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Optimal design of decentralized ammonia production *via* electric Haber–Bosch systems

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Ammonia production, central to global food and energy systems, is highly centralized and fossil-dependent, consuming ~5% of global natural gas and creating supply chain risks due to long-distance transport. Decentralized, electrified Haber–Bosch systems offer a resilient alternative that can diversify supply and reduce emissions. This study develops an optimization model to assess the techno-economic feasibility of decentralized ammonia production across six representative locations (Brazil, India, China, the United States, Italy, and Ethiopia). We evaluate three configurations: autonomous (renewables only), grid-connected, and hybrid systems, under 2025 and 2045 cost scenarios. In 2025, decentralized systems remain uncompetitive, with levelized costs of ammonia often exceeding global market prices by more than 500 USD per tonnes in regions with low renewables potential. By 2045, declining renewables and electrolyzer costs narrow the premium: cost-effectiveness is achieved in the United States and Ethiopia, while China, Brazil, and India approach competitiveness with premiums of 175–435 USD per tonnes. Cost drivers vary by design: capital costs and financing conditions dominate autonomous systems, and electricity prices shape grid-connected plants. We show that coupling of intermittent renewables production, buffer capacities, operational flexibility of electrified Haber–Bosch reactors, and flexibility in ammonia demand are key to determining the cost of ammonia supply. High-pressure reactors and the thermal inertia of Haber–Bosch reactors can limit rapid ramping under variable renewable power, highlighting a core green chemistry challenge: current catalytic and reactor designs are poorly matched to fluctuating, low-carbon energy inputs, thus requiring high buffer capacities or a flexible demand. Sensitivity analyses indicate that higher conversion efficiency, lower specific energy use, and reduced dependence on hydrogen and battery storage or oversized renewable capacity are decisive for cost-competitiveness. These system-level results translate into quantitative design targets for green chemistry, indicating that catalysts, electrolyzers, and synthesis pathways that maintain high efficiency under dynamic and part-load operation are essential for sustainable nitrogen fixation. Overall, reductions in system-level cost and energy demand, and enhancements in operational flexibility and part-load operation are necessary to enable next-generation ammonia reactors that embody the principles of energy efficiency, waste minimization, and decentralized, safer chemical manufacturing to reach competitiveness for industrial-scale deployment.

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1. We develop and solve in relevant global geographies an optimization model to quantify the techno-economic trade-offs of electrified, decentralized ammonia production, comparing autonomous, grid-connected, and hybrid system designs. Results determine the optimal design of small-scale ammonia production *via* electric Haber–Bosch systems.
2. We identify the key challenges of electricity-driven Haber–Bosch systems: high energy demand, limited efficiency on a small scale, and strong impact of intermittent renewables production. We show that these constraints currently limit cost-effectiveness.
3. Because renewables-powered ammonia systems rely on technologies that perform reliably under variable electricity supply, chemists can meaningfully advance green ammonia production by developing synthesis pathways and electrolyzer designs that tolerate dynamic operation and maintain high efficiency at partial loads. Cost-effective systems require innovations that reduce the need for renewable oversizing as well as battery and hydrogen storage.

1. Introduction

Ammonia is emerging as a critical molecule at the interface of food and energy systems.[1] Historically, ammonia-based fertilizers have been indispensable to global agriculture, supporting

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nearly half of the world's population by enabling high-yield farming.[2] In 2020, global ammonia production reached 183 million metric tonnes (Mt NH_3), with about 70% used for fertilizers and the remainder consumed in industrial sectors such as textiles, explosives, pharmaceuticals, and plastics.[3] Global ammonia demand is projected to keep growing, fueled by population expansion, changing diets, and rising incomes.[4,5] Beyond its agricultural role, ammonia is increasingly recognized as a strategic energy vector, serving as both a carbon-free hydrogen carrier and a renewable fuel.[6–9] Meeting this dual demand for food and energy will require transformative changes in production pathways, supply chains, and resource allocation to ensure both climate compatibility and global energy security.[10]

Ammonia is synthesized almost exclusively through the Haber–Bosch process, an energy- and carbon-intensive technology over a century old.[11] Producing one kilogram of ammonia requires 7.7–10.1 kWh, with 90% of this demand tied to hydrogen generation.[12] Today, hydrogen for ammonia is overwhelmingly fossil-based: 70% from natural gas, 26% from coal, and 1% from oil, with just 0.1% from renewable electrolysis.[13] This dependence makes ammonia responsible for ∼450–500 Mt CO_2e annually (≈1.3% of global emissions) and 3–5% of global natural gas use.[14,15] Carbon intensity varies widely by feedstock: natural gas-based plants emit 1.6–1.8 t CO_2 per t NH_3, while coal-based routes emit 3.2–4.5 t CO_2 per t NH_3, excluding upstream methane leakage.[16] Beyond production, fertilizer application adds ∼660 Mt CO_2e each year, largely as nitrous oxide (N_2O), nearly 300 times more potent than CO_2, while transport adds another ∼30 Mt CO_2e.[14,15] Altogether, fertilizers contribute 1100–1300 Mt CO_2e annually, underscoring that although decarbonizing production is urgent for energy and food security, tackling use-phase N_2O emissions remains the greater long-term challenge.[17,18]

Globally, ammonia production is concentrated in 406 large-scale facilities, reinforcing a centralized model that maximizes economies of scale but increases reliance on fossil feedstocks, long-distance transport, and globalized markets.[3] Nearly half of fertilizers are traded internationally, meaning that 1.8 billion people depend directly on imports or imported natural gas for fertilizer supply.[2] This dependence exposes vulnerable regions, particularly in the Global South, to risks from energy price volatility, supply disruptions, and geopolitical shocks.[3] Transportation and distribution add both costs and emissions, while locking farmers into dependence on centralized supply chains.[3,19]

Decarbonizing fertilizer production is therefore urgent, but no single pathway is without trade-offs.[20] Carbon capture and storage (CCS) can reduce process emissions by 70%, yet it entrenches fossil dependence and requires costly infrastructure.[2,21] Biomass-based ammonia synthesis offers low-carbon potential but is constrained by resource availability and competing land uses.[22–25] Electrifying ammonia production through renewable hydrogen and electrically driven Haber–Bosch systems presents a promising pathway toward near-zero emissions.[21,26,27] On a large scale, this approach can replace existing fossil-based facilities, but it requires multi-gigawatt renewable energy infrastructure, significant land and water resources, and substantial upfront capital, often in the order of billions of dollars.[28,29] These constraints raise feasibility and siting challenges, particularly in regions with limited renewables potential or competing demands for land and water.[21,30] The emissions benefits also depend strongly on the power source; if the electricity grid is not fully decarbonized, life-cycle emissions can rival or even exceed those of fossil-based ammonia.[31,32] For this reason, centralized ammonia projects must be evaluated through location-specific assessments that balance production capacity with local resource availability.[21,33]

In parallel, decentralized, small-scale electrolytic ammonia plants are emerging as a complementary model.[26,27] These modular systems can operate closer to end-users, reducing reliance on long-distance transport and buffering agricultural regions against supply chain disruptions.[3,34] By lowering capital intensity and scaling down production to the regional or even farm level, decentralized plants could broaden access to low-carbon fertilizers and enhance both energy and food security.[3,34]

A growing body of research has explored the feasibility of decentralized ammonia production from both techno-economic and environmental perspectives. Early comparative studies benchmarked renewables-driven production processes against conventional centralized supply chains, highlighting cost and emissions trade-offs.[35,36] Subsequent work assessed decentralized solar-based plants in India, demonstrating that local renewable resources could enable viable small-scale systems under specific energy supply scenarios.[37] Decentralized electrocatalytic ammonia production powered by solar energy has also been shown to hold significant environmental advantages, although cost competitiveness remains a challenge.[34,38] Comparative assessments of small-scale electrochemical and plasma-based synthesis pathways further confirmed the technical promise of distributed production, while underscoring efficiency and cost barriers.[39] Parallel studies have evaluated renewable ammonia production under varying wind and solar resource potentials[40] and proposed its use as an energy storage medium for islanded systems.[41]

This study investigates the optimal design of decentralized ammonia fertilizer production *via* electric Haber–Bosch systems, focusing on techno-economic trade-offs across system configurations, cost trajectories, and renewable resource availability. From a green chemistry standpoint, ammonia synthesis represents one of the most energy- and carbon-intensive chemical transformations in modern society, making it a critical target for redesign under the principles of energy efficiency, safer chemical production, and reduced environmental impact. By quantifying the conditions under which decentralized systems can complement centralized production, this work contributes to identifying viable decarbonization pathways that reduce emissions, enhance fertilizer accessibility, and improve resilience in agricultural systems while enabling cleaner, modular chemical manufacturing powered by renewable electricity. Specifically, we conduct a techno-economic pre-feasibility assessment of small-scale Haber–Bosch technologies for on-site fertilizer production, estimating the levelized cost of ammonia (LCOA) under different technology and energy supply configurations. Production costs are shaped by capital and operating expenditures, catalytic and reactor performance, process design, and the integration of renewable or grid-based electricity supply.

The analysis is carried out for six representative global locations (Brazil, India, China, the United States, Italy, and Ethiopia) chosen to reflect diverse agricultural and energy contexts. Brazil is the world's largest soybean producer and heavily dependent on imported fertilizers;[3] India is among the largest fertilizer consumers, with rapidly growing demand;[3] China dominates global ammonia production, yet much of its capacity relies on coal;[3] the United States combines high fertilizer demand with direct ammonia use and established infrastructure;[16] Italy represents European conditions with aging ammonia facilities and strong decarbonization policies;[28] and Ethiopia highlights fertilizer access and food security challenges in Sub-Saharan Africa.[3] Together, these cases capture the interplay between agricultural demand, investment risk, and renewable energy profiles across different regions, illustrating how local energy and resource constraints shape the feasibility of green chemical manufacturing.

The novelty of this study lies in systematically quantifying techno-economic trade-offs across six diverse global regions while explicitly comparing autonomous, grid-connected, and hybrid configurations. We develop a detailed optimization model with hourly resolution, which enables a realistic representation of the dynamics between renewable energy supply and ammonia demand. Our approach explicitly captures temporal variability in electricity generation and system operation, which is central to assessing whether current catalysts, reactors, and electrolyzers can function efficiently under fluctuating, low-carbon power. A further contribution is the identification of optimal storage capacities, including battery and hydrogen storage, and the analysis of how their sizing shifts across diverse local renewable resource conditions and grid contexts, thereby quantifying the material and energy penalties imposed by today's inflexible chemical technologies. Finally, the study advances the literature by systematically quantifying the influence of key techno-economic parameters on the levelized cost of ammonia through a local sensitivity analysis, translating system-level outcomes into performance targets for green chemistry innovations, providing insights into which variables most critically determine system performance and cost-competitiveness.

Quantifying the cost of decentralized ammonia production relative to conventional fossil-based production helps identify the conditions under which localized, low-carbon fertilizers could achieve cost-competitiveness. By connecting chemical reactor performance, energy inputs, and material requirements to sustainability and cost, this work bridges systems engineering with green chemistry. By explicitly linking system design to local renewable energy conditions and grid electricity prices, this study provides insights into the scalability, costs, and trade-offs of decentralized ammonia systems. The findings are relevant to multiple stakeholders, including industrial firms exploring alternative production pathways, venture capital funds investing in clean technologies, policymakers designing incentives for sustainable fertilizer supply chains, and chemists and engineers developing the next generation of catalysts, electrolyzers, and synthesis routes for sustainable nitrogen fixation.

2. Technologies for ammonia and nitrogen fertilizer production

Fig. 1 provides a comprehensive overview of the feedstocks, technologies, and conversion processes involved in the production and application of nitrogen fertilizers. The conventional production method for nitrogen fertilizer production is the Haber–Bosch process, typically relying on large-scale facilities to maximize economies of scale.[42] This process begins with hydrogen production, primarily *via* steam methane reforming or coal gasification,[43,44] followed by ammonia synthesis in a high-temperature Haber–Bosch reactor. As this process relies heavily on fossil fuels (natural gas for reforming and coal for gasification), alternative production technologies, either ammonia-based or ammonia-free, have been investigated.[45–50]

Some innovative ammonia-based technologies (highlighted in blue) preserve the two-step ammonia synthesis conversion process but replace emission-intensive hydrogen production with low-emission technologies (Fig. 1). Among these, water electrolysis[51,52] produces hydrogen by splitting water molecules with oxygen as a by-product, while methane pyrolysis[53,54] decomposes methane into hydrogen and solid carbon. These technologies utilize electricity and heat as energy input depending on the process design (Fig. 1). Ongoing research and development efforts by universities and startups aim at improving the second step of ammonia synthesis by keeping a low unit cost while reducing the size, energy intensity, and carbon footprint of the Haber–Bosch reactor (Fig. 1). These approaches involve developing a low-temperature, small-scale electric Haber–Bosch reactor,[46] which is the objective of the techno-economic analysis in this study, or reactors based on non-thermal plasma synthesis,[48] photocatalytic nitrogen reduction,[55] or direct electrocatalytic nitrogen reduction.[56] In contrast, one-step ammonia production methods enable ammonia synthesis directly from air (oxygen and nitrogen) and electricity, bypassing the need for hydrogen as an intermediate product (Fig. 1).[57] The main ammonia-free route for nitrogen fertilizer production involves non-thermal plasma synthesis based on nitrogen oxidation, forming nitrogen oxides (NOx), which serve as precursors for the production of nitric acid and subsequently nitrate-based fertilizers (Fig. 1).[48,57,58] Although viable as a route for commercial nitrate-based fertilizers, the current industrial production process is predominantly ammonia-based, thus relying on the same large-scale high-

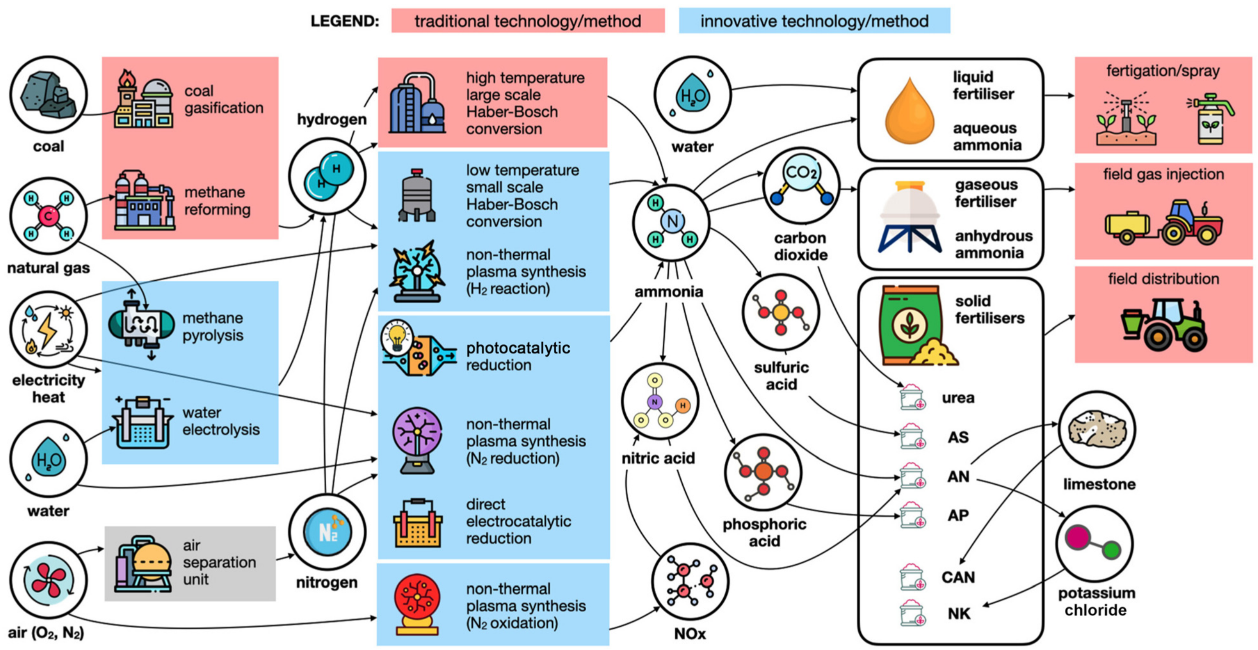

Fig. 1 Feedstocks, technologies, and application methods for synthetic nitrogen fertilizers. Nitrogen fertilizer production can follow fossil-dependent or fossil-free pathways, using ammonia-based or ammonia-free intermediate products. Red squares indicate traditional technologies/methods, while blue squares indicate novel technologies/methods. Main feedstocks include nitrogen from the air, coal and natural gas, and water. After production, ammonia is directly applied, or it is converted into other fertilizers before application on croplands. Fertilizer applications employ different machinery depending on the fertilizer's physical form (liquid, gaseous, or solid). AS: ammonium sulfate; AN: ammonium nitrate; AP: ammonium phosphate; CAN: calcium ammonium nitrate; NK: potassium nitrate.

temperature Haber–Bosch plants, in this case followed by the Ostwald process (Fig. 1).[48,57] Following its synthesis, ammonia molecules are converted into various nitrogenous fertilizers for agricultural application, available in gaseous, solid, or liquid forms, each necessitating distinct application methods.[59]

The application of ammonia in gaseous form offers the advantage of high nitrogen concentration but requires specialized pressurized storage and advanced machinery for underground injections to limit volatilization in air. Its application is primarily in the United States due to the significant investment in equipment, high toxicity, and the requisite of professional expertise for safe handling and application, representing only 3% of the current global nitrogen fertilizer market.[3,15] The production of solid fertilizers involves other compounds beyond ammonia, yielding products widely favored in agriculture due to their ease of transport, storage, and application without specialized equipment. Solid fertilizers in the form of prills, or granules, can be packaged in lightweight forms and distributed efficiently using mechanical fertilizer spreaders (Fig. 1). Urea (CH_4N_2O) is the predominant solid nitrogen fertilizer in the market, accounting for approximately 50% of the global synthetic nitrogen supplied to crops.[3,15] This molecule is synthesized from liquid ammonia reacting at high pressure with carbon dioxide, by-product of the same ammonia synthesis process:[43,44]

$$2NH_3 + CO_2 \rightarrow CH_4N_2O + H_2O \tag{1}$$

Ammonium sulfate (AS, $(NH_4)_2SO_4$) is obtained by reacting ammonia with sulfuric acid (H_2SO_4):[44]

$$2NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4 \tag{2}$$

Ammonium nitrate (AN, NH_4NO_3) is mainly derived from ammonia and the intermediate nitric acid (HNO_3):[43,44]

$$HNO_3 + NH_3 \rightarrow NH_4NO_3 \tag{3}$$

Calcium ammonium nitrate (CAN) is obtained from a solution of AN and calcium carbonate ($CaCO_3$) contained in dolomite or limestone powder,[43,44] while potassium nitrate (NK) is derived from AN and potassium chloride. AS and AN both contribute about 5% of the global market, CAN accounts for approximately 3%, while NK represents less than 1% of the global synthetic nitrogen supplied to crops.[3,15]

Ammonium phosphate (AP), most common in the form of mono- (MAP) or di-ammonium phosphate (DAP), is obtained by reacting ammonia with phosphoric acid (H_3PO_4):[44,60]

$$\begin{aligned} NH_3 + H_3PO_4 &\rightarrow NH_6PO_4\,(\mathrm{MAP}) \\ 2NH_3 + H_3PO_4 &\rightarrow N_2H_9PO_4\,(\mathrm{DAP}) \end{aligned} \tag{4}$$

Other less common phosphate-based nitrogen fertilizers include polyphosphate and nitrophosphate (NP).[60] Ammonium phosphate (AP) represents 7% of nitrogen supply, while NP accounts for 3%.[3,15] Compound fertilizers such as NPK formulations are produced by combining nitrogen-based (N) compounds (*e.g.*, AN, urea) with phosphorus-based (P) and potassium-based (K) compounds in different concentrations, representing roughly 17% of nitrogen delivery.[3,15] Urea-ammonium nitrate (UAN), which is a liquid fertilizer, is produced by combining urea with AN solution and covers 6% of the nitrogen supply.[3,15] Liquid fertilizers consist of aqueous solutions of ammonia (aqueous ammonia or ammonium hydroxide). Despite the lower nitrogen concentration due to dilution in water, liquid fertilizers facilitate application through spraying or existing irrigation infrastructure (fertigation), with simultaneous application of water and fertilizers.[61,62]

3. Methods

This section describes the methodological approach used in the techno-economic assessment of the decentralized electric Haber–Bosch technology for nitrogen fertilizer production. Section 3.1 provides details on the systems considered in this study as three possible configurations to install the technology. Section 3.2 defines the theoretical framework for the optimization problem to identify the system size and the local cost of production for each system configuration. Section 3.3 presents the case studies of this work, by providing details on the fertilizer demand distribution in the selected countries, and the specific areas used for the extraction of local conditions affecting the operation of the technology.

To ensure consistency, we fix a baseline production rate of 1 t NH_3 per hour (8760 t per year), irrespective of location. A detailed Mixed-Integer Linear Programming (MILP) framework is implemented in Pyomo and solved with the Gurobi Optimizer (v12.0.3),[63] optimizing both system sizing and operational strategies to minimize totalized costs, including capital and operational equipment expenditures. The model evaluates three system configurations: (i) a fully autonomous system powered by on-site solar and wind, (ii) a grid-connected system relying exclusively on imported electricity, and (iii) a hybrid combining local renewables with grid supply. Ammonia production through the electrified Haber–Bosch route is represented as a two-step process, water electrolysis followed by ammonia synthesis, with system boundaries encompassing hydrogen and battery storage. The optimization is performed for six representative global regions, selected to capture variation in agricultural demand, investment risks, and geographic conditions (Fig. 2).

3.1 Technology system description

This work focuses on small-scale electric Haber–Bosch technology for the onsite supply and use of ammonia-based synthetic nitrogen fertilizers in the proximity of agricultural farms. As an innovative application, with a limited number of operating pilot plants, this technology lacks a tested and proven standard configuration for commercial production.[13] Here, we explore three different configurations for installation of the technology, depending on the primary electricity supply (panel A in Fig. 2): (a) autonomous, (b) grid-connected, and (c) hybrid. For all the three configurations, we identify the optimal minimum

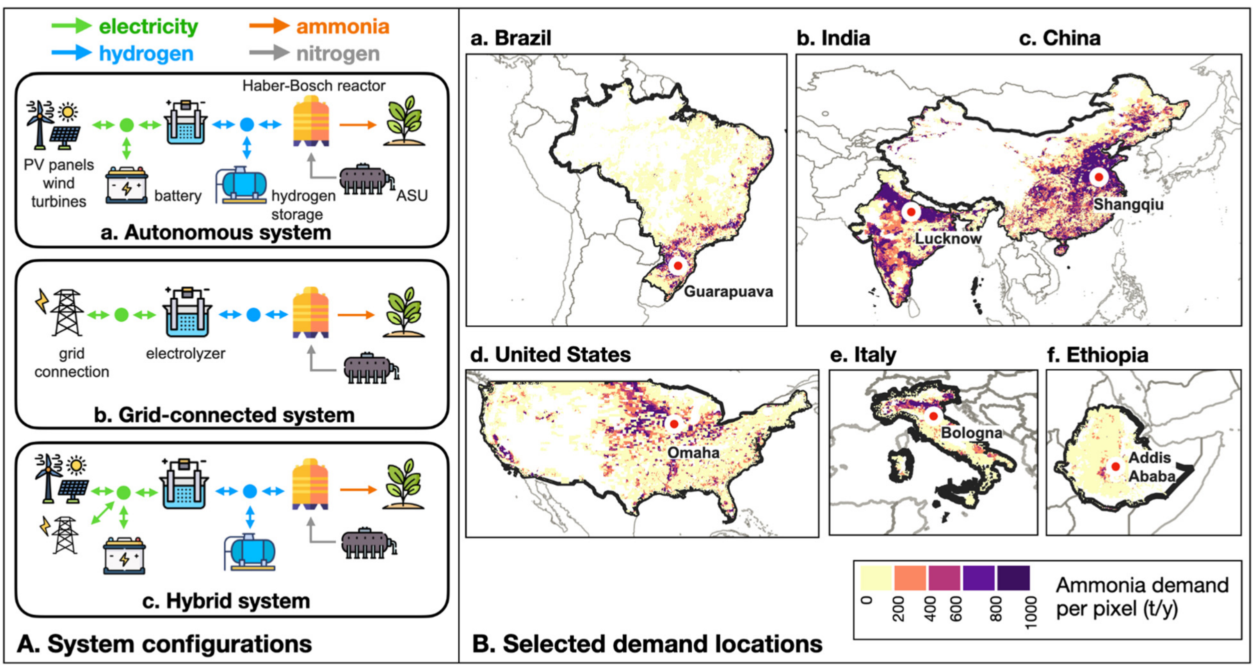

Fig. 2 Case study of analysis. Panel A represents the three system configurations considered for the techno-economic analysis: (a) autonomous system, (b) grid-connected system, and (c) hybrid system. Panel B summarizes the six locations selected to obtain the local conditions for the installation of renewable technologies: (a) Guarapuava in Brazil, (b) Lucknow in India, (c) Shangqiu in China, (d) Omaha in the United States, (e) Bologna in Italy, and (f) Addis Ababa in Ethiopia. Locations have been selected based on the ammonia demand distribution, and the respective data are reported in Table 1.

cost system design based on the average supply of 1 t NH_3 per hour.

3.1.1 Autonomous system. The autonomous system configuration is based on electricity production from an optimal combination of PV panels and wind turbines. This configuration is particularly advantageous in rural areas with limited access to grid connections to operate in islanded (off-grid) mode.[64,65] The size of this system is dependent on the intermittent nature of power production from renewable technologies. To identify the minimum-cost system to supply a predictable amount of ammonia, we allow the optimization model to adopt different ways to compensate for the power production intermittency: (i) oversizing of power production capacity, (ii) power curtailment, (iii) electricity storage in batteries, and (iv) energy storage in the form of hydrogen produced as an intermediate carrier. The model does not include any *a priori* assumptions on their role within the system, which is defined as the result of the optimization problem. Beyond power production and storage, electricity is converted into hydrogen with an electrolyzer which is the input of the Haber–Bosch reactor, fed with part of the electricity produced from the installed renewable technologies. The electric Haber–Bosch reactor, which is an innovative technology, is here modeled based on the reference literature.[46] Nitrogen, which is combined with hydrogen for ammonia synthesis, is supplied by an air separation unit (ASU), equally fed with electricity from the installed renewables. System sizing and operation are affected by limitations in the operation of each system's components. The requirement of operational stability in uninterrupted ammonia supply over a specific period is another technically relevant factor that determines the system size. No power sale injected into the grid is considered for the system under analysis, although it could create a positive cash flow to mitigate the system's costs, depending on country-specific remuneration policies. Additionally, no demand-side flexibility is considered, although its integration could represent a further dimension for cost reduction.

3.1.2 Grid-connected system. The grid-connected system configuration is based on electricity supply from the local power grid. Differently from the autonomous case, the optimization of this system leads to a design that does not require any storage means under the assumption that the system can always be fed with electricity from the local grid.

3.1.3 Hybrid system. The hybrid system combines both the options of electricity supply from the grid and electricity produced from dedicated PV panels and wind turbines. The combination of the different sources of power supply adds an additional dimension to compensate for the intermittent production of renewable technologies. Similarly to the autonomous case, we exclude the possibility of injecting electricity into the grid assuming that in real world applications, excess power would first be curtailed or used to satisfy the local demand of electricity in neighboring buildings before sale into the grid.

3.2 Optimization model and economic metric

3.2.1 Optimization model. The optimal design of the system for ammonia production from decentralized technologies is dependent on the potential and intermittent operation of local renewable technologies. A Mixed Integer Linear Program (MILP) is formulated to model the hourly operation of the system's components and define the optimal system size.[66]

The optimization problem minimizes the total system costs which consist of the total equipment cost assumed to be covered by an initial investment and the yearly operating costs, including feedstock and maintenance costs. Continuous decision variables are used to model the capacity of each component to be installed, and the hourly energy and mass balance. Binary decision variables are used to model the switch between charging and discharging in the operation of equipment storage components. Matrices and vectors of coefficients are derived from the input data of the optimization problem which consists of the ammonia demand, feedstock price, unit capital and operating expenses, and energy and mass conversion coefficients. Accordingly, the constraints of the problem include energy and mass balances, definitions of cost, and operating conditions of the system's components.

An extended description of the model's equations with respect to each system's components, and the main input data, is provided in the SI (section S2 – System optimization model). The model is coded in Python using the Pyomo library and solved with Gurobi Optimizer (version 12.0.3).[63]

3.2.2 Economic metric. Different economic metrics can be considered for the analysis of the cost of fertilizer production, affecting the selection of the metrics used in the comparison of the results. Here we focus on the levelized cost of ammonia (LCOA) (defined in eqn (6)), which allows us to compare the output product of the technology with main products currently traded in the fertilizer's commodity market. An equivalent metric, not used in this work but easy to derive from the LCOA, is the levelized cost of nitrogen delivered to crops (LCON) (eqn (7)). The LCON presents advantages when considering nitrogen fertilizer products from chemical processes that do not involve the intermediate formation of ammonia (*i.e.*, ammonia-free production processes, see Fig. 1). However, since most nitrogen fertilizer products on the market today are produced through processes involving ammonia as an intermediate product (Fig. 2), this study considers only the LCOA.

The LCOA is derived from the total equipment cost (C^{tot} (USD)), the total yearly operating cost (O^{tot} (USD per year)), the yearly ammonia produced (m_a (t per year)), and the cost of capital (r (−)), over the system's lifetime (T (year)):

$$\text{LCOA} = \left(C^{\text{tot}} + \sum_{j=1}^{T}\left(O^{\text{tot}}/(1+r)^j\right)\right) \Big/ \sum_{j=1}^{T}\left(m_\text{a}/(1+r)^j\right) \quad (5)$$

From stoichiometric considerations on the chemical composition of ammonia, which involves the molecular weight of one atom of nitrogen (MW_N = 14 g mol^{-1}) and three atoms of hydrogen (MW_H = 1 g mol^{-1}), the LCON is derived as:

$$\text{LCON} = \text{LCOA}\ (\text{MW}_\text{N} + 3\text{MW}_\text{H})/\text{MW}_\text{N} \quad (6)$$

Based on the assumptions behind the optimization model used (section S2 – System optimization model), the LCOA formula can be simplified as in eqn (7). This form emphasizes the different impact of the cost of capital (r) on the total CapEx (C^{tot}) compared with the total OpEx (O^{tot}) cost components:

$$\text{LCOA} = C^{\text{tot}} / \sum_{y=1}^{T} (m_{\text{a}}/(1+r)^y) + O^{\text{tot}}/m_{\text{a}} \tag{7}$$

The country-specific cost of capital is estimated based on the capital asset pricing model (CAPM):

$$r = R^{\text{f}} + R^{\text{p}} = R^{\text{f}} + \beta R^{\text{c}} \tag{8}$$

where R^{f} (–): mature equity market risk premium computed as the implied equity risk premium of the S&P500; R^{p} (–): country- and sector-specific risk premium; R^{c} (–): country-specific equity risk premium assuming Moody's sovereign rating measuring the country's default risk; and β (–): market-specific relative equity volatility (beta) from historical data of all companies in the green and renewable energy industry within the market region.

Data for country-specific cost of capital calculations are provided in the SI (section S1 – Cost of capital).

3.3 Case studies

We select a total of six countries, each representative of different agricultural activities, financial investment risks, and geographical locations (panel B in Fig. 2). In each country, we pick a reference location close to the region with the highest nitrogen fertilizer demand. It should be noted that the choice of specific reference points coinciding with cities follows communication purposes. Selected points are representative of local conditions for renewables installation near high demand-concentration regions, but they are not intended to indicate specific sites for installing the technologies discussed. Country-specific data discussed in the following are summarized in Table 1.

Brazil was chosen for its substantial total nitrogen fertilizer demand of 5.5 Mt NH_3 per year, associated with a mix of large-scale commercial farms and smallholder farms.[67] Brazil presents a mid-range cost of capital, approximately 6% (derived from a country-default risk of 2.5% (Table S1 in the SI)). Based on the demand concentration in the south of the country (panel B.a in Fig. 2), we considered Guarapuava as the reference point for the extraction of the local hourly capacity factor of solar panels (24.2% yearly average) and wind turbines (21.6% yearly average). The average electricity price is assumed to be 128 USD per MWh.

India and China (panels B.b and c in Fig. 2) were chosen due to their growing economies and nitrogen demand market size. The cost of capital of the two countries is approximately 6% and 5%, respectively (derived from a country-default risk of 2.2% and 0.7% (Table S1 in the SI)). Total nitrogen fertilizer demand in India and China amounts to approx. 20 and 30 Mt NH_3 per year, respectively. Based on the demand distribution, Lucknow was selected as a reference for local renewable conditions in North India (average capacity factor of 22% for solar and 23% for wind), and Shangqiu was selected in Central East China (average capacity factor of 19% for solar and 35% for wind). The average electricity price is assumed to be 126 USD per MWh for India and 94 USD per MWh for China.

The United States (panel B.d in Fig. 2) was selected as a leading country for research and development investments, as well as for the implementation of in-field pilot plants for decentralized nitrogen fertilizer production. The United States has the lowest cost of capital among the countries considered, approximately 4% (based on a country-default risk of 0% (Table S1 in the SI)). Total nitrogen fertilizer demand amounts to 12 Mt NH_3 per year, while average agricultural farms are large-scale and concentrated in the Midwest (the Corn Belt). Accordingly, we chose Omaha as a reference location for local conditions for the installation of renewable technologies, corresponding to an average capacity factor of 23% for solar and 51% for wind. This location has a wind capacity factor that is more than twice those of the other countries considered, except for China. The average electricity price is assumed to be 148 USD per MWh.

Italy (panel B.e in Fig. 2) was chosen as one of the most southern countries in Europe, with agricultural production concentrated in the North Plain area. The assumed cost of capital is 6% (from a country-default risk of 2.2% (Table S1 in the SI)), similar to Brazil and India, and almost half the cost of capital of Ethiopia which is the country with the highest risk considered. Total nitrogen fertilizer demand amounts to 0.6 Mt NH_3 per year and Bologna was considered as the reference area for representative renewable conditions. The average solar and wind capacity factors are approx. 20% and 26%, respectively. Due to high dependency on natural gas supply and power import, the country experiences one of the highest electricity prices in the European area, with an average of 442 USD per MWh.

Table 1 Case studies of analysis: renewables potential at locations considered in this study, country-specific ammonia demand, electricity price, and cost of capital from 100% equity

Case study country	Selected location	Solar PV cap. factor (yearly avg)[68]	Wind turbine cap. factor (yearly avg)[69]	Country's ammonia demand (Mt NH_3 per year)[70]	Electricity price (USD per MWh)[71]	Cost of capital[72]
Brazil	Guarapuava	24.2%	21.6%	5.5	128.0	6.36%
India	Lucknow	21.5%	23.1%	19.8	126.0	6.11%
China	Shangqiu	19.2%	35.0%	28.8	94.0	4.90%
United States	Omaha	23.2%	50.6%	11.8	148.0	4.33%
Italy	Bologna	19.4%	25.9%	0.6	442.0	6.09%
Ethiopia	Addis Ababa	26.4%	17.5%	0.5	19.0	11.64%

Finally, Ethiopia (panel B.f in Fig. 2) was chosen as an African country with a developing economy, high renewables potential and small-sized farms for agricultural production. The risk behind investing in this country is reflected in the high cost of capital of mostly 12% (from a country-default risk of 9% from Table S1 in the SI), which is mostly three times the lowest investment risk among the countries considered (United States). Total nitrogen fertilizer demand amounts to 0.5 Mt NH_3 per year. Although most homogeneously distributed in the inner part of the country, some demand concentration spikes are located close to Addis Ababa, which was selected as the reference location for renewables production. The average capacity factors are 26% and 18% for solar panels and wind turbines, respectively. Although grid electricity supply may be limited by underdeveloped network coverage, the average price of electricity is only 19 USD per MWh, an order of magnitude lower than those in the other countries considered and consistent with local purchasing power.

4. Results

This section presents the results of the optimization problem by focusing on the optimal system components' design (section 4.1), the resulting cost assessment (section 4.2), and the sensitivity analysis of the main parameters (section 4.3).

4.1 Installed capacity and costs of location-optimized systems

Fig. 3 presents the optimal system sizing and the yearly cost of installation of the main components for power production and storage in the three system configurations considered. Fig. 3a shows the capacities of the two power generation technologies, PV panels and wind turbines, the connection capacity for electricity imports from the grid ("grid import"), and the power associated with curtailed electricity ("curtailment"). Fig. 3b shows the capacities of the two storage technologies, battery and hydrogen storage. The respective cost of installation of each system's components and the cost of imports are shown in Fig. 3c and d.

Curtailment is only present in the autonomous system configuration, representing a maximum of 10% of the power produced from the installed PV panels and wind turbines (Fig. 3). In the autonomous system configuration, solar capacity and wind capacity are installed at mostly equal rates in the case presented (low-cost scenario for 2025). The largest PV capacity, 52 MW, is installed in Ethiopia, while the largest wind capacity, 46 MW, is installed in India (Fig. 3a), corresponding to an annualized CapEx of 9 million USD per year and 5 million USD per year, respectively (Fig. 3c). Different heights in the bar chart in Fig. 3a are due to the different capacity factors of the power supply sources, requiring larger capacities in locations with the lowest capacity factors: 87 MW in Ethiopia (autonomous system) with an average solar–wind capacity factor of 22% and 46 MW in the United States with an average solar–wind capacity factor of 37% (Fig. 3a). The grid connected system does not present any variation since a continuous power supply of 14 MW capacity is considered for all locations (Fig. 3a). The hybrid system allows the selection of the cheapest source of power supply. The low-cost price of electricity in Ethiopia implies the hybrid system's configuration to be equal to the grid-connected system, while the high-cost price of electricity in Italy implies the hybrid system's configuration to be mostly equal to the autonomous system.

Fig. 3b presents the installed capacities of storage technologies. No storage is installed in the case of the grid-connected system configuration. The largest storage capacity is installed in India, composed of 11 MWh of battery storage and 1553 MWh of hydrogen storage, which correspond to a yearly investment of 544 k USD per year and 2.2 M USD per year, respectively (Fig. 3d). The main storage technology is based on hydrogen, with a maximum installed battery capacity in Ethiopia of 17 MWh (1.5 M USD per year) (Fig. 3b and d). No storage is required in Ethiopia in the case of the hybrid configuration, due to the optimal system being equivalent to the grid-connected system with no intermittent power supply. In Italy, while the battery is installed in the case of an autonomous system, in the hybrid system configuration, battery storage is replaced by a small amount of power import, with a capacity limited to 15 kW (Fig. 3b compared with Fig. 3a).

4.2 Breakdown production cost of ammonia

Fig. 4 shows the breakdown of the levelized cost of ammonia (LCOA) for the three system configurations in each country considered. The results are presented based on the six locations considered which are representative for different renewables potential, two scenarios (low, high) accounting for parameters' cost variation within the same year, and two years (2025, 2045) accounting for the technological development over 20 years.

Under no conditions, cost-competitiveness is realized for 2025 cost assumptions. In the autonomous and hybrid system configurations (Fig. 4a and b), the largest cost components are related to the cost of capital (dark purple stack), the CapEx of PV panels and wind turbines (light green and yellow stacks), and the CapEx of the electrolyzer (red stack). When compared with the United States average early 2025 market price of 525 USD per ton of ammonia,[74] the cost-competitiveness of decentralized ammonia production is only reached in the 2045 cost scenario, specifically in the United States. China, Brazil and India are not far from cost-competitiveness, yet in these countries the decentralized technologies present a premium with the market reference between 175 and 435 USD per t in 2045 in the average cost scenario (Fig. 4a and b). The installation in Italy is limited by the low-capacity factor for wind, while the installation in Ethiopia is both penalized by a low wind capacity factor and high cost of capital compared to the other locations. In contrast, in the grid-connected system configuration (Fig. 4c), Ethiopia presents the lowest LCOA in 2045. The reasons behind this result reflect both the low electricity price in Ethiopia and the fact that the impact of the cost of capital in the LCOA calculation scales with the total CapEx. In a grid-connected configuration, where the largest fraction of

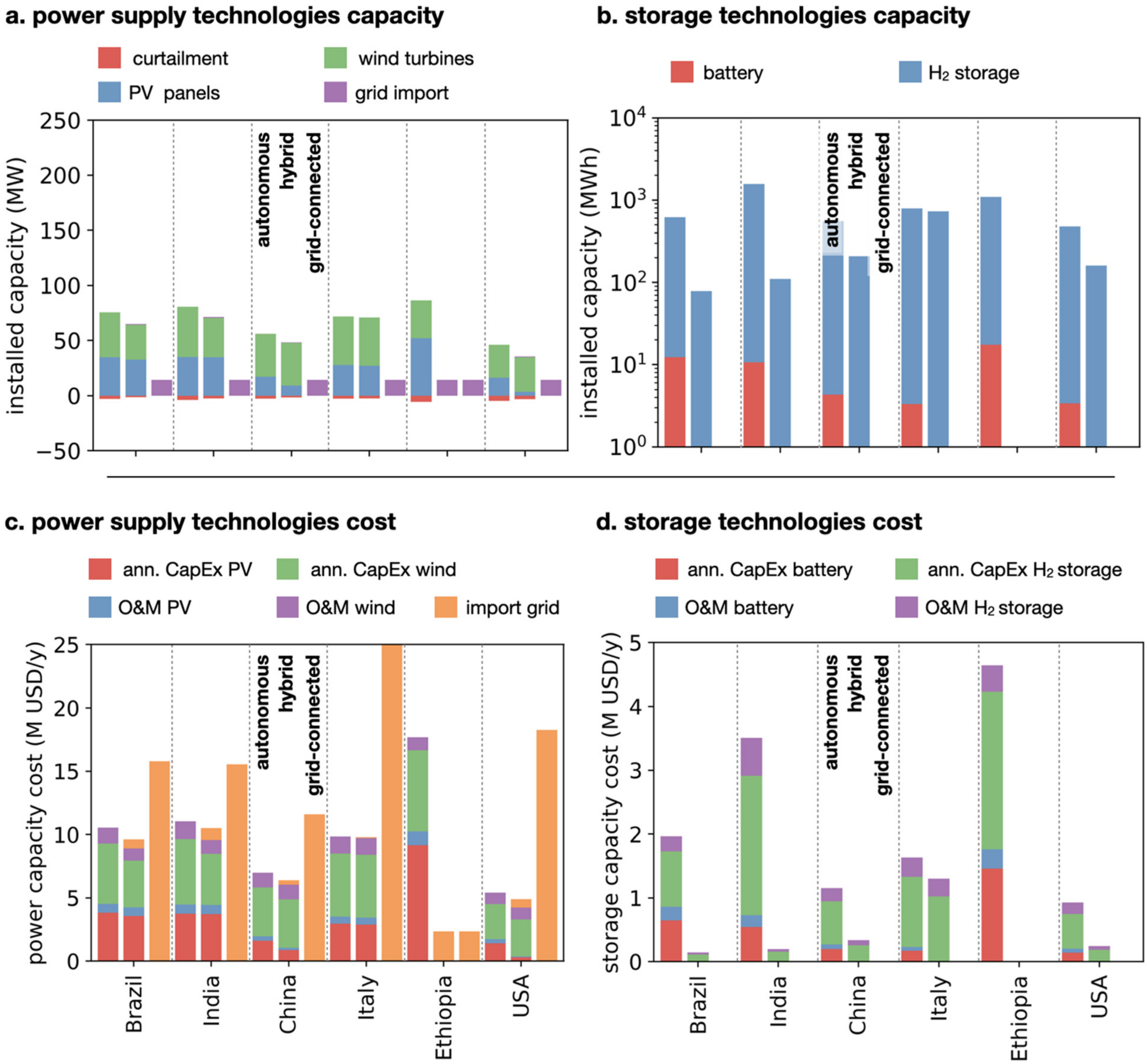

Fig. 3 Capacities and costs of installed power production and storage technologies in different system configurations. (a) The installed capacities of power supply sources, namely PV panels, wind turbines, and grid import. (b) The capacity for battery and hydrogen storage technologies. Technology CapEx is presented as annualized (ann. CapEx) over the 30 years of plant lifetime (see section S5 (Design scenarios comparison) in the SI) for comparison with the yearly cost of electricity imports. (c) The cost of the system's components for power production and (d) the cost of storage components. The installed renewable power capacity is based on local capacity factors (see Table 1), while the curtailment capacity and grid import are based on a load of 8760 h per year. Results are presented for the low-cost scenario in 2025. Log-scale is used for the *y*-axis in (b) to highlight the battery's capacity. Other scenarios are reported in section S5 in the SI.

the costs is the electricity purchase, even a high cost of capital has a limited impact on the LCOA. As expected, the largest LCOA in the grid-connected configuration is presented by the case of Italy, due to electricity prices more than three times higher than those of the other countries. Finally, the hybrid configuration presents the advantage of exploiting both high renewable capacity factors and low electricity prices, leading to cost-competitiveness for both the United States and Ethiopia, and a premium with the market reference between 150 and 350 USD per t NH_3 in 2045 in the average cost scenario for China, Brazil and India. In the case of Italy, the high electricity price leads to hybrid and autonomous systems having the same LCOA, while in the case of Ethiopia, the lowest electricity price leads to hybrid and grid-connected systems having the same LCOA.

The cost of capital affects the LCOA most substantially in the case of high CapEx configuration systems, which include the autonomous and hybrid configurations. In the case of power supply from the grid, the CapEx is limited to the installation of the electrolyzer and the Haber–Bosch reactor, thus limiting the impact on the LCOA. Based on the expressions defining C^{tot} and O^{tot} (see section S2.1 (Model formulation) in

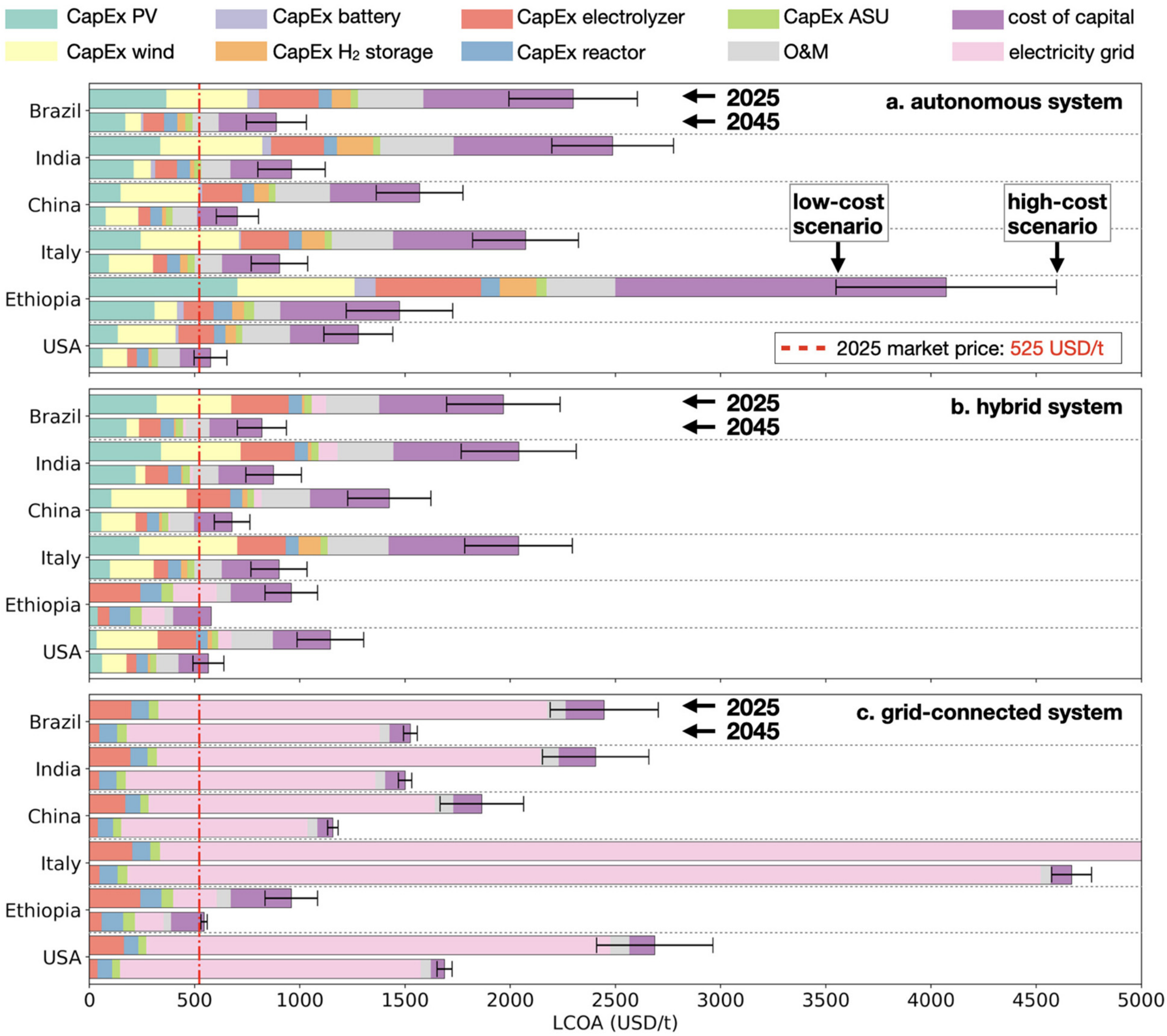

Fig. 4 Breakdown of the levelized cost of ammonia (LCOA) by system's components and cost of capital. The LCOA is specific to the system considered: (a) autonomous, (b) hybrid, and (c) grid-connected. The error bar is representative of the LCOA range of variation depending on different cost-scenarios.

the SI) combined in the total cost of the system, the total system's cost varies linearly with the yearly amount of ammonia produced. Results can be generalized to any ammonia demand, under the assumption that the system design remains the same as the optimal design obtained by considering site-specific renewable conditions and cost scenarios. The main differences in LCOA are observed among different locations, where different solar PV and wind turbine hourly operations determine different storage components' size, curtailment, and import from the grid.

4.3 Sensitivity analysis of production costs

After deriving reference cost estimates for 2025 and 2045, we study the impact of specific variables on the LCOA. Fig. 5 presents a local sensitivity analysis obtained by varying input parameters of the optimization model and by controlling some decision variables in a 2035 cost-scenario (intermediate scenario between 2025 and 2045). To study the impact of system components' size and local parameters on the LCOA, the original MILP problem is converted into a linear problem (LP) as detailed in section S3 (Local sensitivity analysis) of the SI. We run the LP problem while controlling the decision variables whose values, representative of system components' size and operation, depend on the hourly resolution of the model, such as the battery and the hydrogen storage size, and the amount of electricity. It should be noted that the range of variation of the parameters in the sensitivity analysis is derived from the case studies over the different locations analyzed above. This sensitivity analysis helps to estimate a reference LCOA without running a location-specific complete system optimization problem with hourly resolution.

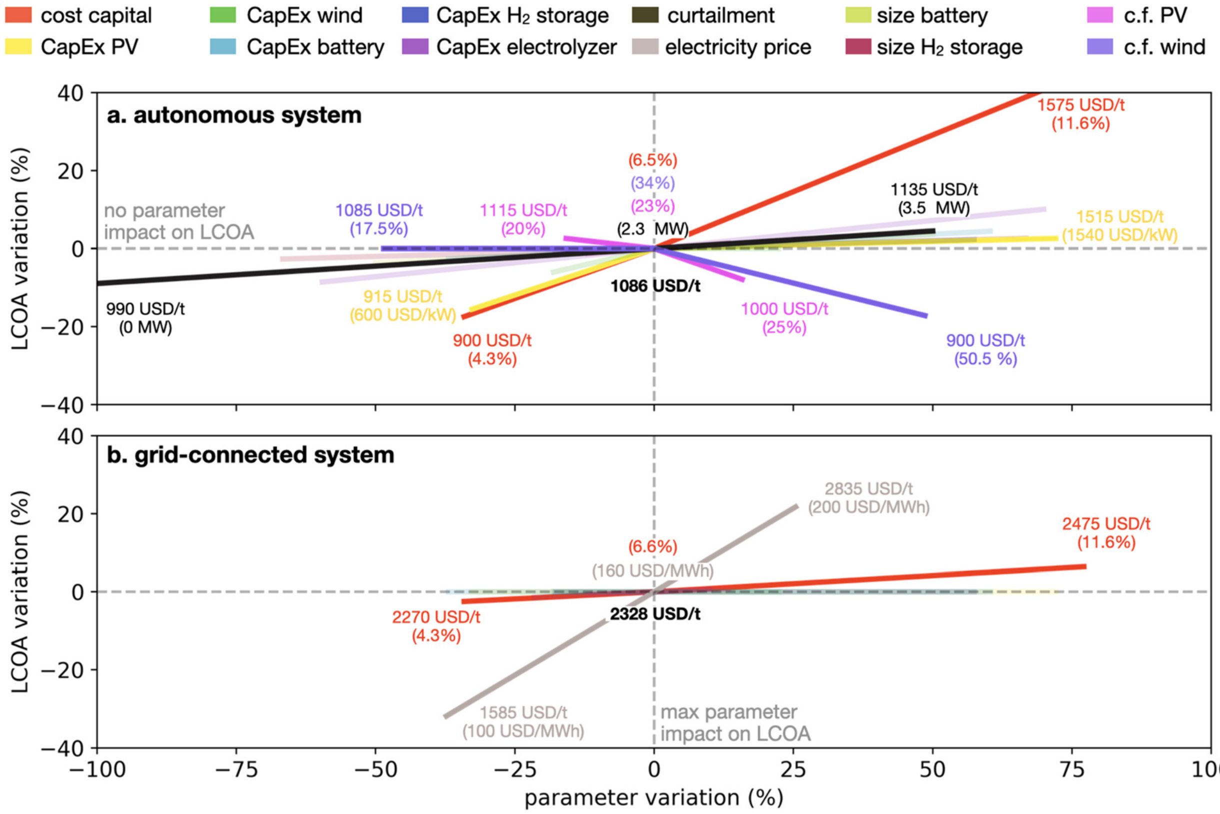

Fig. 5 Sensitivity analysis of LCOA. The analysis is specific to the two extreme system configurations considered: (a) autonomous and (b) grid-connected. The figure shows the influence of selected variables and parameters within their domain of variation. Values in brackets correspond to the control parameter's values, modified within the sensitivity analysis. Variables with the greatest impact on the LCOA (solid colored lines) determine steeper slopes, approaching the vertical dashed line, while variables with minimal impact (light colored lines) determine flatter slopes, approaching the horizontal dashed line. The model used for sensitivity analysis is a linear optimization model with a time resolution of one year. Design variables dependent on hourly resolution are replaced by fixed parameters whose values are set based on the location-specific case studies analyzed within this work. Legend: "c.f." = capacity factor. Table S4 in the SI summarizes the values of the parameters of the optimization model used to run the sensitivity analysis.

In both the autonomous (Fig. 5a) and grid-connected (Fig. 5b) system configurations, the cost of capital (red line) is one of the parameters affecting the LCOA the most. In the autonomous system, which is the most CapEx-intensive system, the cost of capital affects the LCOA between −20% and +40% when varying the cost of capital from the reference 6.5% to the minimum 4.3% (United States) and the maximum 11.6% (Ethiopia). For the same values of cost of capital, the variation of LCOA in the grid-connected system is lower than ±10%. The average capacity factors of PV panels and wind turbines substantially affect the LCOA in the autonomous system cost, leading to approximately 10% reduction of LCOA in the case of a high PV capacity factor (PV capacity of 25% *vs.* 23%) and approximately 20% reduction of LCOA in the case of a high wind turbine capacity factor (wind capacity factor of 50.5% *vs.* 34%) (Fig. 5a). In the autonomous system, curtailment can lead to a 10% reduction in LCOA when it's constrained to 0 MWh and about a 5% increase in LCOA when the curtailment is increased from the reference 2.3 MW (20 GWh) to 3.5 MW (31 GWh). The price of the electricity imported from the grid is one of the factors affecting most substantially the LCOA in the grid-connected system (Fig. 5b). A 25% increase in electricity price, from the reference 160 USD per MWh to 200 USD per MWh, leads to an LCOA increase of 20%, while a 38% reduction, from the reference 160 USD per MWh to 100 USD per MWh, leads to a 32% reduction in LCOA. The total amount of electricity imported in the grid-connected system in the model varies linearly with the ammonia demand, depending only on the electrolyzer and electric Haber–Bosch reactor conversion efficiencies. It should be noted that ammonia demand is not considered among the selected parameters of the local sensitivity analysis due to the independence of the modelled LCOA from the amount of ammonia produced (see section 5).

5. Discussion

This work demonstrates the potential and challenges of decentralized, electrified ammonia production as a complement to the prevailing centralized model. The novelty lies in systematically quantifying techno-economic trade-offs across six diverse global regions while explicitly comparing autonomous, grid-connected, and hybrid configurations. While centralized ammonia production remains dominant, its dependence on fossil fuels, concentration in ~400 facilities, and exposure to geopolitical and price shocks threaten both energy and food security. Decentralization offers a resilience strategy: reducing transport dependence, diversifying supply, and placing production closer to demand.[75]

Our findings underscore that decentralized ammonia production is not a one-size-fits-all solution, but rather a context-dependent technology whose viability varies across regions and system designs (Fig. 4). Under 2025 cost assumptions, no configuration reaches competitiveness with global market prices, with autonomous systems in particular facing prohibitively high costs due to the dominance of capital-intensive components such as solar PV, wind turbines, and electrolyzers. For example, in Ethiopia, high financing costs and low wind capacity factors push autonomous costs far above market levels, while in Italy, high electricity prices make both autonomous and hybrid systems equally uncompetitive (Fig. 4). By contrast, grid-connected systems shift the burden from CapEx to electricity purchases: in Ethiopia, where power prices are low, the grid-connected configuration achieves the lowest LCOA globally by 2045, even though financing remains expensive. By mid-century, technological improvements and cheaper renewables narrow the cost premium substantially, with the United States achieving market parity across all system types, while Brazil, India, and China remain within a 175–435 USD per t NH_3 premium. Hybrid systems show promise by flexibly leveraging both renewables and low-cost electricity: they achieve competitiveness in the USA and Ethiopia by 2045, while narrowing the gap to 150–350 USD per t NH_3 above market levels in China, Brazil, and India.

Sensitivity analysis confirms that financing costs dominate outcomes in CapEx-heavy systems, altering the LCOA by −20% to +40%, while renewable resource quality can lower costs by up to 20%. In grid-connected designs, by contrast, electricity prices are the decisive factor, with a 25% increase raising costs by 20%, and a 38% reduction lowering them by nearly one-third. These results highlight that decentralized ammonia production can only cover a fraction of future fertilizer demand and will do so most effectively when tailored to regional energy conditions, whether as collective-use facilities for cooperatives and plantations, modular units for farms, or hybrid systems balancing renewables with grid supply. Where organic fertilizers such as manure are abundant,[73] green ammonia will struggle to compete, reinforcing the need for a diversified portfolio of nutrient sources.

A key message from this study is the central importance of operational flexibility in ammonia synthesis. The flexibility of the Haber–Bosch reactor – strongly tied to its operating pressure, temperature, and ability to ramp production up or down – directly determines how much electricity and hydrogen storage the system needs.[77] Greater reactor flexibility reduces storage requirements, which in turn lowers the LCOA by cutting the CapEx of storage components. Two technical parameters are particularly influential: (1) the allowable hourly variation in ammonia output, currently limited to ±30% (see eqn (S39) in the SI), which constrains how dynamically the system can respond to fluctuations in renewable power, and (2) the temporal window over which production must match demand, presently set at 30 days (see eqn (S44) in the SI). If a reactor can tolerate wider hourly production swings or balance production over shorter periods, it enables tighter integration with intermittent renewables and significantly improves system-level performance.

Emerging low-temperature, modular technologies, such as electrocatalytic ammonia synthesis[49] and plasma-assisted[49] pathways, offer promising routes to overcome these constraints because they inherently operate under conditions more compatible with fast ramping, partial loads, and distributed deployment. However, these approaches remain at TRL 2–3,[48,49] and more research is still needed to improve efficiency, selectivity, and stability before they can meaningfully shift the system optimum.

A key insight is that the premium of decentralized ammonia production should not be understood solely as an economic disadvantage, but as the cost of decentralization and fertilizer self-sufficiency rather than a carbon price. Importing nations that are heavily reliant on the existing centralized system may view this premium as a strategic investment in supply chain resilience, energy and food security, akin to policies supporting domestic fuel reserves or renewable deployment. By offsetting the decentralization premium through national security frameworks, governments can justify localized production even when electricity is not fully decarbonized, not only on decarbonization grounds but also as a hedge against trade disruptions, supply shocks, and geopolitical dependencies.

Decentralization also carries operational and safety constraints. Gaseous anhydrous ammonia, still directly applied in the USA, poses significant handling risks, requiring strict training and safety protocols.[76] Alternative fertilizers such as urea or ammonium sulfate are safer but entail additional processing steps, energy use, and cost. Addressing these trade-offs is critical if decentralized production is to be viable at the farm gate.[76]

While electrification and decentralization enable pathways toward lower-emission ammonia, they do not guarantee climate benefits. The carbon intensity of electrolytic ammonia production depends critically on the emissions profile of the electricity supply. In regions with carbon-intensive grids, electrolyzer-based hydrogen and electric Haber–Bosch systems can produce more CO_2 per tonne of ammonia than conventional steam-methane reforming,[31,32] despite using cleaner process chemistry. For this reason, we avoid treating electrified ammonia production as inherently "green" and instead frame it as a potentially low-carbon, modular, and flexible production pathway whose environmental performance is contingent on the electricity system it is coupled to. This distinction is essential for green chemistry: sustainability arises not only from cleaner reaction pathways, but also from their integration with low-carbon energy and materials flows. Our results therefore emphasize decentralization, electrification, and operational flexibility as enabling platforms for sustainable ammonia, while recognizing that achieving genuinely low-carbon nitrogen fixation ultimately requires parallel decarbonization of the power sector.

Policy support will be decisive. Our results show that financing costs and electricity price trajectories dominate competitiveness. Concessional loans or guarantees could lower the cost of capital for CapEx-heavy autonomous and hybrid systems, while electricity market reforms could stabilize prices for grid-connected designs. Targeted regional incentives should prioritize areas where decentralized production can undercut imported fertilizers, particularly in Sub-Saharan Africa and parts of Latin America. Beyond economics, policies must also explicitly recognize that the premium represents the cost of strategic autonomy, ensuring continuity of fertilizer supply even when international markets fail.

Finally, this study is bounded by several assumptions. We did not impose constraints on land availability for renewable deployment or limits on grid interconnection capacity, nor did we account for the full lifecycle inventory of decentralized systems.[77,78] Future work should extend the analysis to include environmental trade-offs such as land and water use,[79] N_2O emissions mitigation from improved fertilizer management, and potential displacement by organic sources. Incorporating fertilizer transport costs, national security benefits, and resilience gains into life-cycle assessments will further clarify the context in which decentralized ammonia production provides the strongest value.

Taken together, decentralized ammonia production is best understood as a complementary pathway: not a wholesale replacement of centralized production, but a strategic tool to diversify supply chains, enhance resilience, and decarbonize fertilizer production where conditions are favorable, even when this requires paying a premium as the price of security and self-sufficiency.

6. Conclusions

Improvements in ammonia synthesis should target parameters that strongly influence system-level performance, particularly reactor energy demand, operational flexibility, and electrolyzer efficiency. The sensitivity analysis shows that applications with higher conversion efficiency, lower specific energy consumption, and reduced reliance on large storage volumes or oversized renewable capacity led to production costs that are competitive with centralized ammonia plants. This means that gains in catalyst activity, current density, operating pressure/temperature, or start-up/shut-down flexibility can shift the optimal configuration toward pathways that rely less on capital-intensive power and storage systems. Chemists can therefore contribute by developing ammonia synthesis routes (electrochemical, catalytic, or hybrid) that operate efficiently under variable power input, tolerate dynamic conditions, or reduce compression and separation energy requirements. The study suggests a valuable design target: if a new pathway can reduce energy consumption below the threshold that triggers large hydrogen or battery storage installation, the system transitions to a substantially cheaper optimal design. Thus, chemists can use the identified sensitivity levers (energy intensity, flexibility, and efficiency) as concrete performance benchmarks to guide innovation in next-generation ammonia synthesis.

Author contributions

LR conceived the study. DT and LR designed and wrote the study. DT developed the optimization framework, implemented the coding, and prepared the input data. DT and LR analyzed the results and conducted the research.

Conflicts of interest

The authors declare no conflict of interest.

Data availability

All data required to replicate the results of this study, including input parameters, modeling assumptions, and output data, are provided in the main text and the supplementary information (SI).

Supplementary information with additional results and methods is available. See DOI: https://doi.org/10.1039/d5gc06782k.

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