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Techno-economic assessment of green ammonia plants with multi-scale capacity

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ABSTRACT

Cost reduction of green ammonia production is critical to advancing the hydrogen-ammonia economy, as ammonia capable of cost-effective storage and transportation is a promising hydrogen carrier and energy carrier to alleviate the intermittency and geographical limitations of renewables. Optimisation and techno-economic assessment based on rigorous model are essential to accurately investigate techno-economic feasibility and fully explore optimisation potential. This work estimates the levelized cost of ammonia (LCOA) of an integrated system including a hydrogen generation process employing Proton Exchange Membrane (PEM) water electrolysis, a nitrogen generation process from flue gas recovery, and an ammonia synthesis process based on Haber-Bosch Process. To enhance the reliability of LCOA, detailed equipment sizing and costing is conducted according to stream data from rigorous modelling in Aspen Plus. A novel optimisation strategy is proposed to enhance the computational robustness by sequentially largening the group of optimised variables and improving the quality of initial points. Homotopy-continuation (HC) method is employed to ease the convergence difficulties for solving the flowsheet with multiple recycle streams and scaling up the plant capacities between 100 $tNH_3\ d^{-1}$ and 600 $tNH_3\ d^{-1}$ from an initially feasible point. Heat integration is also considered to realise the combined supply of heat and power by introducing a steam turbine power cycle and utilising the waste heat from exothermic ammonia synthesis.

Keywords: Green ammonia, Rigorous modelling, Process optimisation, Plant scale up

INTRODUCTION

Cost reduction of green ammonia production is critical to advancing the hydrogen-ammonia economy, as ammonia capable of cost-effective storage and transportation is a promising hydrogen carrier and energy carrier to alleviate the intermittency and geographical limitations of renewables. Currently, most current studies estimate the levelized cost of ammonia (LCOA) using oversimplified assumptions [1 – 3] or shortcut models [4, 5], which is inaccurate and unrealistic. In details, linear correlation is inappropriately used to estimate the LCOA in green ammonia systems with all plant scales, as it is derived in a basis of 300 $tNH_3\ d^{-1}$ using 70 USD MWh^{-1} of electricity [5]. Despite shortcut models could provide feasible initialisation for process simulation and optimisation, a technically feasible solution cannot be guaranteed when it is solely based on shortcut modelling, not to mention a reliable cost estimation. Moreover, optimisation scope is restricted to general terms such as equipment capacity and wind-solar mix ratio [1]. Therefore, optimisation and techno-economic assessment based on rigorous model are essential to accurately investigate techno-economic feasibility and fully explore optimisation potential.

Rigorous model of ammonia synthesis employing Neilsen's expression [6] is widely regarded to have the most accurate prediction of ammonia synthesis performance [7], whilst the application of it always focuses on single equipment simulation and cost assessment [8]. Exothermic nature in ammonia synthesis can be well captured by rigorous modelling, and utilisation of this waste heat can further reduce the LCOA to enhance the economic competitiveness.

In this work, detailed equipment sizing and costing are conducted according to stream data from rigorous modelling and in Aspen Plus. A novel optimisation

strategy sequentially largening the group of optimised variables and improving the quality of initial points will be employed to optimise the LCOA for plants between 100 $tNH_3\ d^{-1}$ and 600 $tNH_3\ d^{-1}$ from an initially feasible point.

METHODOLOGY

System description

An integrated system utilising off gas as the nitrogen source for green ammonia production was proposed, as depicted in **Figure 1** [10]. It encompasses an ammonia production system based on the Haber-Bosch process applying an industrial ammonia synthesis convertor (i.e., Topsoe S-200), an electrolysis-based hydrogen production process, and a stepwise nitrogen production technology where a pressure swing adsorption unit is facilitated by an amine-based carbon capture process for nitrogen enrichment. Apart from electric power driven by renewables such as solar and wind, this system also explores heat integration opportunities in ammonia purification process for further energy efficiency improvement and carbon mitigation.

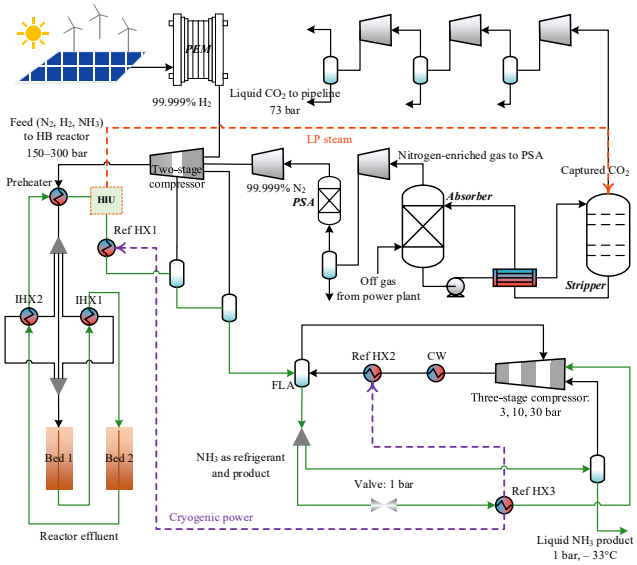

Figure 1. Flowsheet of the green ammonia production system.

Optimisation models

Modelling of ammonia synthesis

The modelling is conducted in Aspen Plus V12.1. The ammonia synthesis convertor (e.g., Topsoe S-200) is modelled by the combination of two internal heat exchangers (modelled by HEATX) and two plug flow reactors (PFR) as the catalytic beds.

The kinetic model of ammonia synthesis employs widely validated Neilsen's expression [6] throughout all sections (e.g. process simulation, optimisation and techno-economic analysis) as follows:

$$r_{NH_3} = \frac{\eta \cdot \kappa_2 \cdot \left(\alpha_{N_2} \cdot K_{eq}^2 - \alpha_{NH_3}^2 \cdot \alpha_{H_2}^{-3}\right)}{0.654 \cdot \left(1 + K_{a,eq} \cdot \alpha_{NH_3} \cdot \alpha_{H_2}^{-1.523}\right)^{1.308}} \cdot V \quad (1)$$

$$\kappa_2 = 7.89 \cdot 10^{10} \cdot e^{-\frac{11171}{RT}} \quad (2)$$

$$K_{a,eq} = -2.94 \cdot 10^{-4} \cdot e^{-\frac{24052}{RT}} \quad (3)$$

$$\log_{10} K_{eq} = 2.69 \cdot (1 - \log_{10} T) - 10^{-7} \cdot (552 \cdot T - 1.85 \cdot T^2) + \frac{2001.6}{T} \quad (4)$$

Objective function

The primary objective of this study is to evaluate and minimise the LCOA, defined in Eq. 5, which represents the average production cost per unit of ammonia (USD tNH_3^{-1}). The LCOA framework integrates both capital and operating expenditures over the lifetime of the plant, thereby providing a consistent economic metric for comparing alternative design (e.g., various plant scales and heat-integration strategies) and operating strategies (electricity prices and optimised operating conditions).

$$LCOA = \frac{ACCR \cdot CAPEX + OPEX}{m_{NH3}} \quad (5)$$

$$C_{TPI} = 1.18 \cdot \left(C_{TBM} + C_{site} + C_{buildings} + C_{offsite}\right) \quad (6)$$

$$C_{BM} = \frac{I}{I_0} \cdot C_{P0} \cdot \left[F_{BM} + \left(F_d \cdot F_p \cdot F_m - 1\right)\right] \quad (7)$$

$$C_{P0} = F \cdot exp\{A_0 + A_1 \cdot (ln\, S) + A_2 \cdot (ln\, S)^2\} \quad (8)$$

The capital component of the LCOA consists of the annualised investment cost associated with major process equipment. Equipment capital costs (Eq. 6–8) are derived from detailed sizing calculations based on rigorous process simulation. Specifically, heat-exchanger costs are correlated to the required heat-transfer area, vessel costs are evaluated as a function of material of construction and shell weight, and compression or expansion equipment costs are determined from shaft power requirements. All equipment sizes are obtained case-by-case from steady-state stream data generated under each candidate design or operating condition. More detailed sizing and costing equations and associated coefficients can be found in the Supplementary Materials.

Operating expenditure includes the cost of raw materials, utilities, and ancillary services necessary for plant operation as shown in Eq. 9. Key contributors are electricity consumption for compression and refrigeration, hydrogen and nitrogen feedstock costs, cooling-water demand, raw materials (e.g., MEA and water) and carbon tax. Variable operating costs are calculated based on process simulation outputs and unit prices, while fixed operating costs such as labour, insurance, and maintenance are incorporated as a fraction of the installed capital cost following standard chemical-engineering

economic practice. Necessary equations and cost assumptions can be found in the Supplementary Materials.

$$OPEX = C_{RM} + C_{utility} + C_{operation} + C_{maintenance} + C_{overhead} + C_{depreciation} + C_{carbon} \quad (9)$$

The optimisation problem is expressed as:

$Min\ LCOA$

$s.t.$

Mass and energy balance

Thermodynamic constraints: RKS-BM

Chemical equilibrium: Correlation of Gillespie and Beattie (Eq. 4)

Reaction kinetics: Neilson's expression (Eq. 1)

Unit models: PFR, Compressor, Heat exchanger, etc.

Boundary conditions: See **Table 1**

Table 1: Boundary conditions of decision variables for the optimisation problem.

Variables	Unit	Lower bound	Upper bound
PCOMP1	Bar	31	149
PCOMP2	Bar	150	300
PFLA	Bar	3	10
TPREHEAT	°C	140	220
TREFRIGERATION	°C	–25	0
TBED1OUT	°C	400	600
TBED2IN	°C	350	500

Solution strategy

Once a feasible scaled-up flowsheet is established, optimisation is performed using the Large-Scale Sparse Successive Quadratic Programming (LSSQP) algorithm. LSSQP is a gradient-based method widely adopted in the chemical process industry, noted for its fast convergence and robustness in solving large-scale nonlinear programming problems [11]. In this study, the derivative information automatically generated in EO mode is incorporated into the optimisation routine, enhancing computational efficiency and solution reliability.

To outlines the transition from an initial feasible point obtained in SM to the EO-based optimisation workflow, the overall procedure is illustrated in **Figure 2** and explained in the following:

Step 1: Generate an initial feasible solution in SM and synchronise the model in EO mode. In this step, all equations from unit models and thermodynamic property models are assembled, and the associated free variables are initialised.

Step 2: Scale up the plant by fixing the required product rate, freeing feed flowrates, scaling up the reactor volume, and initially fixing reactor outlet/inlet temperatures while freeing the internal heat exchanger areas. This ensures that the overall degrees of freedom are balanced (DOF = 0).

Step 3: Perform EO simulation using the LSSQP solver, with the Homotopy-Continuation (HC) method enabled to enhance convergence. If convergence fails, the HC step size is reduced and the simulation is repeated.

Step 4: Switch the selected constant variables to optimisation variables.

Step 5: Apply LSSQP optimisation. If convergence is successful, the optimised variable selections and flowsheet solutions are restored before expanding the set of optimised variables. If convergence fails, the optimisation set is reformulated based on the last feasible selection. After all possible combinations of a given number of optimisation variables have been tested unsuccessfully, the number of active optimisation variables is reduced.

Step 6: Repeat the optimisation–reset cycle until convergence is achieved across the full set of optimisation variables.

Step 7: Once convergence is achieved for all optimisation variables, the global optimal solution is obtained.

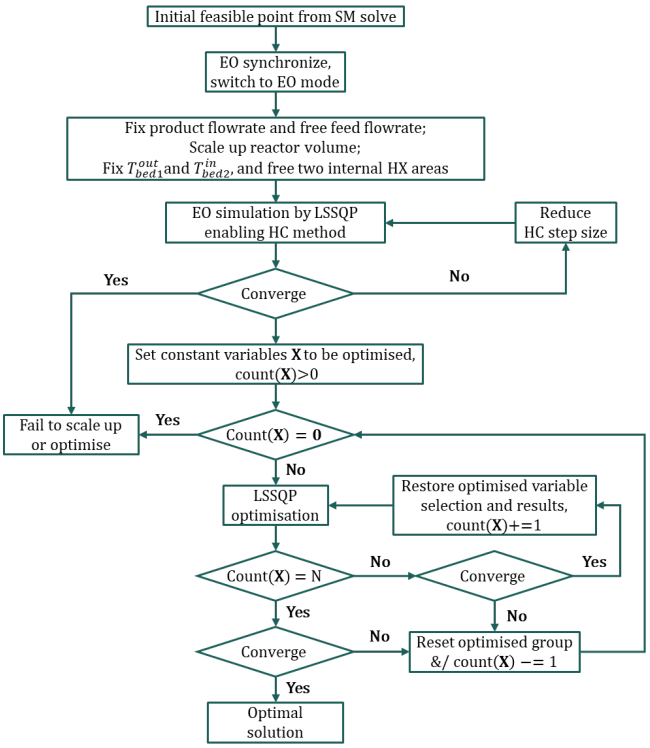

Figure 2. Solution strategy of the optimisation in Aspen Plus Equation-Oriented mode.

RESULTS

Distribution of optimized variables

As the cost of green ammonia production is highly dependent on hydrogen, which in turn originates from green electricity, the assumption regarding electricity price is critical. The International Renewable Energy Agency (IRENA) estimates that the cost of electrolysis-based hydrogen corresponds to electricity prices ranging from 20 USD MWh^{-1} to 65 USD MWh^{-1} over the period 2020–2050. For the optimisation of the base case, an electricity price of 20 USD MWh^{-1} is assumed.

Figure 3 presents the distribution of optimised decision variables for plant capacities of 100–600 $tNH_3\ d^{-1}$. The box plots indicate the 30–70% percentile range, median, and full spread of solutions, revealing which variables consistently converge to well-defined optima and which remain flexible.

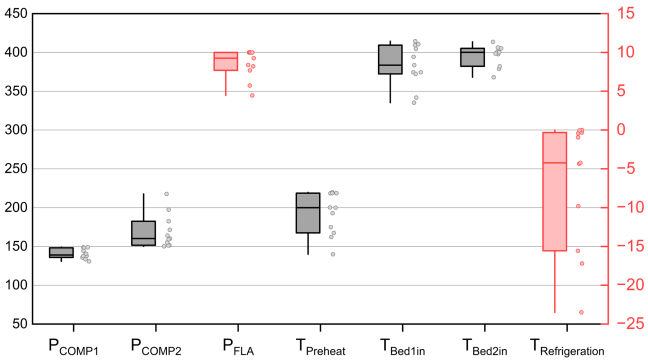

Figure 3. Distribution results of optimised variables

The discharge pressure of the high-pressure compressor (PCOMP2), corresponding to the ammonia synthesis loop pressure, consistently converges to 160–225 bar. This narrow range reflects the core economic trade-off in the Haber–Bosch process: although higher pressure enhances equilibrium conversion, the benefit is offset by higher compression energy demand and increased equipment cost. The medium-pressure compressor (PCOMP1) discharge pressure similarly clusters near its upper bound (ca. 150 bar), indicating a clearly defined optimal compression level to meet synthesis loop requirements.

The inlet temperatures of the catalyst beds (Tbed1 and Tbed2) also show tight distributions around 400 °C. This demonstrates that reactor thermodynamics dominate the optimal solution. The selected temperatures represent the classical compromise between improved reaction kinetics at high temperature and reduced equilibrium conversion.

In contrast, variables associated with downstream separation exhibit wide distributions. The flash pressure (PFLA) spans almost its full allowable range, and the refrigeration temperature varies broadly, including sub-zero conditions. These variables have only a minor impact on LCOA, leading to a relatively flat objective landscape and multiple economically equivalent operating points. The preheat temperature also shows moderate flexibility, as its effect can be compensated by internal heat exchange before the reactor.

Optimized LCOA in various plant scales

Figure 4 shows the dependence of LCOA on plant scale (100–600 $tNH_3\ d^{-1}$) and electricity price (0–120 USD MWh^{-1}). The levelized cost of hydrogen (LCOH) is used as the hydrogen feedstock cost in the LCOA calculation. Plant scale affects both capital-related costs and raw material consumption, while electricity price directly influences electrolysis, compression energy demand, and indirectly the hydrogen production cost.

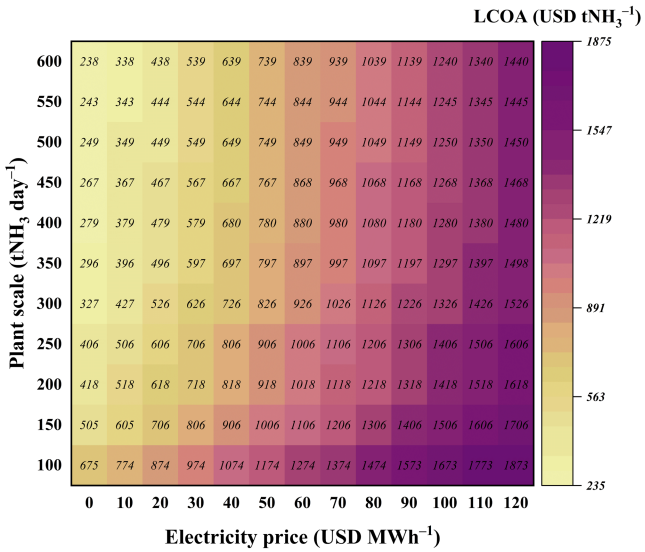

Figure 4. Optimised results, scale-up curve of the ammonia synthesis loop.

Electricity price is the dominant factor controlling LCOA across all plant sizes. Under zero-cost electricity, LCOA ranges from approximately 238 to 675 USD tNH_3^{-1} depending on scale. When electricity price increases to 120 USD MWh^{-1}, LCOA rises sharply to about 1440–1873 USD tNH_3^{-1}.

Plant scale has a secondary but still noticeable effect. Larger plants consistently achieve lower LCOA because capital-intensive equipment, such as reactors and compressors, is amortised over higher annual ammonia output. For instance, at 20 USD MWh^{-1} electricity, increasing capacity from 100 to 600 $tNH_3\ d^{-1}$ reduces LCOA from about 874 to 438 USD tNH_3^{-1}. At this electricity price, the corresponding LCOH is comparable to conventional hydrogen costs, and 600 $tNH_3\ d^{-1}$ represents a typical industrial ammonia plant scale. The resulting LCOA (ca. USD tNH_3^{-1}) is close to the current market price of ammonia (ca. 410 USD tNH_3^{-1}), supporting the credibility

of the economic model.

However, even at the largest scale, electricity prices above 40 USD MWh^{-1} drive LCOA well beyond commonly cited competitiveness ranges for green ammonia (400–600 USD tNH_3^{-1}). This indicates that economies of scale alone cannot compensate for high electricity costs, and that access to inexpensive renewable electricity remains the key requirement for economically viable green ammonia production.

To clarify how plant scale influences both the magnitude and structure of ammonia production cost, **Figure 5** and **Figure 6** decompose the LCOA into annualised capital cost (ACC), cost of manufacturing (COM), raw material, and utility costs. An electricity price of 20 USD MWh^{-1} is assumed for all plant capacities.

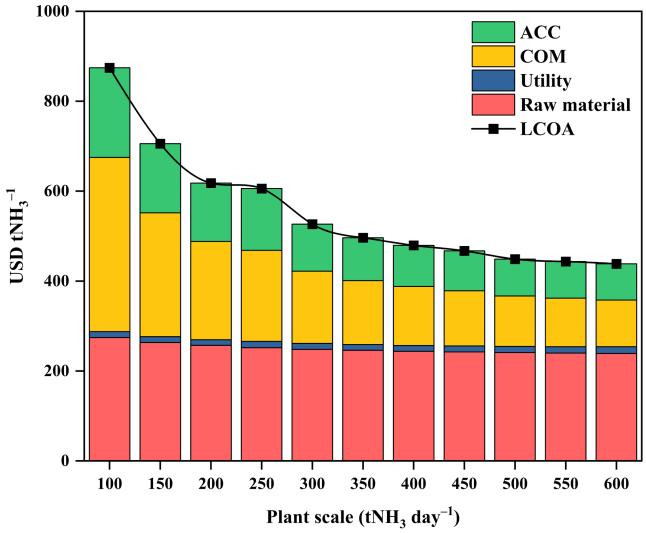

Figure 5. Optimised results, scale-up curve of the ammonia synthesis loop.

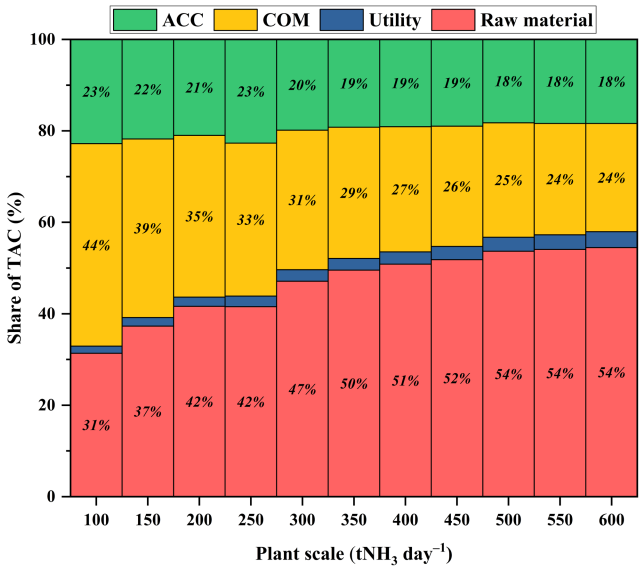

Figure 6. Breakdown of TAC.

Figure 5 shows a pronounced economy-of-scale effect, with total LCOA decreasing significantly as plant capacity increases from 100 to 600 $tNH_3\ d^{-1}$. At the smallest scale (100 $tNH_3\ d^{-1}$), LCOA is close to 900 USD tNH_3^{-1}, while at 600 $tNH_3\ d^{-1}$ it drops to about 440 USD tNH_3^{-1}. The reduction is steep between 100 and 300 $tNH_3\ d^{-1}$ and becomes more gradual beyond 400 $tNH_3\ d^{-1}$, indicating diminishing marginal benefits from further scale-up.

The stacked cost breakdown indicates that the decline in LCOA is mainly driven by reductions in ACC and COM. Both components decrease with scale because capital-intensive equipment is utilised more effectively and fixed costs are distributed over higher production rates. In particular, depreciation, maintenance, and equipment-related operating expenses are key contributors to COM. In contrast, raw material cost changes only slightly in absolute terms, and utility cost remains relatively small and nearly constant across plant sizes. Consequently, small-scale plants are dominated by capital and manufacturing burdens, whereas at large scale the cost structure becomes increasingly governed by raw material inputs.

Figure 6 presents the cost structure in percentage terms, showing the contribution of each component to the total annualised cost (TAC). A clear structural transition occurs as plant scale increases. At 100 $tNH_3\ d^{-1}$, COM is the largest contributor (44%), followed by raw materials (31%) and ACC (23%). With increasing capacity, the COM share steadily declines to about 24% at 600 $tNH_3\ d^{-1}$, while the ACC fraction decreases more moderately from about 23% to 18%.

In contrast, the raw material share increases significantly, rising from roughly 31% at small scale to more than 50% at large scale, eventually becoming the dominant cost component. The utility share remains small across all scales and increases only slightly. This behaviour is consistent with the optimisation results, where operating conditions tend to minimise compression work while maintaining relatively high ammonia synthesis conversion, thereby limiting additional utility penalties at larger scales.

CONCLUSION

This work estimates the levelized cost of ammonia (LCOA) of an integrated system including a hydrogen generation process employing Proton Exchange Membrane (PEM) water electrolysis, a nitrogen generation process from flue gas recovery, and an ammonia synthesis process based on Haber-Bosch Process. In particular, CO2 in flue gas is removed by Monoethanolamine (MEA)-based carbon capture process and nitrogen is enriched to 90%, contributing to a higher efficiency and cost reduction of nitrogen purification, compared with considering air as the nitrogen source with 79% of nitrogen. An

industrial ammonia synthesis convertor (e.g., Topsoe S-200), consisting of two reactor beds and two internal heat exchangers, is employed to make our work closer to a real-life project. To enhance the reliability of LCOA, detailed equipment sizing and costing is conducted according to stream data from rigorous modelling in Aspen Plus. A novel optimisation strategy is proposed to enhance the computational robustness by sequentially largening the group of optimised variables and improving the quality of initial points. Homotopy-continuation (HC) method is employed to ease the convergence difficulties for solving the flowsheet with multiple recycle streams and scaling up the plant capacities between 100 $tNH_3\ d^{-1}$ and 600 $tNH_3\ d^{-1}$ from an initially feasible point.

Overall, the optimisation results reveal a clear hierarchy in the factors governing the techno-economic performance of green ammonia production. Reactor operating conditions, particularly synthesis pressure and catalyst bed inlet temperature, consistently converge to narrow ranges, demonstrating that reactor thermodynamics and compression trade-offs dominate the optimal process configuration. In contrast, separation and auxiliary thermal variables show wide feasible ranges, indicating a relatively weak influence on the LCOA. From an economic perspective, electricity price is the most critical external parameter, exerting a nearly linear and dominant impact on LCOA across all plant scales due to the electricity-intensive nature of hydrogen production and compression. Plant scale introduces a strong but secondary economy-of-scale effect, substantially reducing LCOA by diluting capital and manufacturing costs, especially between 100 and 300 $tNH_3\ d^{-1}$. However, as capacity increases, the capital- and manufacturing-related expenses become less dominant, while raw material costs (primarily linked to electricity for hydrogen production) emerge as the controlling factor. These results indicate that, beyond industrial-scale capacities, further cost reductions depend more on access to low-cost renewable electricity and improvements in process efficiency than on additional scale-up, while fixing strongly converged reactor operating conditions can enhance optimisation robustness with minimal economic penalty.

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