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Multi-Scale Design for Clean Energy Systems: Industrial Electrification and Flexible Operation of Ammonia Synthesis

Nicholas N. Kalamaris[a], Christos T. Maravelias[ab]*

[a] Princeton University, Department of Chemical Engineering, Princeton, New Jersey, United States of America
[b] Andlinger Center for Energy and the Environment, Princeton, New Jersey, United States of America
* Corresponding Author: maravelias@princeton.edu.

ABSTRACT

Flexible, electrified systems for chemical and energy production are promising alternatives to traditional, hydrocarbon-based processes. Flexible systems have the potential to reduce costs and emissions, but the interconnection between design and operation makes these systems challenging to implement. We use an operation-informed design framework to model a flexible, electrified ammonia synthesis system. We examine the levelized cost and carbon intensity of ammonia in response to different grid emissions (0-420 kg/MWh). We find levelized costs from 700-1200 $/ton-$NH_3$ and observe non-monotonicity in carbon-intensity with respect to grid emissions. We rationalize this trend as a design transition from large, grid-reliant systems to smaller, flexible designs that are grid independent. We then study how synergies in demand and unit-operation flexibility can lower both the price and carbon-intensity of ammonia production. We find that for seasonal, or yearly demand (rather than hourly), a fully flexible Haber Bosch process can achieve 20% lower costs and reduce its carbon-intensity by ~70-100%. We highlight major challenge in decarbonization, but also the importance flexibility plays in reducing carbon-intensity. Together, these analyses demonstrate that flexibility helps electrified industrial systems achieve financial and environmental goals.

Keywords: Multiscale Modelling, Energy Systems, Process Design

INTRODUCTION

Global manufacturing relies on chemical and energy systems to interconvert matter and energy. Fundamental production processes for energy, commodity chemicals, and construction material are the basis of the international supply chain. Fossil fuels serve as cheap precursors for these processes, but petroleum resources dwindle as material and energy demand increase. The future security of manufacturing requires a switch to sustainable production.

Flexible, electrified systems are attractive alternatives to traditional processes because they can selectively access intermittent renewable power, avoid operation during energy price spikes, and participate in demand response programs. Despite these benefits, flexible systems struggle to penetrate the chemical sector due to challenges in design and operation. Many unit operations have limited flexibility, requiring mass and energy storage devices to buffer their exposure to variability. The interplay between storage, flexible, and inflexible units creates a challenging problem; the optimal design depends on the holistic operation of the system. Newly developed frameworks for operation-informed design can be implemented to understand how chemical and energy systems respond to multi-scale variability [1]. These frameworks can also be used to identify transitions in design and operation for different conditions such as energy availability, grid renewability, and demand side flexibility.

To identify and address systemic challenges in decarbonization, we implement an operation-informed design framework to perform a case study on electrified ammonia synthesis. Previous studies have examined the levelized cost of ammonia (LCOA) for electrified systems [2, 3, 4]. However, these studies do not fully examine the

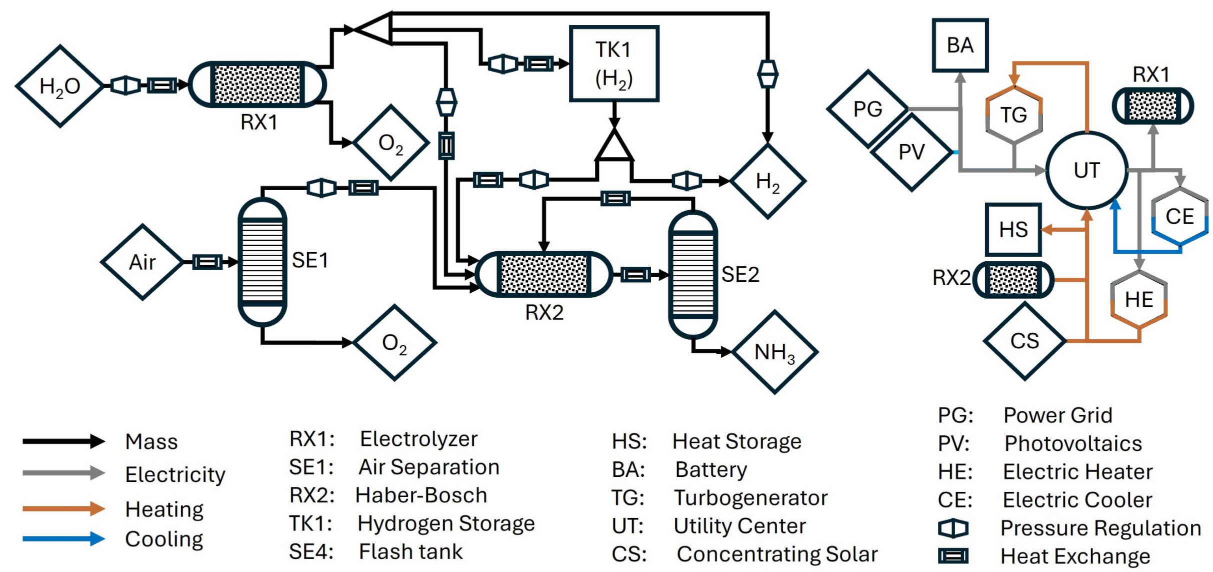

Figure 1. Superstructure for flexible, electrifed, ammonia sythesis. The system is connected to the power grid, and can also generate and interconvert power from solar irradiance onsite. Mass and energy storage allow for flexible operation in response to variability in energy price, availability, and associated emissions.

interplay between optimal design and operation. They are either simulation based (and require a pre-supposed design) or focus on operation under uncertainty, and sacrifice detail in terms of the system design and unit models. Recently, studies have suggested that process flexibility can positively impact the environmental and economic outcomes of ammonia synthesis [5, 6]. However, they utilize coarse grain system models and focus broadly on ammonia synthesis across different locations and modes of production. More detailed models exist in the context of process control, but do not optimize design [7].

The operation-informed design framework we use captures non-linearities in design (economies of scale) and operation (thermodynamics) in a single mathematical program. We use this to study the impact of grid emissions on the environmental and economic outcomes of this system. We then understand these outcomes by examining transitions in optimal design and operation. We also analyze the synergy between unit-operation and demand flexibility to identify conditions that can reduce the cost and carbon intensity of electrified ammonia production.

METHODS

Superstructure

We consider a system superstructure for flexible, electrified ammonia synthesis (Figure 1). The system can utilize grid electricity (≤ 1 GW) or generate power onsite using photovoltaics and/or concentrating solar units (≤ 10 km^2 total panel area). We utilize an emission penalty of 300 \$/ton-CO_2 for grid related emissions [8]. Heating, cooling, and electricity can be interconverted using power conversion units (heaters, coolers, turbogenerators). Hydrogen is generated via water electrolysis, and nitrogen is purified using cryogenic distillation of air. Hydrogen and nitrogen are converted to ammonia according to the Haber-Bosch reaction. The system can install hydrogen storage (≤ 1500 m^3), as well as electricity and heat storage (≤ 500 MWh each). All units are assumed to be flexible except for the Haber-Bosch reactor, which has limited flexibility.

Time Structure

The time-structure for the system is a 30-year time horizon with six epochs, each corresponding to five-years. An epoch is represented by a one-year operating period composed of four seasons. Each season contains representative days chosen from 3-years of power-grid data (Figure 2). The representative period accounts for hourly variability in electricity price, grid emissions, and solar irradiance using data from the CAISO grid [9, 10, 11].

Representative days for a season are generated using an IP clustering algorithm which groups individual days around a representative [1]. The algorithm minimizes the distance between all days and their representative at a fixed cost per representative. The time points in a representative day are weighted by the number of days they represent; representatives for larger clusters are weighted more heavily than smaller clusters (which typically represent atypical days). The representative days are hierarchy concatenated to form a season and subsequently a year, which is used as the operating period for the epoch. We allow for discontinuity in process operation between, but not within, seasons. We do not consider retrofitting in this analysis, and the operation across epochs is repeated.

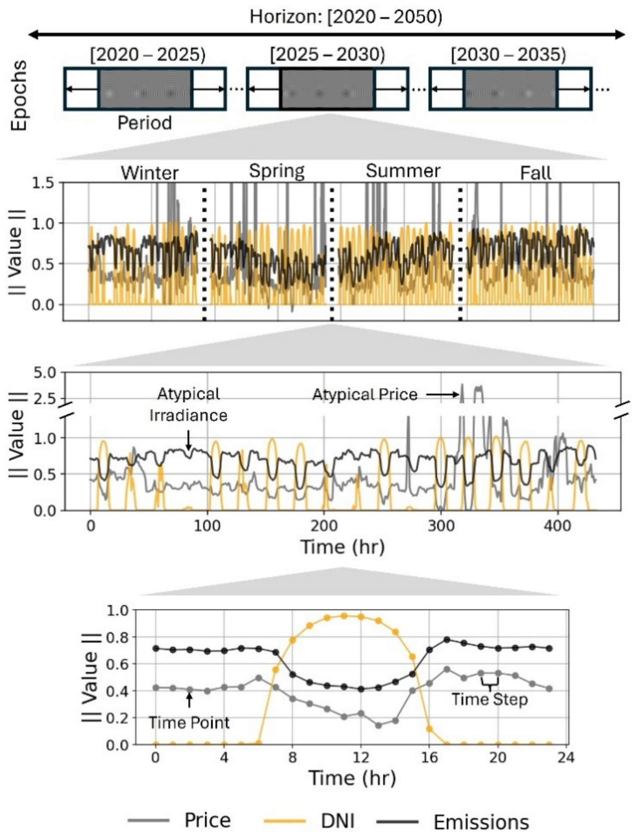

Figure 2. A 30 year horizon is partitioned into six epochs of five years. Epochs corresponds to a representative year with four seasons. Seasons are composed of representative days at an hourly resolution.

Mathematical Program

We utilize an operation-informed design framework to formulate a mathematical program for the system. This framework includes unit models for conversion reactors, separators, heaters, coolers, expanders, compressors, as well as mass and energy storage. Each unit has constraints enforcing mass (eq. 1) and energy (eq. 2) balances, as well as thermodynamic relationships (eq. 3) as described in [1].

$$
\begin{aligned}
\min \quad & C_{NH3} & & \\
\text{s.t.} \quad & \mathbf{m}(\mathbf{x}_t, \mathbf{x}_{t-1}) = 0 & \forall\, t \in \mathbf{T} \setminus \mathbf{T}^0 \quad & (1) \\
& \mathbf{e}(\mathbf{x}_t, \mathbf{x}_{t-1}) = 0 & \forall\, t \in \mathbf{T} \setminus \mathbf{T}^0 \quad & (2) \\
& \mathbf{h}(\mathbf{x}_t) = 0 & \forall\, t \in \mathbf{T} \quad & (3) \\
& \mathbf{l}(\mathbf{y}) \leq \mathbf{o}(\mathbf{x}_t) \leq \mathbf{u}(\mathbf{y}) & \forall\, t \in \mathbf{T} \quad & (4) \\
& \text{NPV} = 0 & & (5)
\end{aligned}
$$

Here, $\mathbf{x}_t$ are the operating variables at time t and $\mathbf{y}$ are design variables. Limits on operation $\mathbf{o}(\mathbf{x}_t)$ are set relative to functions of the design: $\mathbf{l}(\mathbf{y}), \mathbf{u}(\mathbf{y})$ (eq. 4). $\mathbf{T}$ is the set of time points in the time structure, and $\mathbf{T}^0$ is the first time point in a season. The cost for unit operations is calculated based on their capacity, and the total capital expenditure is amortized over the process horizon. The system generates revenue by selling ammonia, and has operating expenses related to maintenance and labor, electricity purchase, and emissions penalties. There is a 21% corporate tax on profit. We find the system LCOA by minimizing the selling price of ammonia (C_{NH3}) subject to a net present value of zero (eq. 5).

First, we demonstrate how the optimal system LCOA, design, and operation change with respect to different levels of grid emissions. We consider representative profiles for the power grid with average emissions from 0-420 kg/MWh. The ammonia production capacity is a design variable between 5 and 100 tons/hr. We assume that there is no demand flexibility, such that the system maintains production at its nominal capacity. For this analysis we use a time structure containing 16 representative days for a period (Figure SI.1a).

Then, to understand how flexibility impacts the LCOA of the system, we fix ammonia production to 45 tons/hr and examine different combinations of demand and process flexibility. We consider systems with hourly demand (eq. 6), seasonal demand (eq. 7), and yearly demand (eq. 8). Average grid emissions are 220 kg/MWh. The sensitivity analysis utilizes 16 representative days for a period. We then analyze design and operation of flexible and inflexible systems using a 77-day time structure (Figure SI.1b).

$$M_{t,NH3} = \delta \;\forall\, t \in \mathbf{T} \quad (6)$$

$$\sum_{t \in \mathbf{T}_s^S} \omega_t M_{t,NH3} = \frac{1}{4}\delta \;\forall\, s \in \mathbf{S} \quad (7)$$

$$\sum_{t \in \mathbf{T}_p^P} \omega_t M_{t,NH3} = \delta \;\forall\, p \in \mathbf{P} \quad (8)$$

$\mathbf{P}$ the set of periods, $\mathbf{S}$ is the set of seasons, $\mathbf{T}_s^S$ is the set of time points for a season, and $\mathbf{T}_p^P$ is the set of time points for a period. $M_{t,NH3}$ is the production of ammonia at time t, δ is the ammonia demand, and ω_t is the weight for a time point (weights sum to one over $\mathbf{T}_p^P$). For each demand type, we quantify the LCOA for different levels (0-100%) of hourly flexibility from the nominal design of the Haber-Bosch reactor. We then examine how design and operational changes improve the LCOA.

The model is solved using CONOPT. Computations were performed on the Princeton Della computing cluster, using 2.8 GHz Intel Cascade Lake CPUs. Additional details can be found in the supplemental information.

RESULTS

Grid Renewability Analysis

We find a range of LCOA from 700-1200 $/ton over a range of grid emissions from 0-420 kg-CO_2/MWh. We identify that the trend in LCOA increases linearly from 0-140 kg-CO_2/MWh before exhibiting a non-linear response to changes in grid emissions (figure 3a).

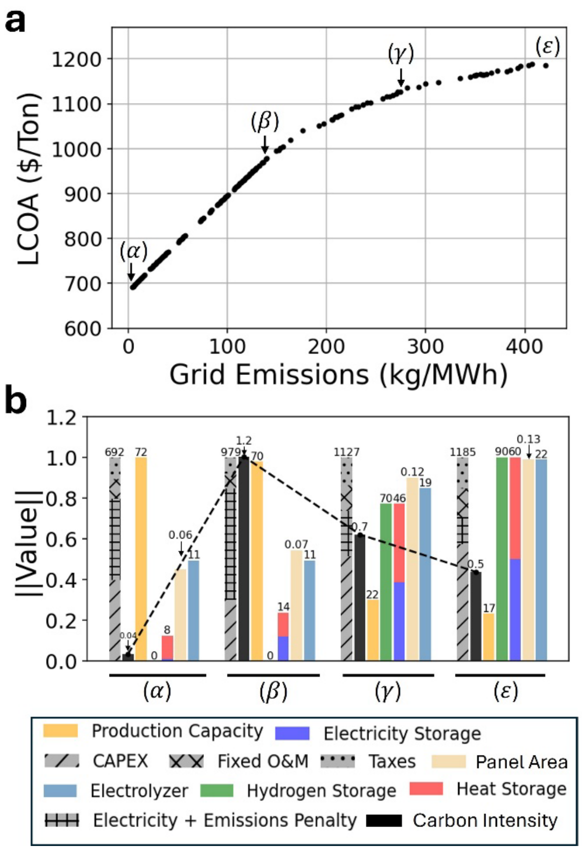

Figure 3. The levelized cost of ammonia for different average grid emissions (a). The contributions to the LCOA are shown in grey, along with production capacity in orange (ton-NH_3/hr), and carbon intensity in black (ton-CO_2/ton-NH_3). Relative to production capacity, mass storage (m^3), energy storage (MWh), solar facility panel area (km^2), and electyrolyzer capacity (MW) are also shown (b). Values have been normalized to lie between zero and one for the purpose of visualization; actual values appear above each bar.

This change is rationalized as a transition point in design and operation when examining instances $\alpha, \beta, \gamma, \varepsilon$. From 0-140 kg-$CO_2$/MWh, the production capacity remains constant, but the fraction of expenses due to emissions rises steadily. In this range, the process has a high production capacity but relies on the grid to provide power during the night, when onsite renewables are inactive. At ~140 kg-CO_2/MWh, operating costs dominate capital expenditure, and it becomes optimal to redesign the process: production capacity decreases, and the proportional level of mass and energy storage increase. This allows the process to operate more flexibly. Increased storage reduces power usage from the grid during levels of low solar irradiance. In turn, operating costs drop but capital costs increase disproportionately due to decreased economies of scale and overdesign (Figure 3b). Specifically, as emissions rise from 140 to 420 kg-CO_2/MWh, the relative electrolyzer capacity and solar facility size double. Overdesign allows these systems to operate independently from the grid but drastically increases capital costs.

The interplay between capital and operating expenditure causes non-monotonic behavior in the carbon-intensity of the system. Systems operating in low or high emission grids produce ammonia at a lower carbon intensity than grids with intermediate emissions. This presents a major challenge to ammonia decarbonization through electrification. Moderate improvements in grid renewability may not improve system level emissions. Carbon intensive grids must decarbonize significantly for green ammonia production to be competitive. Unfortunately, changes to the grid are often slow and incremental. However, these results suggest that increasing system flexibility is the key to achieving lower emissions and prices.

System Flexibility Analysis

Storage is not the only sources of flexibility; it can also be achieved by unit operations or the demand side.

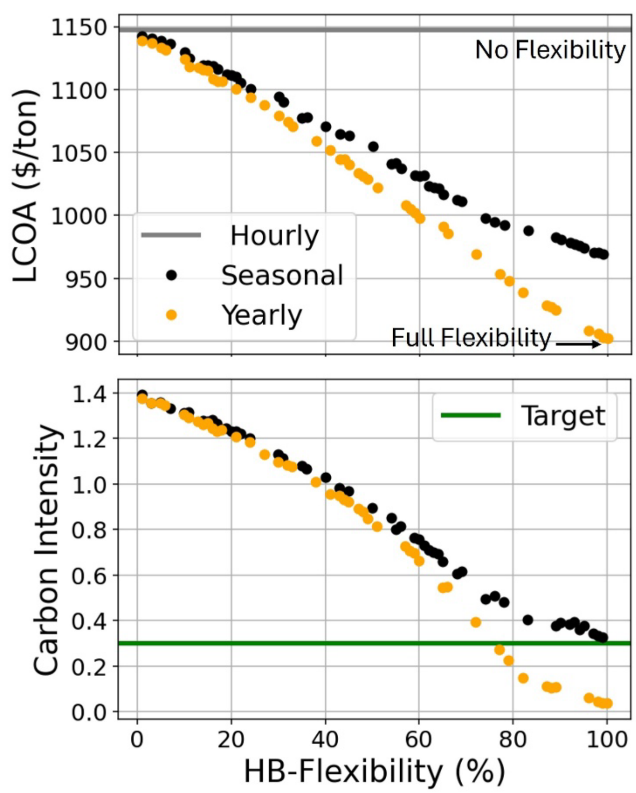

Figure 4. Levelized cost of ammonia and carbon intensity (ton-CO2/ton-NH_3) for different levels of Haber-Bosch (HB) flexibility with hourly, seasonal or yearly demand.

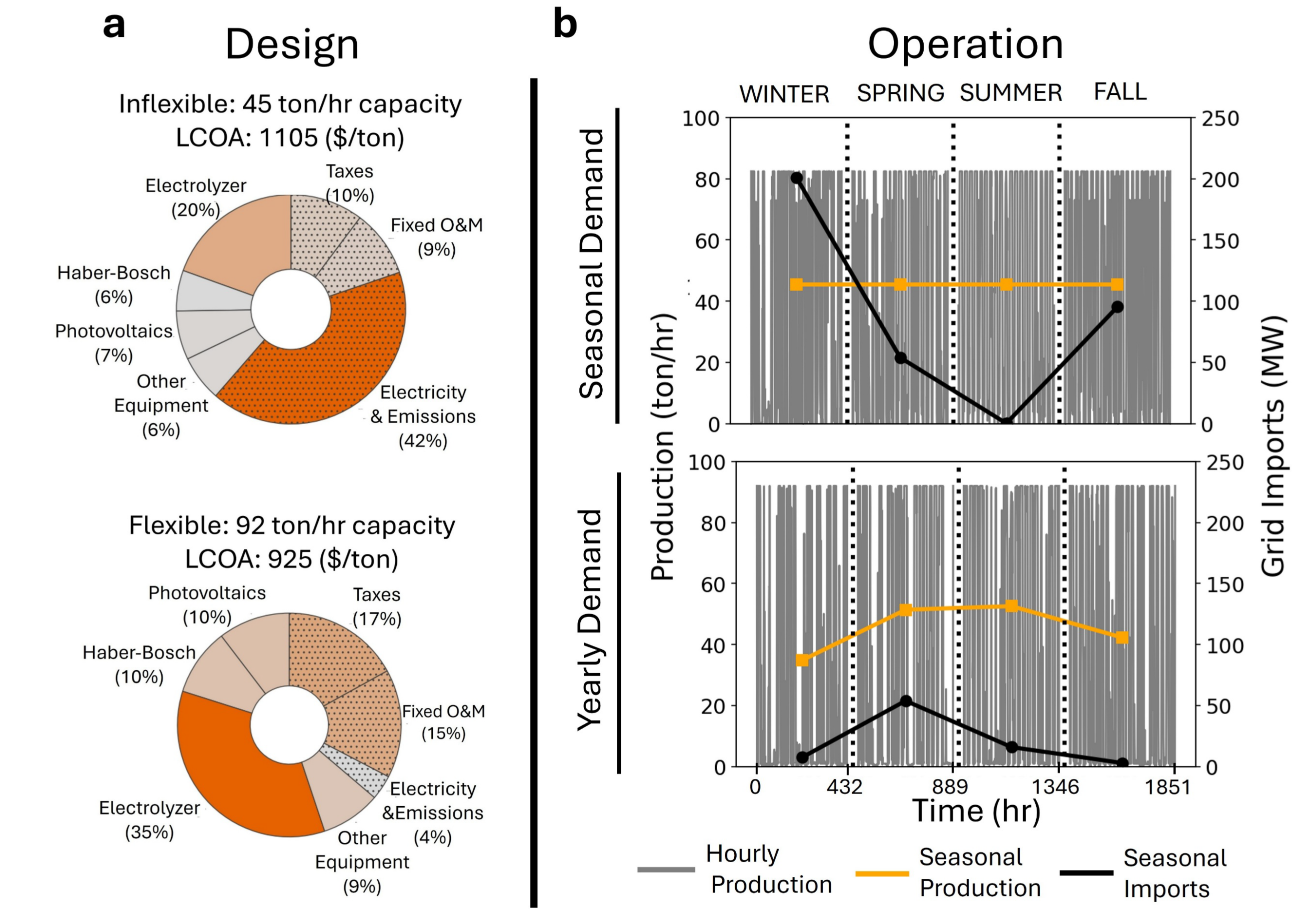

Figure 5. Contributions to the LCOA for an inflexible and flexible system (a). Hourly production of ammonia, as well as the seasonal average production and electricity imports from the power grid (b).

We find that synergies between demand and unit operation flexibility drastically reduce ammonia price and emissions. When considering seasonal or yearly demand, Haber-Bosch flexibility can reduce the LCOA by almost 20% (Figure 4a) without requiring inordinate storage capacity. Increased flexibility in the Haber-Bosch process can also move electrified systems towards, and even below, the target carbon intensity for green ammonia (0.3 ton-CO_2/ton-NH_3); unit flexibility, when coupled with seasonal or yearly demand flexibility, reduces the systems emissions by almost 70% and 100%, respectively.

When examining the LCOA of inflexible and flexible processes, we see that a high level of flexibility results in an islanded process that purchases very little electricity from the power grid. The flexible design is dominated by capital expenditure and is designed at approximately twice the nominal capacity of the inflexible design (Figure 5a). Examining the operation, it is observed that flexible processes produce twice as much material per hour during the day when compared to the inflexible designs but forgo operation during hours of low solar irradiance. Flexible systems benefit from increased economies of scale, and because they do not rely on the grid for power, they also are insensitive to spikes in electricity price and emissions, which often coincide with hour of low solar irradiation.

While the difference in the LCOA and carbon intensity between systems with seasonal and yearly demand is negligible at low to moderate levels of unit flexibility, the difference becomes pronounced at high levels of unit flexibility. Systems with seasonal demand have a different relationship with the power grid than those with yearly demand. Irradiance is low in the winter and fall, so systems with seasonal demand meet the demand requirement by supplementing their onsite power production with grid electricity. For yearly demand, higher production during the spring and summer make up for decreased production during the winter and fall. These seasonal changes in operation allow systems with yearly demand flexibility to achieve almost complete utility independence (Figure 5b); electricity is purchased sparingly from the grid during the spring and summer, and only because very low prices and emissions are achieved during the day.

CONCLUSIONS

Using a framework for operation-informed design, we have modeled a flexible, electrified ammonia synthesis system. We use this model to quantify how the levelized cost of ammonia changes for different grid emissions and understand the transitions in design and operation associated with these different grids. We also find non-monotonicity in the carbon intensity of this system due to transitions in production capacity. At low grid emissions, large, grid-reliant processes are optimal due to economies of scale. These designs remain optimal even as grid emissions rise, causing a sharp increase in carbon intensity. At emission rates of approximately 140 kg-CO_2/MWh, the operating expenditure for electricity and emissions penalties justify a significant downscaling of production capacity. Smaller systems can better leverage onsite energy and mass storage, operating with increased flexibility and reduced grid-reliance. It is important to note that these systems do utilize more land relative to production when compared to grid-reliant systems. Considering the ecological impact of land usage was outside the scope of this work, but in regions with limited land availbility, or sensitive ecosystems, solar power may not be a viable option physically or environmentally. The trends identified in this analysis highlight the importance of operation-informed design, and the role of flexibility in achieving ammonia decarbonization.

We also identify synergies between demand and unit-operation flexibility. We find that improved Haber-Bosch flexibility can lower LCOA by 20% and significantly reduce carbon-intensity for systems with seasonal or yearly demand. Highly flexible systems are designed at much higher capacities than inflexible systems but only operate during hour of peak solar irradiation. Flexible systems are not dependent on the grid, even during hours of low irradiance. Systems with fully flexible unit operations and seasonal demand can achieve a carbon-intensity of approximately 0.3 ton-CO_2/ton-NH_3 (a target for green ammonia). With yearly demand, these systems can achieve nearly zero emissions by adjusting operation to match seasonal changes in energy availbility.

The results demonstrate the importance of flexibility in achieving economic and environmental targets. They also illustrate synergy between multiple forms of flexibility: unit-level, demand-side, storage. Because optimal flexible systems can have drastically different designs from their inflexible counterparts (and even from one other), it is important to evaluate all contributions to flexibility. Operation-informed design frameworks are particularly powerful for these analyses. While there are many challenges to decarbonization through industrial electrification, studying optimal design and operation together uncovers nuanced trends in these systems, and allows us to make informed and intelligent decision about the transition to sustainability.

DIGITAL SUPPLEMENTARY MATERIAL

Supplementary Text S1: Detailed system specifications, parametric data, and additional figures can be found at LAPSE:2026.0018.

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AUTHOR IDENTIFIERS

Author ORCIDs:
Kalamaris NN: 0000-0002-3886-1979
Maravelias CT: 0000-0002-4929-1748

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