
When $C_{Me}(t) > C_{Mf}(t)$, electricity production should be maximized and fertilizer production should be minimized; the opposite must hold when $C_{Me}(t) < C_{Mf}(t)$. Accordingly, we divide the yearly hours $m$ into $m_\alpha$ and $m_\beta$, introduced in Definition 4. $m_\alpha$ corresponds to the number of hours in year $i$ when $C_{Me}(t) > C_{Mf}(t)$ whereas $m_\beta$ corresponds to the number of hours when $C_{Me}(t) < C_{Mf}(t)$.\footnote{in (15) and (16) is the Lebesgue Measure over the set of real numbers between and [46].} Clearly, $m = m_\alpha + m_\beta$ for every year $i$.

**Definition 4.**

$$m_\alpha = \mu([m_\alpha]) = \mu\left(\{ t | 0 \leq t \leq m, C_{Me}(t) > C_{Mf}(t) \}\right)$$

$$m_\beta = \mu([m_\beta]) = \mu\left(\{ t | 0 \leq t \leq m, C_{Me}(t) < C_{Mf}(t) \}\right)$$

Flexibility enables choosing the highest contribution margin in every time period. Thus, we define the difference between $C_{Me}(t)$ and $C_{Mf}(t)$ as the ‘incremental contribution margin of flexibility’ (ICMF). In a given year $i$, ICMFe is the yearly-averaged sum of flexibility-enabled contribution margin over $m_\alpha$ hours, attributed to switching hydrogen allocation from fertilizer to electricity. Equivalently, ICMFe is the yearly-averaged sum of flexibility-enabled contribution margin over $m_\beta$ hours, attributed to switching hydrogen allocation from electricity to fertilizer. ICMFe ($$/kg_a$$) and ICMFf ($$/kg_a$$) are introduced in Definition 5. By design, both terms are always positive.

**Definition 5.**

$$ICMFe = \frac{1}{m} \int_{m_\alpha} [C_{Me}(t) - C_{Mf}(t)] dt$$

$$ICMFi = \frac{1}{m} \int_{m_\beta} [C_{Mf}(t) - C_{Me}(t)] dt$$

The formulation of ICMF illustrates the beneficial impacts of price volatility on the economics of flexible PES. Consistent with the earlier assumption that only electricity price $P_e(t)$ changes over time, the effect of higher volatility in $P_a(t)$ is captured in two ways: higher $P_e(t)$ leads to higher $C_{Me}(t)$ during $m_\alpha$ hours and therefore higher ICMFe, and lower $P_a(t)$ leads to lower $C_{Mf}(t)$ during $m_\beta$ hours and therefore higher ICMFi. In short, the higher the price volatility (around the same price average), the higher the incremental contribution margin of flexibility.

Similar to the time-averaged variable cost in (6), the time-averaged incremental contribution margins of flexibility ICMFe ($$/kg_a$$) and ICMFi ($$/kg_a$$) are derived from ICMFe and ICMFi in (19) and (20), respectively.

$$ICMFe = \sum_{i} \frac{ICMFe_i \cdot X_a \cdot y_i^d}{\sum_{i} X_i \cdot y_i^d}$$

$$ICMFi = \sum_{i} \frac{ICMFi_i \cdot X_i \cdot y_i^d}{\sum_{i} X_i \cdot y_i^d}$$

As a result, we can now assess the economic feasibility of the flexible PES in this simplified scenario by formulating two mathematically equivalent statements of Proposition 2a.

**Proposition 2a.** A flexible PES is cost-competitive if and only if:

$$|X_f \cdot [P_f - X_f \cdot LIC_f - X_a \cdot LIC_a] + (1 - \lambda_{max}) \cdot [ICMF_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a)] - (1 - \lambda_{min}) \cdot [ICMF_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a)] > LCOH$$

Equivalently, the flexible PES is cost-competitive if and only if:

$$X_a \cdot [P_e - LIC_e] + (1 - \lambda_{max}) \cdot [ICMF_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a)] - (1 - \lambda_{min}) \cdot [ICMF_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a)] > LCOH$$

As proven in Appendix A, the left-hand sides in (21) and (22) are identical. The formulation in (21) benchmarks flexible polygeneration against static fertilizer monogeneration. Specifically, the net revenue from hydrogen conversion is divided into three terms. As in Scenario 1, the first term $[X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a]$ corresponds to the net revenue from the static monogeneration of fertilizer. The second and third terms correspond to the additional net revenues from flexibility. $\lambda_{max}[ICMF_f - X_a \cdot (c_a + j_a)]$ represents the net revenue associated with flexible switching from fertilizer to electricity; the flexibility-enabled incremental contribution margin is weighed against the flexibility-required capacity and fixed operating costs of generating electricity. This ‘gained’ net revenue is scaled by $\lambda_{max}$, the maximum fraction of hydrogen capacity allocated to electricity. On the other hand, electricity generation cannot drop below a lower limit defined by $\lambda_{min}$, so the corresponding net revenue associated with flexible switching from electricity to fertilizer is ‘lost’. This net revenue is captured in $\lambda_{min} \cdot [ICMF_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a)]$, which balances the flexibility-enabled incremental contribution margin against the flexibility-required capacity and fixed operating costs of generating ammonia then fertilizer.

The formulation in (22) has a similar and symmetric structure to (21), but it benchmarks the economics of the flexible polygeneration against static electricity monogeneration. In this case, the ‘gained’ and ‘lost’ net-revenue terms associated with flexibility are scaled by $(1 - \lambda_{min})$ and $(1 - \lambda_{max})$, corresponding to the maximum and minimum fractions of hydrogen that can be converted to fertilizer, respectively.

In both (21) and (22), the ‘gained’ and ‘lost’ net-revenue terms associated with flexibility are positive only when the incremental contribution margin surpasses the capacity and fixed operating costs. Thus, Proposition 2a shows that adding flexibility to a PES may not result in superior economic value; the latter depends on the specifications of the investigated facility. We analyze this dependency in more detail in Section 4. Also, (21) and (22) show that maximizing the revenue of flexible polygeneration requires exploiting the ability to vary $X(t)$ between $\lambda_{min}$ and $\lambda_{max}$; setting $\lambda_{min} = 0$ and $\lambda_{max} = 1$ reduces Proposition 2a to Proposition 1.
maximized during $m_f$ hours. Equating the yearly variable output from the ammonia subsystem to the yearly fixed input into the ferti-
lizer subsystem results in $K = [m_x \cdot (1 - \lambda_{\text{max}}) + m_f \cdot (1 - \lambda_{\text{min}})] / m$.

$$[m_x \cdot (1 - \lambda_{\text{max}}) + m_f \cdot (1 - \lambda_{\text{min}})] \cdot X_f = m \cdot K \cdot X_f \quad (23)$$

With these modifications, we can now assess the economic feasibil-
ity of flexible polygeneration in this scenario by deriving two equiv-
lalent statements of the new Proposition 2b.

**Proposition 2b.** A flexible PES is cost-competitive if and only if:

$$[X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a] + \lambda_{\text{max}} \cdot [ICMF \cdot X_a - X_a \cdot (c_a + j_a)]$$

$$- \lambda_{\text{min}} \cdot [ICMF \cdot X_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a)]$$

$$+ [(1 - \lambda_{\text{min}} - K) \cdot X_f \cdot (c_f + j_f)] > LCOH \quad (24)$$

Equivalently, the flexible PES is cost-competitive if and only if:

$$X_e \cdot (P_e - LIC_e) + (1 - \lambda) \cdot [X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a]$$

$$- \lambda_{\text{max}} \cdot [ICMF \cdot X_f - X_f \cdot (c_f + j_f)]$$

$$+ [(1 - \lambda_{\text{min}} - K) \cdot X_f \cdot (c_f + j_f)] > LCOH \quad (25)$$

A detailed derivation of (24) and (25) is presented in Appendix A. The formulations in (24) and (25) are identical to those in (21) and (22) for Scenario 2a, except for two differences. First, to account for storage, the levelized-cost terms of ammonia, $c_a$, $j_a$, and $w_a$ are updated to $c_a$, $j_a$, and $w_a$, respectively; other metrics incorporating these terms are also updated accordingly. Second, reducing the fertilizer capacity from $1 - \lambda_{\text{min}}$ in Scenario 2a to $K$ in Scenario 2b results in a net-revenue ‘gain’ of

$$[(1 - \lambda_{\text{min}} - K) \cdot X_f \cdot (c_f + j_f)],$$

which accounts for savings in capacity and fixed operating costs. All other economic expressions introduced in Scenario 2a remain valid here. Notably, the flexible PES still captures the full economic benefits of flexibility even though the fertilizer subsystem is static. Because storage allows all generated ammonia to be eventually converted to fertilizer, flexible ammonia generation is sufficient to sustain the economic benefits of flexible fertilizer generation.

$$1 - \lambda_{\text{min}} - K = \frac{m_x \cdot (\lambda_{\text{max}} - \lambda_{\text{min}})}{m} \quad (26)$$

Using (23) to expand the formulation of $K$, we find that

$$(1 - \lambda_{\text{min}} - K)$$

is directly proportional to $m_t$, as shown in (26). A larger $m_t$ means that the flexible PES spends more time maximizing electricity generation on the expense of fertilizer generation. In this case, a smaller static fertilizer subsystem with intermediate ammonia storage (Scenario 2b) may achieve better economics than a larger flexible fertilizer subsystem with no storage (Scenario 2a), even if the latter is technically feasible.

### 4. Profitability and real-option values

Our findings in Scenarios 1 and 2 show that different operation modes result in different economic values for PES. Compared to a static single-output plant, a polygeneration plant offers ‘the option’ of diversifying the static output (Scenario 1) as well as ‘the option’ of substituting part of the static output capacity with flexible capacity (Scenario 2). To quantify the value of these ‘real options’, we first need to characterize the ‘profitability’ of PES. The overall net present value (NPV) associated with investing in the capacity to deliver one kilogram of hydrogen per hour ($N_h = 1$) is given in (27). $PM$ is the ‘profit-margin’, which denotes the difference between the net revenue for one kilogram of hydrogen and its levelized cost. We use $PM$ as a profitability metric to assess and compare PES under different operation modes.

$$\text{NPV}(\$$) = $PM \cdot m \cdot CF \cdot \sum_{i=1}^{r} X_i \quad (27)$$

$PM_0$ measures the unit profit-margin of a static single-output plant. $PM_{of}(\$$/kg$_f$) refers to the profit-margin of a static plant that converts all hydrogen to ammonia and then fertilizer ($\lambda = 0$). Similarly, $PM_{of}(\$$/kg_a)$ refers to the profit-margin of a static power plant that converts all hydrogen to electricity ($\lambda = 1$). $PM_{of}$ and $PM_{ow}$ are formally defined in (28) and (29), respectively.

$$PM_{of} = X_f \cdot P_f - X_f \cdot LIC_f - X_f \cdot LIC_a - LCOH \quad (28)$$

$$PM_{ow} = X_e \cdot P_e - X_e \cdot LIC_e - LCOH \quad (29)$$

Let $PM_1(\$$/kg$_f$) denote the unit profit-margin of the static PES in Scenario 1, which can be directly deduced from Proposition 1. $PM_1$ is derived in (30) by re-arranging the terms in (10).

$$PM_1 = \lambda \cdot X_e \cdot (P_e - LIC_e) + (1 - \lambda) \cdot (X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a) - LCOH \quad (30)$$

Similarly, $PM_2(\$$/kg$_f$)$ refers to the unit profit-margin of the flexible PES in Scenario 2, which is obtained directly from Proposition 2b. $PM_2$ can be expressed in two forms, $PM_{2f}(\$$/kg$_f$)$ and $PM_{2e}(\$$/kg$_f$)$, presented in (31) and (32), respectively. $PM_{2f}$ is derived from (24) where the economic value of a flexible PES is benchmarked against that of a static fertilizer plant, and $PM_{2e}$ is derived from (25) where the economic value of a flexible PES is benchmarked against that of a static power plant. Importantly, we note that $PM_{2e} = PM_{2f}$.

$$PM_{2f} = [X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a] + \lambda_{\text{max}} \cdot [ICMF \cdot X_a - X_a \cdot (c_a + j_a)]$$

$$- \lambda_{\text{min}} \cdot [ICMF \cdot X_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a)]$$

$$+ [(1 - \lambda_{\text{min}} - K) \cdot X_f \cdot (c_f + j_f)] - LCOH \quad (31)$$

$$PM_{2e} = X_e \cdot (P_e - LIC_e) + (1 - \lambda) \cdot [X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a] - \lambda_{\text{max}} \cdot [ICMF \cdot X_f - X_f \cdot (c_f + j_f)]$$

$$+ [(1 - \lambda_{\text{min}} - K) \cdot X_f \cdot (c_f + j_f)] - LCOH \quad (32)$$

These profitability metrics can be directly used to quantify the value of real options enabled by polygeneration. We first define $VOD$ as the ‘value of diversification’ from a single output to a portfolio of multiple outputs. $VOD_i(\$$/kg$_{of}$)$ is the difference between the profit-margin of static polygeneration $PM_i$ and that of static monogeneration of fertilizer $PM_{of};$ similarly, $VOD_e(\$$/kg$_{of}$)$ is the difference between $PM_1$ and $PM_{ow}$. Clearly, both $VOD_i$ and $VOD_e$ are dependent on $\lambda$, as shown in (33) and (34), respectively.

$$VOD_i(\lambda) = PM_i(\lambda) - PM_{of} \quad (33)$$

$$VOD_e(\lambda) = PM_i(\lambda) - PM_{ow} \quad (34)$$

$PM_i$ is between $PM_{of}$ and $PM_{ow}$, so the value of diversification need not be always positive. In our model, $VOD_i(\lambda > 0)$ implies that $VOD_i(\lambda < 0)$, and vice versa. Thus, in practice, when comparing alternative investments of the same hydrogen capacity, one might prioritize investing in the most profitable single-output system. However, market or regulatory constraints (e.g. market saturation or emissions regulation) may make such investment infeasible, in which case polygeneration becomes the second-best option.

We then define the ‘value of flexibility’ $VOF(\$$/kg$_{of}$)$ associated with varying power and ammonia production rates with time. $VOF$ is the difference between the profit-margin of flexible polygeneration $PM_{2f}$ and that of static polygeneration $PM_1$, and it is
dependent on $\lambda$, as highlighted in (35). This formulation shows that flexible polygeneration is more profitable than static polygeneration only if $VOP(\lambda) > 0$. There might exist some value of $\lambda$ for which a static PES could outperform a flexible PES, in which case $VOP(\lambda)$ is negative.

$$VOP(\lambda) = PM_f - PM_s(\lambda) = PM_{a2} - PM_{t}(\lambda)$$

(35)

Overall, we define the value of polygeneration $VOP$ ($$/kg CO_2$$) as the sum of the real-option values associated with both diversification and flexibility. As shown in (36) and (37), one VOP metric is needed for each end-product; $VOP_f$ ($$/kg CO_2$$) compares the profit-margin of a flexible PES to that of a static fertilizer plant, and $VOP_e$ ($$/kg CO_2$$) compares the profit-margin of a flexible PES to that of a static power plant.

$$VOP_f = VOP(\lambda) + VOP_f(\lambda) = PM_f - PM_{f}$$

(36)

$$VOP_e = VOP(\lambda) + VOP_e(\lambda) = PM_{a2} - PM_{a2}$$

(37)

When $VOP_f > 0$, flexible polygeneration is more profitable than static fertilizer monogeneration. Similarly, when $VOP_e > 0$, flexible polygeneration is more profitable than static power monogeneration. However, we showed in (33) and (34) that static polygeneration is less profitable than the static monogeneration of at least one end-product. Accordingly, when both $VOP_f$ and $VOP_e$ are positive, flexible polygeneration is more profitable than both static monogeneration and static polygeneration. In that regard, while $VOP(\lambda)$ identifies the condition for a flexible PES to be more profitable than a specific static PES with a specific $\lambda$, $VOP$ identifies the condition for a flexible PES to be more profitable than any static PES with any $\lambda$.

5. Additional modeling considerations

5.1. Carbon capture and storage

The proposed economic assessment of PES can be robustly expanded to account for technical supplements such as carbon capture and storage (CCS). The net CO2 output, defined as the gross CO2 production less the CO2 used for fertilizer synthesis, may be compressed then transported in pipelines to be either geologically sequestered or used for enhanced oil recovery [23]. Since CO2 is produced by a steady-state process (gasification) and partially utilized by another steady-state process (fertilizer synthesis), its net output is a fixed flow, regardless of whether the PES is static or flexible.

CCS is treated as a separate subsystem of production capacity $U_t \cdot N_{cc}$ (kg/h), where $U_t$ (kg/kg CO2) denotes the net CO2 output rate per one kilogram of produced hydrogen. As before, $LIC_e$ refers to the sum of $c_i$, $l_i$, and $w_i$, which correspond to the cost of capacity, time-averaged fixed operating cost, and time-averaged variable cost of CCS per unit of CO2 ($$/kg CO_2$$), respectively. Also, if sold for enhanced oil recovery, the CO2 output generates revenue proportional to its price $P_t$ ($$/kg CO_2$$). As such, Propositions 1 and 2b can be revised to incorporate CCS in a static and a flexible PES, as shown in (38) and (39), respectively. All other economic metrics and propositions can be updated accordingly.

**Proposition 1.** A static PES with CCS is cost-competitive if and only if:

$$\lambda \cdot X_e \cdot (P_e - LIC_e) + (1 - \lambda) \cdot (X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a) + U_t \cdot (P_t - LIC_e) > LCOH$$

(38)

**Proposition 2b.** A flexible PES with CCS is cost-competitive if and only if:

$$\left[ X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a \right] + \lambda_{\max} \cdot \left[ CMF_e - X_e \cdot (c_e + j_e) \right] - \lambda_{\min} \cdot \left[ CMF_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a) \right] + \left[ 1 - \lambda_{\min} - K \right] \cdot X_f \cdot (c_f + j_f) + U_t \cdot (P_t - LIC_e) > LCOH$$

(39)

5.2. Time-dependency of prices and variable costs

So far, we have assumed that, except for the price of electricity, all prices and variable costs are fixed within a given year. If this assumption is not met, the aforementioned analysis will still generate the same exact results in Scenario 1 and Scenario 2a, but slightly modified results in Scenario 2b where fertilizer production is fixed. In this particular case, ‘correction’ terms should be added to the formulations of Proposition 2b to account for the different averaging of the fertilizer contribution margin $CM_{f}(t)$ over different time periods. Specifically, (40) and (41) introduce the two correction terms $\Phi_f ($/kg CO2$)$ and $\Phi_e ($/kg CO2$)$ in year $i$.

$$\Phi_f = \frac{1}{m} \frac{1}{m} \int_0^m \left[ CM_f(t) \right] d(t) - \int_0^m \left[ CM_f(t) \right] d(t)$$

(40)

$$\Phi_e = \frac{1}{m} \frac{1}{m} \int_0^m \left[ CM_e(t) \right] d(t) - \int_0^m \left[ CM_e(t) \right] d(t)$$

(41)

If all prices and variable costs are allowed to vary with time, Proposition 2b can be easily revised to incorporate $\Phi_f$ and $\Phi_e$, as illustrated in (42).

**Proposition 2b.** A flexible PES is cost-competitive if and only if:

$$\left[ X_f \cdot P_f - X_f \cdot LIC_f - X_a \cdot LIC_a \right] + \lambda_{\max} \cdot \left[ CMF_e - X_e \cdot (c_e + j_e) \right] - \lambda_{\min} \cdot \left[ CMF_f - X_f \cdot (c_f + j_f) - X_a \cdot (c_a + j_a) \right] + \left[ 1 - \lambda_{\min} - K \right] \cdot X_f \cdot (c_f + j_f) + \left[ \lambda_{\max} \cdot \Phi_f + \lambda_{\min} \cdot \Phi_e \right] > LCOH$$

(42)

6. Case study: Hydrogen Energy California

To demonstrate the usefulness of our model analysis in the previous sections, we now assess the economic performance of Hydrogen Energy California (HECA), a polygeneration facility currently under development in California.

6.1. Technical configuration

Consistent with the technical configuration presented in Section 2.2, HECA uses a gasification technology to convert coal and petcoke into clean-burning hydrogen. As an intermediate product, hydrogen is then converted to electricity and ammonia, which is further processed into urea and UAN – a solution of urea and ammonium nitrate [31,32]. The operational configuration of HECA allows flexible generation of electricity and ammonia, but it requires static generation of hydrogen, urea, and UAN; the facility also includes a CO2 compression unit, which can be treated as a separate static CCS subsystem.

The first task is to quantify all technical parameters needed for the economic evaluation. A list of HECA’s technical parameters and their values is provided in Table 1. With a capacity factor of $CF = 0.835$ and an expected operational lifetime of 25 years, the facility consumes coal and petcoke at rates equal to roughly...
4,209 tonne/day and 1,053 tonne/day, respectively [33]. The syngas generated from the gasification of coal and petcoke undergoes shift-reaction to convert most of the carbon monoxide into carbon dioxide, 90% of which is captured. A fraction of the captured CO₂, corresponding to \( U = 12.1 \text{ kg}_\text{CO}_2/\text{kg}_\text{O}_2 \), is compressed and sold to nearby oil fields for enhanced oil recovery.

Produced at a fixed flowrate of \( N_y = 28.748 \text{ kg}_\text{g}/\text{h} \), hydrogen is converted to electricity and ammonia at rates equal to \( X_e = 19.66 \text{ kWh/kg}_\text{H}_2 \) and \( X_a = 5.63 \text{ kg}_\text{NH}_3/\text{kg}_\text{H}_2 \), respectively. On a daily basis, the facility operates under two modes: “electricity peak” mode from 7 a.m. to 11 p.m., followed by “electricity off-peak” mode for the rest of the time. During “peak” hours of electricity demand, the plant runs at maximum power and minimum ammonia generation capacities, corresponding to \( \lambda_{\text{max}} = 0.717 \). Alternatively, during “off-peak” hours, the plant runs at minimum power and maximum ammonia generation capacities, corresponding to \( \lambda_{\text{min}} = 0.521 \) [26]. Summing over one year, this results in \( m_e = 5840 \text{ h} \) and \( m_f = 2920 \text{ h} \). Importantly, \( m_e \) and \( m_f \) are ‘exogenously imposed’ in this case instead of being ‘endogenously optimized’ through (15) and (16). This regime will have significant impacts on the economic value of the facility, as we explain in the next section.

Table 2 outlines the auxiliary load requirements for the system under each operation mode [34]. As shown, both operation modes consume 247–248 MW of the gross power output, which is less than \( \lambda_{\text{min}} \cdot X_e \cdot N_y = 295 \text{ MW} \). In reality, HECA continues to generate a positive net power output to the grid even under the “off-peak” mode [34].

<table>
<thead>
<tr>
<th>System/unit</th>
<th>Peak mode</th>
<th>Off-peak mode</th>
<th>Unit</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen subsystem</td>
<td>170</td>
<td>164</td>
<td>MW</td>
<td>[34]</td>
</tr>
<tr>
<td>Electricity subsystem</td>
<td>12</td>
<td>12</td>
<td>MW</td>
<td>[34]</td>
</tr>
<tr>
<td>Ammonia subsystem</td>
<td>10</td>
<td>17</td>
<td>MW</td>
<td>[Estimated]</td>
</tr>
<tr>
<td>Urea + UAN subsystem</td>
<td>15</td>
<td>15</td>
<td>MW</td>
<td>[Estimated]</td>
</tr>
<tr>
<td>CO₂ subsystem</td>
<td>40</td>
<td>40</td>
<td>MW</td>
<td>[34]</td>
</tr>
<tr>
<td>Total</td>
<td>247</td>
<td>248</td>
<td>MW</td>
<td>[34]</td>
</tr>
</tbody>
</table>

The produced ammonia reacts with a fraction of the captured CO₂ to synthesize urea, part of which is then further processed with more ammonia to produce UAN. Because hydrogen is effectively processed into two fertilizer end-products, every unit of hydrogen allocated to fertilizer synthesis is split into two fractions: \( y_{\text{urea}} = 0.532 \) for urea and \( y_{\text{UAN}} = 0.468 \) for UAN. We then define \( X_{\text{urea}} = 9.93 \text{ kg}_\text{urea}/\text{kg}_\text{H}_2 \) and \( X_{\text{UAN}} = 13.72 \text{ kg}_\text{UAN}/\text{kg}_\text{H}_2 \), as the conversion rates of hydrogen to urea and UAN, respectively. Finally, to buffer the variable ammonia output and secure a constant input for urea and UAN synthesis, ammonia storage is needed. The storage capacity is \( S_\text{a} = 9,474,036 \text{ kg}_\text{a} \), equivalent to 7 days of full loading at a rate of \( K \cdot X_a \cdot N_y = 56,393 \text{ kg}_\text{a}/\text{h} \) [35].

6.2. Economic analysis

6.2.1. Cost and revenue

The cost figures for the hydrogen, electricity, and CCS subsystems are based on a study by the International Energy Agency that analyzes the economics of coal gasification for co-production of electricity and hydrogen [36]. The cost of CCS in this case covers CO₂ transportation and sequestration. In addition, the costs associated with ammonia production, ammonia storage, urea production, and UAN production, are based on studies by Bartels [37], Leigh [38] and Morgan [39], Lennon [40], and Damas [41], respectively. Furthermore, because the urea and UAN units are static, we combine them into one ‘fertilizer’ subsystem. This approach allows us to directly use the economic metrics derived in Sections 3 and 4.

For convenience, the costs of this joint fertilizer subsystem are expressed per unit of produced urea, so the definition of \( X_f \) and \( \text{LIC}_f (\$/\text{kg}_\text{urea}) \) should be updated according to (43) and (44), respectively. All monetary figures are adjusted to 2012 U.S. dollars, assuming a 1.33 conversion factor from Euro to U.S. dollar when needed. Finally, as mentioned in Section 2.1, taxes are not accounted for in this analysis.

\[
X_f = y_{\text{urea}} \cdot X_{\text{urea}}
\]

\[
\text{LIC}_f = \frac{y_{\text{urea}} \cdot X_{\text{urea}} \cdot \text{LIC}_{\text{urea}} + y_{\text{UAN}} \cdot X_{\text{UAN}} \cdot \text{LIC}_{\text{UAN}}}{X_f}
\]

The levelized capacity, fixed operating, and variable costs are presented in Tables 3–5, respectively; a more detailed breakdown of the cost figures is provided in Appendix B. We assume a constant...
annual discount rate of τ = 0.07 and no degradation in productivity over the years (x = 1) for all cost figures.

Table 3 lists the levelized costs of capacity for the five major subsystems of HECA. Since the size of HECA is comparable to that of the facilities analyzed in the referenced literature, linear scaling factors are used to calculate the capacity cost of each subsystem. Also, we recall that cxs and cys correspond to the capacity costs of the ammonia subsystem with and without intermediate storage, respectively.

The yearly fixed operating costs are calculated as a constant fraction of the overall capacity cost (refer to Appendix B), and they remain unchanged every year throughout the lifetime of the project. Accordingly, the levelized time-averaged fixed operating costs of HECA’s subsystems are listed in Table 4.

The variable cost for the hydrogen subsystem incorporates the costs of coal and petcoke as fuel, Selexol™, flux, catalysts, other chemicals, waste-water treatment, and the unit’s auxiliary load. For all other subsystems, the auxiliary loads are assumed to be the only variable costs. The prices of all physical commodities are fixed with time, assuming they are purchased through long-term contracts (refer to Appendix B). However, we assume that HECA’s net power output is sold in the wholesale market, and the cost of auxiliary power equals the price of sold power. Hence, the yearly costs of the auxiliary loads in Table 2 are obtained by summing up the hourly costs, which are calculated using variable electricity prices. To simulate a real-life performance, we use the 2012 wholesale one-day-ahead electricity prices from the SP26 pricing hub, which covers the Southern California region where HECA plans to operate [29]. The yearly price data, plotted in Fig. 3, is assumed to be replicated every year throughout the facility's lifetime. Under these assumptions, the time-averaged variable cost equals the yearly-averaged variable cost for each subsystem, and those costs are presented in Table 5. Finally, important to note, the variable cost of ammonia storage is assumed to be negligible, resulting in Wvm = Wxs.

The last important set of economic data is the prices of end-products, which account for HECA’s revenues. The revenues from both fertilizers, urea and UAN, are combined in $P$ (kg/urea). This price of fertilizers’ term, expressed per unit of produced urea, is derived in (45) using a similar formulation to that of LICf in (43). In addition to fertilizers, Table 6 shows the time-averaged prices of electricity and CO2 sales. More detailed price figures are provided in Appendix B.

6.2.2. Economic value

The aforementioned data allows us to calculate the derived metrics in Sections 3 and 4 and therefore to assess the economic value of HECA under several operation modes. The results are presented in Table 7.

The levelized cost of hydrogen production is estimated at $LCOH = 1.373 \$/kg$. This cost can be combined with the cost of the electricity and CCS subsystems to calculate an LCOE for HECA, as illustrated in (46). Notably, the obtained $LCOE = 0.0953 \$/kWh$ is comparable to that of coal power plants with CO2 capture, currently estimated at about 0.089–0.139 \$/kWh [42–44].

$$LCOE = LCOH/X_0 + LIC_0 + U_0 \cdot LIC_0/X_0$$  \tag{46}$$

To calculate HECA’s unit profit-margin, we use the profitability metrics from Section 4, with a few updates. Starting with the static mode of operation, PMf, PMo, and PM1 are updated in accordance with (38) in Section 5.1 to account for the CCS subsystem. With $PM_f = 1.934 \$/kg$, HECA is obviously profitable if run as a static fertilizer-only plant. However, the facility would not break even if

\begin{table}[h]
\centering
\caption{Yearly wholesale prices of electricity in HECA’s region [29].}
\begin{tabular}{lll}
\hline
\textbf{Price} & \textbf{Value} & \textbf{Unit} \\
\hline
$P_e$ & 0.0295 & $/kWh$
\end{tabular}
\end{table}
run as a static power-only plant, with \( PM_{0e} = -0.992 \ $/kg_{so} \). The profit-margin of the static polygeneration mode \( PM_1 \) is between \( PM_{0e} \) and \( PM_{0f} \); the exact value of \( PM_1 \) changes with the hydrogen allocation fraction \( \lambda \), as illustrated in Fig. 4. Under assumed prices and costs, a static HECA breaks even around \( \lambda = 0.66 \). Confirming our argument in Section 4, the value of diversification is not always positive. In this case, diversifying away from power monogeneration increases profitability, evident by the positive \( VOD_1 \). Conversely, diversifying away from fertilizer monogeneration severely reduces profitability, evident by the negative \( VOD_1 \).

Ultimately, increasing electricity generation reduces both profitability and the associated values of diversification, as illustrated in Fig. 4.

Shifting to the flexible polygeneration mode, \( PM_{2e} \) and \( PM_{2f} \) are updated per Sections 5.1 and 5.2 to account for the CCS subsystem and the correction factors for the time-dependent variable costs, respectively. \( \Phi_2 \) and \( \Phi_f \) in Table 7 correct for the fact that the variable costs change on an hourly basis due to HECA subsystems' need for auxiliary power. In addition, although \( m_e \) and \( m_f \) are exogenously imposed rather than endogenously optimized through (15) and (16), the incremental flexibility contribution margins \( ICMF_e \) and \( ICMF_f \) are calculated by following their definitions in (19) and (20). Referring to Table 7, \( ICMF_f \) is clearly positive because the contribution margin from fertilizers exceeds that from electricity during \( m_f \) hours. However, \( ICMF_e \) is negative, contrary to our assertion in Section 3.2 that it should also be positive. Caused by the exogeneity of \( m_e \) and \( m_f \), this result essentially means that urea and UAN generate higher revenue than electricity even during \( m_e \) hours when electricity prices are highest. Therefore, flexible power generation may seem like a poor line of business.

However, flexibility enables a two-way substitution, so a flexible electricity capacity requires an equivalent flexible fertilizer capacity. For HECA, while a flexible power capacity may not be beneficial because electricity prices are relatively low, flexible fertilizer capacity is indeed beneficial for the exact same reason. This is better understood by looking at \( PM_2 \) and the corresponding \( VOF \). The profit-margin of a flexible HECA is \( PM_{2e} = PM_{2f} = -0.0439 \ $/kg_{so} \), so the facility almost breaks even. As shown in Fig. 4, a flexible HECA can be less or more profitable than a static HECA, depending on the exact value of \( \lambda \) for the latter. For a small \( \lambda \), the static HECA is dominated by fertilizer generation, so adding flexibility leads to switching from high-price fertilizers to low-price electricity during the exogenously imposed \( m_e \). In this case, flexibility is not useful, and \( PM_2 \) is lower than \( PM_1 \), evident by the negative \( VOF \). Conversely, when \( \lambda \) is large, the static mode of HECA is dominated by electricity generation, so adding flexibility leads to switching from low-price electricity to high-price fertilizers during \( m_f \). In this case, flexibility is useful, and \( PM_2 \) is higher than \( PM_1 \), evident by the positive \( VOF \).

Ultimately, \( VOF \) converges to \( VOP \) at either extreme value of \( \lambda \). When \( \lambda = 0 \), \( VOF \) is at its minimum value and equal to \( VOP_1 \). Conversely, when \( \lambda = 1 \), \( VOF \) is at its maximum value and equal to \( VOP_f \). We conclude that HECA benefits from flexible polygeneration if the company's other feasible alternative is investing in a static power-only plant, but it does not benefit from flexible polygeneration if the other feasible alternative is investing in a static fertilizer-only plant.

For completeness, we briefly analyze HECA's performance under a hypothetical optimal operational schedule, where \( m_e \) and \( m_f \) are obtained endogenously. Under assumed prices and costs, we find that \( m_e = 0 \) and \( m_f = m \), suggesting – as expected – that the facility should run as a static fertilizer-only plant. Increasing electricity prices, nonetheless, leads to a different conclusion, as illustrated in Fig. 5. First, we proportionally increase all prices of electricity depicted in Fig. 3, which increases the average price \( P_e \), while preserving the relative volatility. As electricity prices increase, \( m_e \) increases, signifying the economic favorability of installing flexible capacity and switching to electricity generation. When \( P_e \) is 550–574% times its current value, both \( VOP_1 \) and \( VOP_f \) are positive; in this case, flexible polygeneration becomes the most profitable alternative for HECA, better than all static polygeneration or monogeneration alternatives.

### 6.2.3 Sensitivity analysis

Since HECA is a first-of-a-kind facility, it seems particularly important to check the sensitivity of our results. Specifically, we analyze the sensitivity of HECA’s profitability to the following variables: price of fertilizers, price of electricity, price of CO₂, and discount rate. Fig. 6 shows that the unit profit-margin of a flexible HECA \( PM_2 \) is highly sensitive to both the fertilizers price \( P_f \) and the discount rate \( r \). In fact, the facility can break even only upon modest increase in \( P_f \) beyond 3.1% or upon modest decrease in \( r \) beyond 7.5%. Conversely, HECA’s unit profit-margin seems to be less sensitive to changes in \( CO₂ \) price \( P_c \) and least sensitive to changes in electricity prices, characterized by \( P_e \). To achieve break-even, \( P_e \) would need to increase by more than 14.5%, whereas \( P_f \) would need to increase by more 34%. The aforementioned prices and discount rate affect the unit profit-margin of a static HECA \( PM_1 \) in a very similar manner.
7. Conclusions

The levelized cost of electricity is an important economic concept that can be expanded to assess the economic value of hydrogen-based polygeneration energy systems (PES). In this study, we derive a set of metrics that quantify the cost, profitability, and real options associated with fossil-fuel PES. Because a PES can be divided into a distinct set of operational subsystems, we first define the levelized cost of hydrogen (LCOH) and the levelized incremental cost (LIC) of converting hydrogen to market commodities such as electricity and fertilizers. All cost figures can be combined into one term, the levelized cost of polygeneration (LCOP), expressed as a monetary value per unit of produced hydrogen ($/kg\text{H}_2$). Given that polygeneration systems share hydrogen as an intermediate product, this approach allows a systematic comparison of polygeneration costs under multiple technical configurations and operation modes.

By adding end-products’ sales, we derive the optimal unit profit-margin of PES under two operation modes: static production of electricity and fertilizer (PM$_1$), and flexible production of electricity and fertilizer (PM$_2$). We then compare both metrics to the unit profit-margin of static monogeneration of electricity or fertilizer (PM$_0$). The difference between PM$_1$ and PM$_0$ is coined as the value of diversification (VOD), and it captures the economic trade-offs associated with allocating hydrogen to multiple end-product units. Similarly, the difference between PM$_2$ and PM$_0$ is coined as the value of flexibility (VOF), and it captures the economic trade-offs associated with varying hydrogen allocation to each end-product unit over time. VOF and VOD can be combined into one term, referred to as the value of polygeneration (VOP). Also, we demonstrate how to update these metrics to assess PES with carbon capture and storage (CCS).

Through a series of derived economic propositions, we show that static polygeneration is more profitable than static monogeneration if VOD is positive. Similarly, flexible polygeneration is more profitable than static polygeneration if VOF is positive, and flexible polygeneration is more profitable than static monogeneration if VOP is positive. Notably, however, VOD, VOF, and VOP need not always be positive because of the aforementioned economic trade-offs. As such, no specific operation mode is unconditionally superior; the relative competitiveness of static monogeneration, static polygeneration, and flexible polygeneration is highly dependent on the assumed commodity prices and investment costs.

Applying the aforementioned economic metrics to a real polygeneration project, Hydrogen Energy California, reveals their practical significance. Given a set of technical and financial assumptions, HECA proves to be profitable as a static fertilizer-only plant with PM$_{0}$$_F$ = 1.934 $/kg\text{H}_2$. However, with PM$_{0}$$_e$ = −0.992 $/kg\text{H}_2$, HECA fails to break even as a static electricity-only plant although its cost at LCOE = 0.0953 $/kWh$ is comparable to coal power plants with carbon capture. As a static PES, HECA’s profit-margin PM$_1$ is between PM$_{0}$$_e$ and PM$_{0}$$_F$, with the exact value dependent on the exact splitting of produced hydrogen between the two end-products. As a flexible PES, HECA almost succeeds to break even, with PM$_2$ = −0.0439 $/kg\text{H}_2$. In this case study, the flexible polygeneration is unequivocally superior to all other operation modes only if electricity prices increase 5.5–5.74 folds under an endogenously optimized operational schedule.

Moving forward, several opportunities still exist to expand this work. One potential area of research involves analyzing the economic value of polygeneration systems powered by renewable energy. While producing the same end-products (e.g. electricity and fertilizer), renewable polygeneration might differ from fossil-fuel polygeneration in two major ways, namely, hydrogen production and the need for CCS. Multiple technologies are available to produce hydrogen in renewable polygeneration, including biomass gasification and water electrolysis powered by solar PV and wind turbines. Interestingly, in this case, a separate source of carbon would be needed to synthesize chemicals, and renewable PES may result in negative emissions if combined with CCS. In addition, hydrogen can be treated as a form of energy-storage if used to regenerate electricity.

Furthermore, it would be rather important to examine the effect of taxes, including tax subsidies, on polygeneration. Such endeavor requires a more careful analysis of investment tax credits, effective corporate income tax rates, and accelerated depreciation rates that could be applicable to both fossil-fuel and renewable polygeneration. Finally, this work assumes deterministic prices of commodity inputs and outputs as well as known energy policies. A more realistic approach is to consider uncertain market prices then optimize the operational schedule of PES as prices vary with time. A similar approach can be followed to incorporate uncertain environmental regulations in the form of future carbon pricing.

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Appendices A and B. Supplementary data

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References


