

Designing a Load-Flexible Renewable Ammonia Plant for Variable Green Hydrogen Supply

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ABSTRACT

Decarbonizing ammonia by replacing grey with green hydrogen directly affects the operation of the Haber-Bosch (HB) process. When directly coupled to green hydrogen production from renewable energy, the HB process should be able to operate flexibly to match variable hydrogen supply. This study presents a structured approach for designing a load-flexible HB plant, supported by a rigorous process model. First, we screen 2,000 designs at high (100%) and low (10%) hydrogen loads to assess operability. Only 1,100 designs are feasible for both loads, underscoring the need to account for multivariable interactions during design. Next, we assess the economic feasibility of a base design, comparing HB operation under constant and flexible loads. Flexible operation reduces the levelized cost of ammonia (LCOA) by about 5.8%, primarily by lowering green hydrogen production costs. This cost reduction results from downregulating hydrogen production during periods of high electricity prices. By contrast, HB design improvements yield only small LCOA reductions (about 0.4%), though lower reactor pressure and a larger reactor volume remain the best HB design options to further reduce renewable ammonia costs.

Keywords: Process Design, Process Operations, Renewable and Sustainable Energy, Green Ammonia

INTRODUCTION

Ammonia is one of the most-produced chemicals worldwide. It is primarily used as a fertilizer, but could also serve as an energy carrier or fuel in the future [1, 2]. Most ammonia is produced from hydrogen via steam methane reforming, also called grey hydrogen. Since grey hydrogen is produced from natural gas, ammonia production inherently accounts for approximately 2% of global greenhouse gas emissions [2]. To reduce the environmental impact of ammonia production, studies suggest replacing grey hydrogen with green hydrogen as the primary feedstock [1, 2]. Pure grey and green hydrogen are chemically identical; however, their production behavior can significantly affect ammonia plant operations. Today's commercial ammonia plants all rely on the Haber-Bosch (HB) process, in which hydrogen and nitrogen are converted to ammonia over a metal catalyst at high pressure and temperature. The HB process is expected to remain the preferred option, at least in the mid-term, even when coupled to a green hydrogen supply.

The main difference between producing ammonia

from green or grey hydrogen lies in the availability and flexibility of hydrogen supply. Typically, ammonia production is coupled directly with a hydrogen production process to minimize the cost of hydrogen storage and transport [3, 4]. Grey hydrogen, produced continuously from methane, enables the HB process to operate continuously at a constant hydrogen load. In contrast, green hydrogen production via electrolysis powered by renewable energy can exhibit significant load variations, mainly due to the intermittent nature of renewable electricity supply. Although modern electrolyzers can rapidly adapt to changing conditions [5], incorporating this flexibility into load-flexible HB plant design and operation remains an open challenge, increasing the design complexity.

Many previous studies have focused on the core of the HB process, the reactor system [6]. The reactor system usually consists of a combination of adiabatic beds and cooling systems to drive the strongly exothermic reaction $3\text{H}_2 + \text{N}_2 \rightarrow 2\text{NH}_3$. Most conventional HB plants today still rely on the reactor system, which couples multiple adiabatic reactor beds with quench cooling (AQCR). However, Morud and Skogestad first noted that this

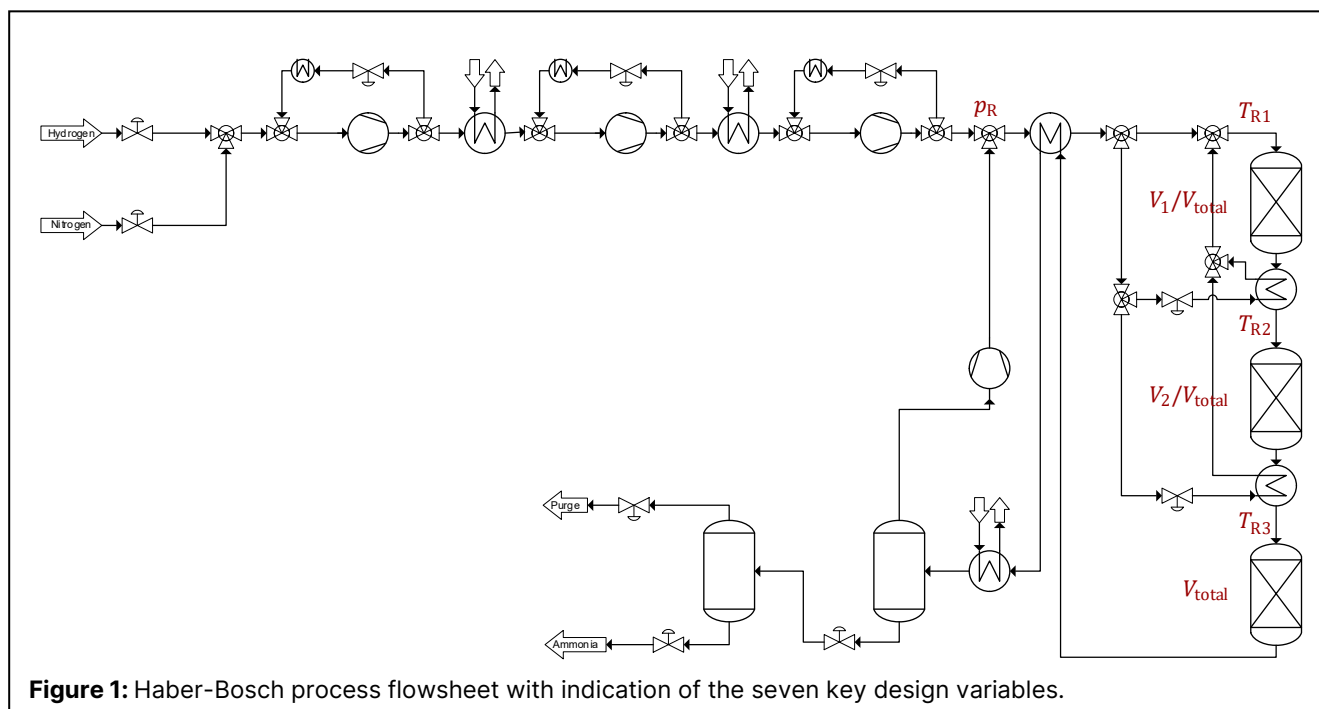


Figure 1: Haber-Bosch process flowsheet with indication of the seven key design variables.

AQCR system could experience stability issues during load changes [7]. In contrast, Rosbo *et al.* found that adiabatic indirect-cooled reactor (AICR) systems can handle load changes well and achieve higher conversion rates than AQCR systems [6]. Since then, several studies have focused on operating HB plants for green ammonia production using AICR systems, assuming variable hydrogen supply rates ranging from 100% to 10% of the nominal capacity [4, 8]. Furthermore, given the described advantages, ammonia plant licensors are increasingly focusing on AICR systems rather than AQCR systems, particularly for green hydrogen applications [8, 9]. Recently, the world's first large-scale demonstration plant for dynamic ammonia production opened in Denmark, operating solely on renewable energy and using an AICR system [9]. AICR systems use three reactor beds with interbed cooling in series. The coolers are usually heat-integrated, resulting in a complex HB design. Key design choices include compressor dimensions, reactor bed volumes, and heat exchanger sizes. However, dimensions are rarely publicly available.

Given the degrees of freedom, traditional process design focuses on a single steady-state operating point. In the HB process, this point corresponds to a nominal hydrogen supply rate. But, coupling the HB process to a green hydrogen source often results in a variable feed supply, making single-point designs potentially infeasible or uneconomical. Studies show that certain HB process designs can operate at reduced hydrogen feed rates through various low-load operating procedures [4, 10]. Opinions diverge on whether the reactor pressure should be reduced from the nominal setpoint during low-load operation [4] or remain constant [10]. While some studies

showed better performance under varying pressure [4], we believe that, given concerns about mechanical stress from frequent pressure changes, operating at constant reactor conditions is preferable.

In this study, we provide guidance for designing a flexible HB plant to produce green ammonia using green hydrogen. We explore the range of feasible AICR system designs using a detailed, rigorous simulation model and demonstrate the potential economic advantages of flexible operation. We also examine how HB process design can be adapted and improved to further reduce costs when coupled to a green hydrogen supply.

METHODOLOGY

In this chapter, we first detail the HB process model and its key design variables, including reactor pressure, bed inlet temperatures, and reactor bed volumes. We then introduce a sampling algorithm to efficiently explore the feasible design space defined by these variables. Further, we present how to calculate and quantify the costs of green ammonia production. Finally, we explain how dynamic electricity prices can serve as decision variables for operating the green hydrogen production and HB plant at variable loads.

Green Ammonia Process Design

The green ammonia process design follows the same basic flowsheet as the well-known HB process, developed by Fritz Haber and Carl Bosch in the early 20th century, and largely unchanged since then. Our model, shown in Figure 1, comprises three main parts: (i) the feed compression of reactants (hydrogen and nitrogen), (ii)

the reactor system for converting the reactants to ammonia, and (iii) the separation system for recovering unreacted gases and product purification. The plant is designed to produce 500, 000 tonnes of ammonia per year using the commercial AVEVA Process Simulation (APS) software. For modelling details, we refer to our previous work [11], as the process design here investigated follows a very similar setup with similar assumptions.

In the process, three compressors with intermediate cooling in series compress the reactant gas from 10 bar to the specified reactor pressure. Each compressor is equipped with an anti-surge recycle that opens at feed flow rates below 60% of the nominal load to prevent surging. The reactor system is based on an AICR design with three adiabatic fixed beds and interbed cooling. Due to the exothermic reaction, the effluent from each reactor bed is hot and therefore cooled by the cold reactor feed stream. The remaining heat from the last bed is integrated to heat the reactor feed stream via the feed-effluent heat exchanger. Since single-pass conversion in the AICR system is limited by chemical equilibrium to about 30% (depending on operating conditions) [6], the reactor effluent still contains high concentrations of nitrogen and hydrogen. These gases must be recovered and recycled for efficient operation. To maximize recovery, the reactor effluent stream is further cooled and separated into two phases in a flash drum. The reactant gases in the distillate stream are recompressed to reactor pressure and recycled, while the ammonia-rich bottom stream is further purified. A second flash at lower pressure vaporizes the remaining impurities from the product, achieving 99.8 mol-% ammonia purity.

The most impactful and complex design decisions concern the selection of the AICR system's size and operating conditions. Key variables include reactor pressure, individual reactor beds' inlet temperatures, and the individual volumes of the three reactor beds. These key variables not only affect reactor conversion but also influence equipment specifications, such as compressor dimensions, reactor bed volumes, heat exchanger sizes, and, consequently, equipment costs and the required amount of utilities.

Sampling of Design Alternatives

The values of the seven previously defined key design variables must be carefully selected by the responsible design engineer, as not all possible combinations of design variable values yield feasible design solutions; certain regions of the design space may be inherently infeasible due to process constraints. This problem becomes even more complex if the design must be operable over a broad range, rather than at a single operating point, as required for green ammonia production.

To efficiently explore the design space, we define broad bounds for all key design variables (see Table 1).

We assume uniform distributions within these bounds and use Latin Hypercube Sampling (LHS), a quasi-random, space-filling technique, to generate numerous design alternatives. Each alternative is a unique combination of the key design variables and is evaluated using the rigorous process model in APS. We classify the results as feasible or infeasible based on process system constraints. To account for different operating loads, we test the feasibility at both the high hydrogen load (same as nominal) and the low hydrogen load (10% of nominal).

Table 1: Base design and bounds for the HB process key design variables.

Design Variable	Base	Bounds
Reactor Pressure (p_R) in bar	218	[200, 250]
Total Reactor Vol. (V_{total}) in m ³	65	[50, 80]
Ratio Volume Bed 1 (V_{R1}/V_{total})	0.3	[0.1, 0.4]
Ratio Volume Bed 2 (V_{R2}/V_{total})	0.3	[0.2, 0.4]
Inlet Temp. Bed 1 (T_{R1}) in K	670	[620, 700]
Inlet Temp. Bed 2 (T_{R2}) in K	620	[620, 700]
Inlet Temp. Bed 3 (T_{R2}) in K	620	[620, 700]

Economic Evaluation

Several economic metrics can evaluate green ammonia production, such as net present value (NPV), payback time (PBT), minimum selling price (MSP), and leveled cost of ammonia (LCOA). NPV and PBT depend on financing, discount rate, and market prices, making them suitable for evaluating individual investments. In contrast, MSP and LCOA measure economic performance per unit, allowing comparison across projects. We use LCOA as our primary metric because it provides the average cost of ammonia production over the plant's lifetime, independent of market prices. Table 2 summarizes all prices and economic parameters used.

The LCOA is calculated using Equation 1: The annualized total capital investment (TCI) is split over the plant's lifetime using the capital recovery factor (CRF) (see Equation 2), then operational expenditures (OPEX) are added, and the result is divided by the annual ammonia production size.

$$LCOA = \frac{TCI \cdot CRF + OPEX}{M_{NH_3, annual}} \quad (1)$$

$$CRF = \frac{r(1+r)^n}{(1+r)^n - 1} \quad (2)$$

The TCI is calculated by summing the fixed capital investment (FCI) and additional working capital (WC) costs (see Equation 3). For the FCI calculation, the costs for all process equipments are summed up and scaled by the respective 2024 Chemical Engineering Plant Cost Index (CEPCI) [12]. In the final step, we multiply this sum by the Lang factor for fluid-processing plants (see Table 2) to estimate total installation costs [13].

$$TCI = \sum (C_{\text{equip}} * \frac{CEPCI_{2024}}{567}) * f_i * (1 + f_{WC}) \quad (3)$$

We calculate the cost for each piece of equipment using the equations and assumptions implemented in APS. Due to the harsh conditions (high pressure and temperature) in the HB plant, we assume stainless steel as the construction material for all equipment. The compressors are modeled as centrifugal units driven by an electric motor, with an overall compression efficiency of 95%. For the heat exchangers, we assume a counter-current design and, if necessary, cooling with cooling water. To calculate the heat exchanger area, we use an overall heat transfer coefficient (value depends on the fluids, see Table 2), along with the logarithmic mean temperature difference between the tube and shell sides, and assume a minimum temperature difference of 10 K. The flash units are assumed to be vertical drums with hemispherical heads, each with a residence time of 50 min and a length-to-diameter ratio of three. The AICR system is assumed to be placed in a vertical shell with inner and outer bed diameters of 2 and 3.5 m, and a total length determined by the selected reactor bed volumes. The required thicknesses of the hemispherical heads of the AICR and flash vessels are determined in accordance with the ASME Boiler and Pressure Vessel Code, Section VIII, Division 1, UG-32(f) [14].

Table 2: Parameters for the techno-economic assessment.

Parameter	Value
CEPCI 2024 ($CEPCI_{2024}$)	800 [12]
Lang factor (f_i)	5.93 [13]
Working capital factor (f_{WC})	15% [15]
Plant lifetime (n)	25 yr
Discount rate (r)	6%
Overall heat transfer coefficient pressured gas – pressured gas	0.5 kW/m ² /K
Overall heat transfer coefficient pressured gas – liquid	0.4 kW/m ² /K
Price cooling water	0.35 €/GJ [15]
Price catalyst	15.36 €/kg [16]
Energy demand nitrogen	0.37 kWh/kg [17]
Catalyst lifetime	5 yr
Electricity fees and taxes	26.26 €/MWh [18]

We calculate OPEX (Equation 4) from reactants costs (hydrogen and nitrogen) and utilities (compression energy, cooling water, and catalyst replacement as a continuous cost). We use fixed prices for cooling water and catalyst per unit, and variable electricity prices to calculate hydrogen, nitrogen, and compression costs. The levelized cost of operation of hydrogen (LCOH) are calculated using the European Hydrogen Observatory calculator with default values for a PEM electrolyzer [19],

splitting the cost into CAPEX, electricity, and OPEX (see Equation 5). We source electricity prices from Danish databases [20] and adjust operating times to match the plant operation as described in the next subsection.

$$OPEX = (C_{H_2} + C_{N_2}) + (C_{\text{comp}} + C_{\text{cw}} + C_{\text{cat}}) \quad (4)$$

$$C_{H_2} = \dot{m}_{H_2} * (c_{H_2, \text{CAPEX}} + c_{H_2, \text{Elec}} + c_{H_2, \text{OtherOPEX}}) \quad (5)$$

For load-flexible operation, we average OPEX across the two main operating points (high and low load), assuming instantaneous changes between. In reality, the HB plant, compared to the PEM system, is the limiting factor for transition time between operating points, and transitions are not rapid [4–6]. However, recent studies show that fast transitions of 3% load change per minute are possible [4, 8]. Further, we use representative electricity prices at the two operating loads to account for realistic costs when using load-flexible operation.

Load-Flexible Operation

Green hydrogen and ammonia production depend heavily on renewable energy supply. In practice, a green ammonia plant would most likely be built alongside electrolyzer units close to renewable electricity sources, such as solar or wind farms. However, modeling renewable electricity generation is heavily dependent on location and technology and is beyond the scope of this study. To still account for variability in renewable electricity generation, we consider dynamic electricity prices driven by regional demand and supply. In particular, we use historic hourly distributed prices from the day-ahead market in West Denmark from 2024 [20]. Figure 2 displays the mean price and the histogram of all prices, which range from slightly negative to above 800 €/MWh. With these prices we calculate LCOH and LCOA to approximate the dynamic price effect on renewable production plants.

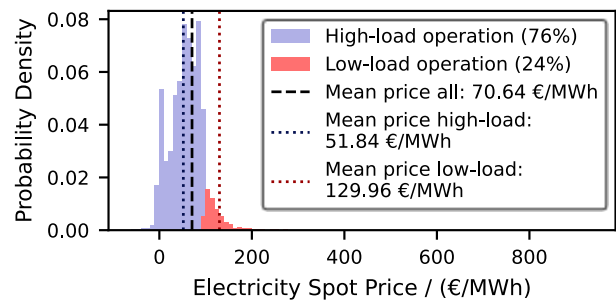


Figure 2. Electricity spot price probability distribution from hourly day-ahead market data from West Denmark in 2024 [20], including the indication of mean price and representative prices for load-flexible operation.

For constant operation, each electricity price would have the same impact on average production costs. However, with a load-flexible system, production at high prices can be reduced to a low-load operating point,

while at low prices, the production can be shifted back to the high operating point. In this study, we compare a constant operation at high load with the annual average electricity price to a load-flexible approach using two representative prices. The lower of these prices represents the lower 76% of the historic prices, while the high price represents the upper 24%.

RESULTS AND DISCUSSION

In this section, we systematically explore the design space of the HB plant to identify feasible process designs that account for different loads. Then, we evaluate the economics of constant ammonia production relative to load-flexible operation and, lastly, show how an improved HB process design can influence the total LCOA.

Finding a Feasible Process Design

The most important task when designing a load-flexible process is to identify a design that is operable over the full operating range, rather than at a single operating point. Thus, different designs must be evaluated under different loads. Since we assume that the HB process is primarily operated at two extreme load levels (high and low), we evaluate the designs at these two operating points. In total, we sample 2000 different designs and thus perform 4000 evaluations with our rigorous process model. Of the sampled designs, 1103 yield feasible solutions for both loads. Figure 3 visualizes the feasible design space by projecting it onto planes of two variables at a time and differentiating between all sampled (grey) and feasible designs (blue).

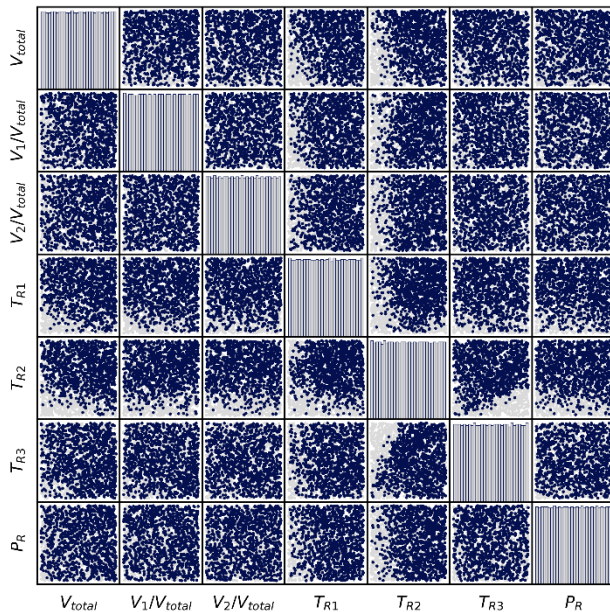


Figure 3. Input (grey) and feasible (blue) design-space projections in two-dimensional space.

The success of 55% of all sampled designs implies that a feasible design solution satisfying all process constraints at both loads is indeed possible, but not straightforward. Feasible design solutions exist for most combinations of one or two fixed design variables since only some regions of the two-dimensional projections of the full design space appear completely or largely infeasible, like very low T_{R2} values or combinations of low V_{total} and low T_{R1} . However, the contrast between the largely feasible region in plane projections and the large number of infeasible designs indicates that interactions among multiple variables are significant for feasibility. These multi-variable interactions should be considered during the process design procedure. We also note that nearly all infeasibilities arise from high-load simulations, suggesting that the design at this operating point should be assessed first.

Based on the insights from the design space evaluation, we select a feasible base design near the center of the total design space for the following assessments. The values of the design variables for the base design are listed in Table 1.

Comparison of Operational Approaches

Moving forward, when designing a load-flexible plant, the most important objective is that flexible operation reduces costs relative to constant operation at high load. In the following, we compare two operational approaches for integrating green hydrogen and the HB plant based on the LCOA, using the feasible base design identified earlier. Before, in the next subsection, we replace the base design with an improved alternative.

As explained earlier, for flexible operation, the plant operates at high load (76% of the time) with lower electricity prices and at low load (24% of the time) with higher prices. Electricity prices affect green hydrogen costs and other OPEX, such as nitrogen and compression costs. The total equipment costs do not scale with the load since the nominal plant size remains unchanged, but operating costs vary. However, compressor power does not scale proportionally with the load because, for low loads, anti-surge recycling is required. Table 3 highlights key differences between the operation of the base design at high and low loads.

With above assumptions for the two operational modes, the first two bars in Figure 4 directly compare the LCOA for constant versus load-flexible HB process operation using the base design. The figure details the separate contributions of HB TCI and all OPEX components. Overall, the load-flexible approach yields an LCOA about 5.8% lower than constant operation. Comparing this LCOA to literature is challenging because key parameters, such as electrolyzer technology and electricity price, vary widely. For example, our LCOA matches the values reported by Sánchez and Martín [21] (1.35 €/kg),

which are well above current grey ammonia prices. In contrast, Hartvigsen *et al.* [22] report an LCOA of 792 €/kg for green ammonia in Denmark, using alkaline electrolyzers with far lower electricity prices for 2030.

Table 3: Comparison between high and low load operation of HB process.

	High	Low
Faction of time in operation	76%	24%
Hydrogen feed rate in t/d	250	25
Ammonia production rate in t/d	1368.6	136.81
Average electricity price + fees and taxes in €/MWh	78.10	156.22
Compression Demand in MW	26.18	15.51
Cost for Compression in €/h	2045	2423
TCI in M€	285.85	285.85

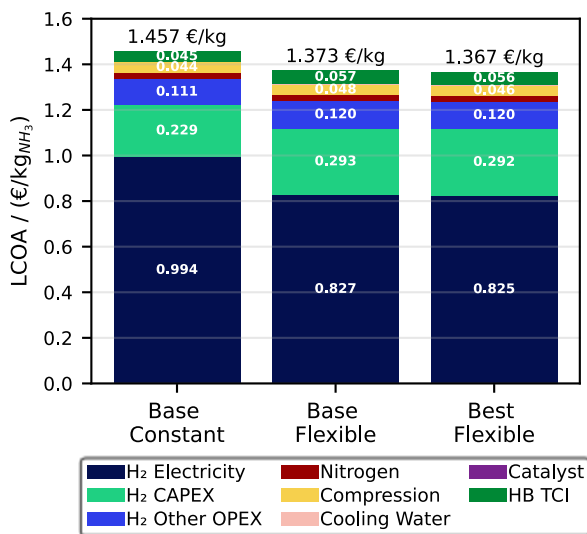


Figure 4. LCOA and its components for the three different case studies: Constant operated base design, load-flexible operated base design, and load-flexible operated best (LCOA) design.

As shown by the individual contributions, the green hydrogen price accounts for more than 91.5% of the total LCOA in the constant and 90.3% in the load-flexible case. The LCOH itself depends heavily on the price of green electricity; thus, using load-flexible operation for green hydrogen production reduces the share of electricity costs in the LCOH from 74.5% to 66.7%. This reduction is then inherently responsible for the lower LCOA when the HB process also operates flexibly. In the future, adding hydrogen storage between the PEM system and the HB process could be a case worth comparing. Introducing a buffer offers the advantage that PEM and HB process operations can be flexibilized separately, which could yield further LCOA reductions, despite high investment in the hydrogen storage system [5].

Another result highlighted by Figure 4 is that under

flexible operation, the shares of CAPEX for the hydrogen generation process and the HB process increase. The higher share of equipment costs stems from the lower total output from the same plant during periods of low load. Thus, in particular, lower electrolyzer costs could significantly affect the LCOH and LCOA, especially when operated flexibly. In contrast, the effect of reducing the TCI or utility costs of the HB process itself on the LCOA is limited, accounting for only about 10% of the total LCOA. However, the ratio of hydrogen consumed to ammonia produced in the HB process could have a significant impact, and the HB design should be closely assessed in this regard.

Benefit of HB Process Design Enhancements

Having examined differences in LCOA between constant and load-flexible operation, we investigate how improvements of the HB process design could further reduce the green ammonia costs. In particular, we focus on the three most influential factors related to the HB process identified in the analysis of the LCOA components: the ratio of hydrogen feed to ammonia produced (at high load), the TCI of the HB plant, and the cost for electric compression (at both loads). Figure 5 shows the LCOA for each of the three influencing factors across all feasible designs, identified during the LHS-based design evaluation. The scatter plots show that all three factors indeed influence the total LCOA, and that, starting from the base design, minimizing each factor individually also reduces the LCOA.

The LCOA of the selected base design equals the average LCOA of all feasible designs and the standard deviation of LCOA across designs is very low (0.003 €/kg), supporting the claim that the HB process design has little influence on the total LCOA. Selecting the design with the lowest LCOA yields a 0.4% reduction compared to the base design (see Figure 4, second and third bar).

The best design alternative with the lowest LCOA (Best LCOA) also yields the lowest TCI, indicating that a focus on reducing equipment costs can have a positive overall effect. However, the design with the lowest hydrogen-to-ammonia ratio (Best HtA) and the lowest compression power has only a negligibly higher LCOA. Table 4 compares the two best designs and shows similarities in the values of the key design variables.

Both designs operate almost at the lower bound of the pressure range to minimize compression and compressor costs. This suggests that, in the future, even lower pressures could be assessed if compatible with the chosen catalyst. Recently, research has focused on so-called low-pressure HB processes using special catalysts that enable pressures below 150 bar, potentially reducing overall compression costs [2]. Further, our selected two best design candidates also almost maximize the total

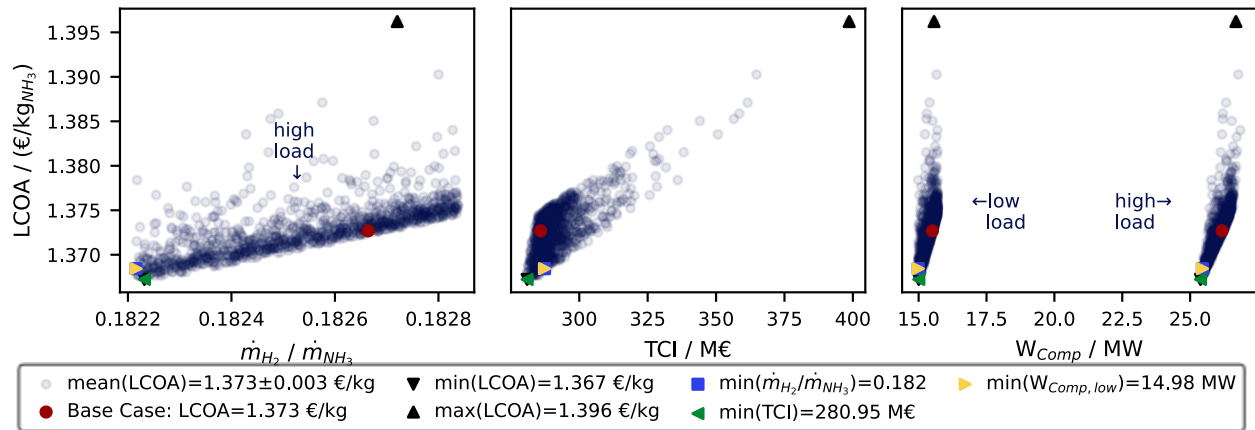


Figure 5: LCOA related to three HB process metrics: hydrogen-to-ammonia ratio, TCI, and compression demand.

reactor volume to its upper limit. As seen in Figure 4, catalyst costs affect the LCOA only minimally; thus, a higher reactor volume that improves single-pass conversion and reduces the demand for recycle stream compression could potentially lead to a reduction of the total LCOA. Lastly, comparing the volume shares among the three reactor beds and the reactor bed inlet temperatures for both design candidates does not reveal close similarities. However, the choice of reactor bed volume together with the reactor bed inlet temperature is essential for the feasibility of the design, as discussed earlier.

Table 4: Best feasible HB process designs related to the lowest LCOA and the lowest hydrogen-to-ammonia (HtA) ratio.

Design Variable	Best LCOA	Best HtA
Reactor Pressure (p_R) in bar	200.7	200.0
Total Reactor Vol. (V_{total}) in m^3	80.0	79.4
Ratio Volume Bed 1 (V_{R1}/V_{total})	0.263	0.333
Ratio Volume Bed 2 (V_{R2}/V_{total})	0.373	0.388
Inlet Temp. Bed 1 (T_{R1}) in K	654.0	638.9
Inlet Temp. Bed 2 (T_{R2}) in K	675.2	679.3
Inlet Temp. Bed 3 (T_{R2}) in K	667.3	628.5
LCOA	1.367	1.368

In summary, while the total impact of all key design variables on the LCOA could be evaluated more quantitatively by calculating sensitivity indices, the overall impact of the HB process design on the total LCOA remains small relative to the cost of green hydrogen. Thus, we find this effort is not worthwhile. The same applies to the use of optimization techniques to minimize the LCOA, treating the key design variables as decision variables.

CONCLUSION

This work addresses the central challenge of

coupling ammonia synthesis to variable green hydrogen: high fluctuations in renewable electricity and, hence, stochastic hydrogen availability and price. We proposed a structured design-space exploration to identify Haber-Bosch (HB) designs that remain operable at extreme load variations. Further, we compared constant production with load-flexible operation based on the levelized cost of ammonia (LCOA). The key finding is that load-flexible operation can lower the LCOA relative to constant operation because electricity-driven hydrogen costs dominate overall economics, and shifting production toward periods with low electricity prices reduces the average green hydrogen price. By contrast, HB process design variations have only a secondary influence on the total LCOA. We indicate that a lower reactor pressure (within catalyst constraints) and a larger total reactor volume can reduce the overall LCOA by lowering compression duty and compressor sizes, yet the aggregate cost benefits of improved HB designs remain modest relative to the price of green hydrogen.

These conclusions should be interpreted in light of the scope and modeling choices. The analysis compared two steady-state load points and did not include dynamic transients. Control constraints were enforced implicitly by feasibility, not by explicit plant-wide control design. Moreover, exogenous electricity prices and renewable availability were also not modeled at hourly resolution. To address these limitations, future work should focus on rigorous modeling of renewable generation, electrolyzer dynamics, and plant controls, while accounting for time-series market and weather data. Stochastic, multi-objective assessments (cost, emissions, reliability) can then quantify when added design complexity is justified. Overall, the dominant levers for renewable ammonia lie upstream, in electricity price trajectories, electrolyzer cost, and integration strategies, while HB design refinements provide only incremental gains.

DIGITAL SUPPLEMENTARY MATERIAL

All code and simulations are available on GitHub:
https://github.com/gsi-lab/FlexiblePtA_Economics

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