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Research Article

Spatial Variation in Cost of Electricity-Driven Continuous Ammonia Production in the United States

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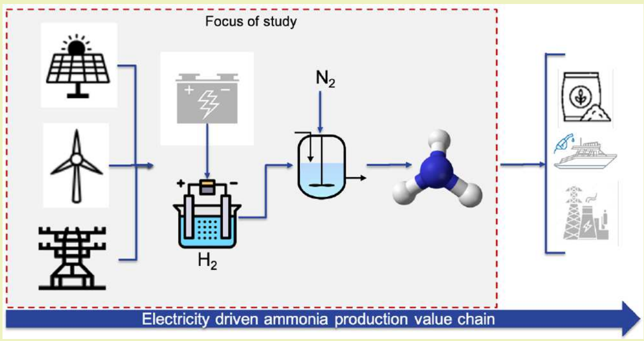
ABSTRACT: Cost-effective, low-carbon ammonia production is necessary for decarbonizing its existing uses but could also enable decarbonization of other difficult to electrify end uses such as shipping, where the energy density is a key criterion. Here, we assess the levelized cost of ammonia production (95% availability) at industrial-scale quantities (250 tonnes/day) in 2030 from integrating commercial technologies for renewable electricity generation, electrolysis, ammonia synthesis, and energy storage. Our analysis accounts for the spatial and temporal variability in cost and emissions attributes of the electricity supply from variable renewable energy (VRE) sources and the grid and its implications on plant design, operations, cost, and emissions. On the basis of 2030 technology cost and grid projections, we find that grid-connected ammonia in midcontinental U.S. costs 0.54−0.64 $/kg, in comparison to 0.3−0.4 $/kg for natural-gas-based ammonia and, depending on the generation mix of the grid, may have higher or lower CO_2 emissions. Fully VRE based ammonia production, even with simultaneous wind and PV utilization, is more expensive than grid-connected outcomes, due to the need for storage to manage VRE intermittency and continuous ammonia production. Using a combination of VRE and grid electricity at locations of existing ammonia facilities in the midcontinental U.S. can achieve 2−80% CO_2 emissions reduction per tonne of ammonia in comparison to natural gas routes and corresponds to a levelized cost range of 0.57−0.85 $/kg NH_3. Further cost reductions are shown to be possible if the ammonia synthesis loop can be made more flexible, which reduces the need for a round-the-clock electricity supply and substitutes use of battery storage with ammonia storage.



KEYWORDS: *Ammonia, Hydrogen, Decarbonization, Renewable energy, Techno-economic analysis, Electrified processes, Optimization*

INTRODUCTION

Global efforts to reduce greenhouse gas (GHG) emissions over the past decade have seen the most success in the electric power sector, while emissions from other sectors have seen only modest decreases or remained stagnant. For example, in the U.S., CO_2 emissions from the power sector decreased by 26% during 2008−2018, while for the same period, transportation CO_2 emissions increased by 1.4% and industrial CO_2 emissions decreased by 9%.[1] Decarbonization strategies for these sectors often cite electrification as a potential pathway, which shifts the burden of emissions reduction from these sectors to the power sector, where continued growth of wind and solar generation is expected to further reduce the emissions intensity of the electricity supply. While direct electrification of certain end uses is poised to grow rapidly (e.g., light-duty vehicles), it may be challenging in particular applications such as heavy-duty transport such as shipping and aviation where high energy density requirements remain a key performance criterion. For these end uses, using alternative energy carriers such as hydrogen (H_2) and by extension hydrogen-rich molecules such as ammonia (NH_3) and other liquid fuels, produced using low-carbon pathways, remain an appealing prospect.

Ammonia offers some distinct advantages over other energy carriers, such as being carbon-free at the point of use and having an increased volumetric energy density vs compressed H_2, ease of storage and transport in comparison to liquid or gaseous H_2, and long track record for safe handling at scale.[2−4] The predominant route for ammonia production today relies on fossil fuels such as natural gas and coal as sources of energy and hydrogen for the thermochemical Haber-Bosch (H-B) synthesis and is estimated to result in about 2.3 tonnes of CO_2 per tonne of NH_3 produced.[5] The reliance on natural gas for ammonia production also implies that the cost of natural gas is a key driver of the effective landed cost of the ammonia,

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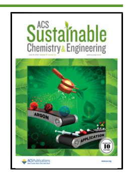

Table 1. Summary of Recent Work on Electricity Driven Ammonia Production Techno-Economic Modeling

ref	VRE sources considered	modeled operations variability?	grid connection?	H-B synthesis loop process model?	storage options	H-B process flexibility?	region
Nayak-Luke et al.[25]	PV, wind	yes	no	no	H_2 only	yes	UK
Guerra et al.[22]	no	no	PPA	no	NH_3 only	no	Chile
Maia et al.[20]	wind	no	no	no	NH_3 only	no	Iceland
Osman et al.[28]	PV, CSP	yes	no	yes	H_2, N_2, NH_3	no	UAE
Morgan et al.[30]	wind	no	yes	no	H_2, N_2, NH_3	no	USA
Beerbuhl et al.[35]	no	yes	yes	no	H_2 only	no	Germany
Allman et al.[36]	wind	yes	no	no	H_2, N_2, NH_3	no	USA
Nosherwani et al.[21]	wind	yes	no	yes	H_2, N_2, NH_3	no	Brazil
Liang et al.[27]				yes		yes	Netherlands
Zhang et al.[37]			yes	yes		no	Italy
Palys and Daoutidis[32]	PV, wind	yes	no	no	H_2, N_2, NH_3	yes	USA
current work	PV, wind	yes	yes	yes	H_2, N_2, NH_3, Li ion	yes	USA

ranging from 300 to 400 $/tonne in the U.S. context[6] to higher prices of near 700 $/tonne for other regions with a limited domestic natural gas supply and infrastructure constraints, such as India and Africa.[7−9]

Declining costs of variable renewable energy (VRE) based electricity and electrolyzers have raised interest in producing low-carbon H_2 via electrolysis, as well as its use in the decarbonization of industrial ammonia production.[10−13] This route is among the most technologically mature process concepts for electricity-based ammonia production[14−16] and paves the way for emerging electrochemical ammonia production pathways that are modular and, hence, amenable to deployment at smaller scales in comparison to the conventional fossil-fuel-driven process.[14,17] As was noted earlier, electrically driven ammonia production is potentially appealing for many developing countries with relatively high natural gas costs and where ammonia use for fertilizer is projected to grow rapidly over the next few decades.[17] Finally, the ease of handling and storage of liquid ammonia relative to hydrogen also opens up the potential for the use of ammonia as a potential energy storage vector in a carbon-constrained world.[5,18]

Several recent studies have investigated the techno-economics of an electrically driven ammonia production process via a low-temperature electrolytic hydrogen production coupled with a thermochemical H-B synthesis. These studies tend to focus on one or more of the following aspects: (a) NH_3 costs in a particular geographical region, including the Middle East,[19] Iceland,[20] Germany,[21] Chile,[22] China,[23] and India,[24] (b) alternate electricity supply options, ranging from a colocated VRE supply as part of islanded systems[25] to a grid + contractual VRE supply via power purchase agreements,[26] (c) representation of ammonia production requirements and process operational constraints, which are included in varying detail by some studies[21,27,28] but overlooked in other cases,[25,29−31] and (d) inclusion of alternative on-site storage technologies to manage the temporal variability of the electricity supply, either from the grid or on-site or contracted VRE sources.[22,26,28,32] Here, we note the salient contributions of some of these studies, while noting their differentiating aspects related to model fidelity (i.e., temporal resolution, demand, and operational constraints), regional characteristics, and level of decarbonization evaluated (see Table 1). Nayak-Luke et al.[25] evaluated the effect of VRE electricity on running a thermochemical Haber−Bosch process reactor with an electrolytic H_2 supply. They model electricity supply from different combinations of colocated PV and wind generation while optimizing for the H-B system size that also accounts for process flexibility. However, the authors did not model a grid-based electricity supply or the full spectrum of storage options to manage VRE variability. Banares-Alcantara et al.[33] evaluated the levelized cost for an islanded ammonia generation facility but overlooked temporal variations in VRE generation. Morgan et al.[30] studied offshore wind-driven ammonia production in the United States (U.S.) context while incorporating intermediate storage for the physical ammonia process components but overlooked the time and price variations in grid and wind farm power output and its effect on hourly process operations and overall cost. Osman et al.[28] developed a techno-economic model that incorporated the effects of variability in solar resources, the flexibility of the subsystems such as air separation unit (ASU), and electrolyzers as well as an ASPEN-based process model, to study the design and operations of a renewable ammonia system in the Middle East. However, they overlooked the role of grid integration which, as we discuss in later sections, may allow for lowering ammonia costs and eventually CO_2 emissions as well. Along similar lines, Armijo et al.[34] focused on studying the potential for renewable ammonia production in Chile and Argentina through a temporally resolved optimization model and conclude that the combination of wind and solar resources for electricity supply can drive down costs by reducing the overall variability in energy supply. The authors also studied the role of flexible H-B process operation as a key driver for the eventual reduction of costs. Schulte Beerbühl et al.[35] developed a design and operations model for electricity-based ammonia production that included nonlinear constraints related to some unit operation (e.g., electrolyzer), which was shown to provide a more accurate representation of process flexibility. Related to this, Allman et al.[36] have focused on evaluating the effects of wind intermittency on the cost of ammonia production in the US upper Midwest. The authors also studied the role of intermediate N_2 and H_2 storage to ensure round-the-clock operation. Palys and Daoutidis also considered the storage of intermediate H_2 and N_2 along with NH_3 as part of designing a renewable energy storage and supply system for meeting MW-

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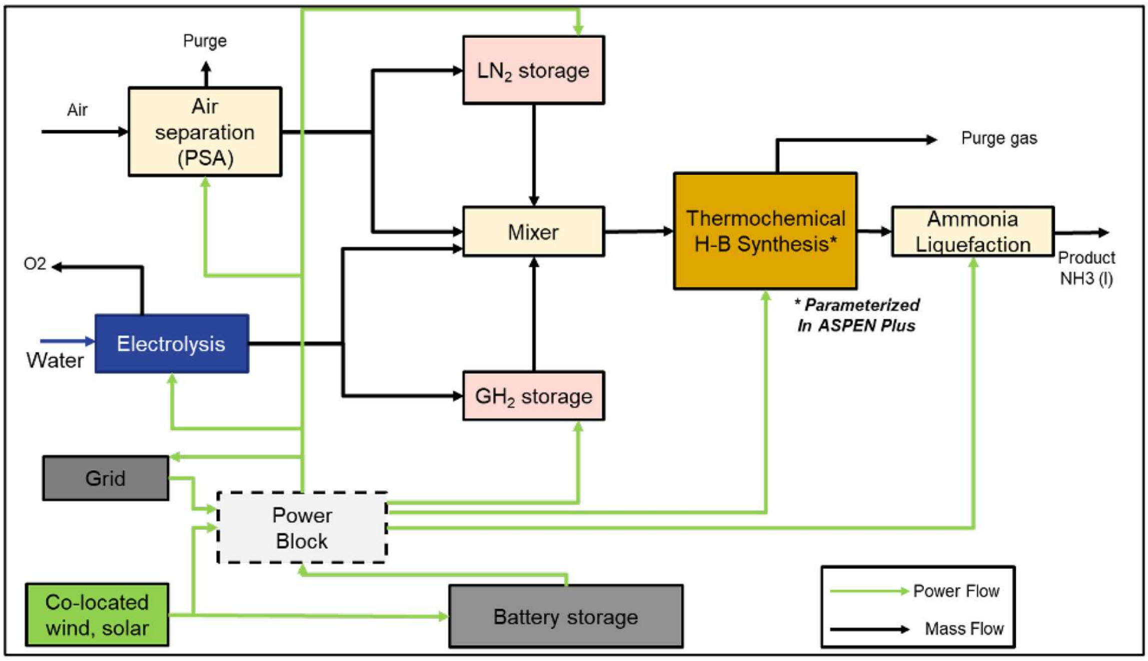

Figure 1. Simplified process flow diagram of an ammonia production process based on an electrolytic H_2 supply and thermochemical Haber−Bosch (H-B) synthesis. A detailed ASPEN model used to evaluate the H-B synthesis is provided in the appendix (see Figure S10) in the Supporting Information. Abbreviations: PSA, pressure swing adsorption; H-B , Haber-Bosch; LN2, liquid nitrogen; GH2, gaseous hydrogen.

scale electricity demand.[32] Due to the many unit operation choices being considered, the resulting design optimization model considers plant operation over a limited number (672) of representative periods while preserving a chronology that is important to model seasonal energy storage.[32]

In this study, we perform a detailed spatial and temporally resolved analysis of electrically driven ammonia production via the process depicted in Figure 1. Our analysis is based on modeling the least-cost design and operation of the process while considering three key attributes influencing the overall process economics: (a) temporal variability in electricity supply from grid and colocated VRE generation, (b) detailed process considerations, including the operational inflexibility of the thermochemical H-B synthesis as well economies of scale of investment in certain unit operations, and (c) use of alternate on-site storage options to manage temporal variability in energy inputs, including chemical storage and electricity storage. We use the developed model to evaluate the cost of an electricity-based NH_3 supply for various regions in the continental U.S. under various technology cost assumptions and carbon policy and electricity supply scenarios (dedicated VRE or grid based, VRE + grid) for 2030. Finally, we use the model to explore the economic value and process design implications of introducing limited operational flexibility in thermochemical H-B synthesis.

METHODOLOGY

The integrated design and operations modeling framework used in this study is adapted from prior work[38] and incorporates the unique features influencing design and operations of industrial processes such as ammonia production: (a) round-the-clock operation to maximize capacity utilization, (b) centralized production to maximize economies of scale of thermochemical processes, (c) limited operational flexibility due to the large thermal inertia of units, and (d) extensive heat and mass integration within the process. We formulate the design and operations assessment as a mixed integer linear program (MILP) with an objective function corresponding to the sum of the annualized investment (CAPEX) and operating (OPEX) cost of running the ammonia production facility shown in Figure 1. This objective is minimized subject to a variety of operational and policy constraints that are enforced to model plant operations throughout the year at a hourly resolution, resulting in 8760 operational periods. The resulting MILP model is solved via a Gurobi[39] run on a Xeon-g6 processor with 4 GB of RAM across 32 cores on each compute node.[40] The average time to converge for each run ranges from 200 to 900 s considering an optimality gap of 5% or lower. Additional computational statistics for the runs can be found in Table S5 in the Supporting Information. The base system design parameters are shown in Table 2. Below, we describe the modeling of

Table 2. Design Assumptions for Electricity-Driven Ammonia Process

param	value	units
ammonia production capacity	250	tonnes/day
plant minimum down time	48	hours
CAPEX contingency factor	21	percent
discount rate	8	percent
weather year for renewable availability data	2011	
cooling water use	1000	tonnes/tonne of NH_3
cooling water cost	0.0148	\$/tonne
plant annual availability	95	percent
grid interconnection cost	30	\$/kW

the various unit operations in the process along with a summary of the key cost and performance assumptions affecting their design and operations, with additional details being provided in the Supporting Information.

Electrolyzer. H_2 production via low-temperature electrolysis is modeled on the basis of available cost and performance projections for proton exchange membrane (PEM) electrolyzers for 2030[41] (see Table S1 in the Supporting Information for assumptions). PEM electrolyzer capital costs projections reported in the literature vary greatly, reflecting the emerging nature of this technology as well as scales at which capital costs are quoted (e.g., kW vs 1 or 10s of MW[42]). Here we model PEM capital costs of $500/kW (see Table S1 in the Supporting Information), on the basis of projections for multi-MW scale systems[41−43] that would be needed for the modeled ammonia production facility (250 tonnes/day). We assume a electrolyzer lifetime of 20 years, with the cost of periodic stack replacement included as part of the FOM cost (5%, see Table S1 in the Supporting Information). PEM electrolyzers can produce pressurized H_2 at 30 bar which could be stored as a compressed gas for later use as a feed for the H-B synthesis. The model sizes the optimal electrolyzer capacity as well as enforces hourly operational constraints to track the power inflow into the system and produced H_2 streamflow rates to the storage and H-B unit (eqs S17 and S18 in the Supporting Information). We also enforce the requirement that PEM electrolyzer production must be constrained above a minimum loading level, set at 5% of nameplate capacity, or switched off.[42] This behavior is modeled using a binary variable in each time period that tracks whether the electrolyzer is on or off (eq S28 in the Supporting Information). The cost impact of including this operating constraint is negligible (0.3%; see Figure S9 in the Supporting Information), presumably because the minimum power load is quite low. However, the model with the additional variables and constraints to model the minimum power load takes about 4 times longer to solve in comparison to the model without these variables or constraints, implying that ignoring them could have a small cost impact but relatively large run time impact.

Storage. We model four forms of storage using a common structure that separates sizing decisions related to storage capacity (energy or mass) and maximum rate of charging or discharging storage. The four storage types include (a) Li-ion battery, (b) gaseous hydrogen (above-ground storage), (c) liquid nitrogen, and (d) ammonia as a pressurized gas or liquid. Storage operation is modeled to follow constraints that track storage inventory levels from one hour to the next, as well as adherence to the installed capacity limits (see eqs S3−S6 in the Supporting Information). We consider the availability of ammonia storage only in the case when the H-B process is modeled to be flexible. Storage parameters are summarized in Table S4 in the Supporting Information.

Air Separation Unit. Nitrogen (N_2) generation is modeled as per the specifications of the pressure swing adsorption (PSA) process (see Table S2 in the Supporting Information), which can adjust its hourly output flexibly. PSA units tend to operate in a cyclical steady state, and this mode of operations allows for operational flexibility that can be leveraged in an electrically driven ammonia production process.[44] To account for the economies of scale in the PSA process, we model the capital cost of the system as a piecewise linear function of capacity using five piece-wise linear segments (see eqs S12−S14 in the Supporting Information). The N_2 output from PSA is then split into two streams—directly flowing into the H-B synthesis loop or being liquefied for storage. The stored liquid N_2 is pumped into the H-B stream at the reactor pressure (250 bar) for further use.

Haber−Bosch (H-B) Synthesis Loop. The H-B synthesis loop section is simulated in ASPEN plus on the basis of the flowsheet shown in Figure 1, starting with the input of pure H_2 and N_2 streams from the upstream production facilities. The H-B synthesis loop consists primarily of three sections: (a) the compressor train to compress the input feed gas (mixture of H_2 and N_2) to 250 bar for the H-B reactor, (b) the H-B reactor, which is maintained at a temperature of 500 °C with a heat recovery exchanger to recover waste heat from the output stream (eqs S23−S38 in the Supporting Information), and (c) finally a flash tank which separates and liquefies the output NH_3 in the system to produce liquid ammonia (99% purity) (eqs S34 and S35 in the Supporting Information). For the MILP model, the H-B synthesis loop is treated as a black box with predefined process operating parameters related to power and cooling water inputs from the ASPEN simulation (see Table S2 in the Supporting Information).

Currently deployed H-B synthesis facilities tend to operate at a steady state, and we have incorporated this constraint in our modeling. At the same time, to understand the role of flexible H-B synthesis and the impact on cost we introduce three parameters to understand the nature of flexibility in the synthesis loop: minimum stable production level, minimum shutdown times, and ramp rates. The minimum shutdown constraint (eq S28 in the Supporting Information) enforces that the plant has to be remain shutdown for a minimum amount of time (assumed to be 48 h on the basis of a 10 °C/h rate of temperature increase for the reactor)[45] before being brought back to full production (eqs S29 and S30 in the Supporting Information).

Electricity Supply. Electricity is the only energy input for the entire process, and we consider the availability of VRE resources (solar (PV) and wind) as well as connections to the grid (including grid interconnection + electricity supply costs and emissions) as a part of the set of available electricity sources. The model takes inputs in the form of hourly VRE capacity factor data as well as electricity price time series (see eqs S7 and S8 in the Supporting Information).

VRE Resource Modeling. To characterize VRE availability over the continental U.S., we define a grid consisting of 1487 nodal points across the region (Table 3). Then for each grid point, the renewable energy resource availability profile is generated in line with Brown and Botterud[46] and summarized in the Supporting Information. We consider renewable availability data for 2011 as a representative weather year for our analysis.

Table 3. VRE Resource Cost Assumptions[a]

resource	CAPEX ($/kW)	FOM (%)	lifetime (years)	ref
PV	500	1	20	47
wind	1200	2	20	47

[a]Cost assumptions reflect 2030 projections available from the literature.[47]

Grid Electricity Input. To evaluate the cost and emissions impact of the grid electricity supply on electricity-based ammonia production, we evaluated model scenarios using spatially and temporally resolved electricity system projections for 2030 available from the National Renewable Energy Laboratory (NREL) 2020 standard scenarios.[48,49] Specifically, we use simulated electricity prices and marginal emission factors data for 2030 for each balancing area corresponding to NREL's midrange renewable penetration scenario. The spatial distribution in CO_2 emissions intensity and marginal electricity prices for the region under focus in our study is presented in Figure 2 and Figure S1 in the Supporting Information, respectively.

While there are no direct CO_2 emissions from the process shown in Figure 1, we account for the CO_2 emissions associated with the grid electricity supply in the model, which allows for a holistic assessment of shifting from natural gas to electricity-driven processes. Therefore, the hourly electricity requirement from the grid is tracked and the corresponding marginal CO_2 emissions intensity of the supplied grid electricity at each time period is incorporated in computing the CO_2 emissions intensity of ammonia production. Marginal emission factors are modeled in place of average emissions to account for the hourly variability in grid operations.[50] As discussed in the results, this representation of grid electricity use allows for exploring tradeoffs between grid supply vs colocated VRE supply under various CO_2 policy scenarios.

RESULTS AND DISCUSSION

Operational Dynamics of Electricity-Driven Ammonia Production. We highlight the functionalities of the developed integrated design and operations model by discussing the model outcomes for two locations in the United States—first (A) Amarillo, TX, and second (B) Greenfield, IN—on the basis of the aforementioned 2030 technology cost assumptions and under scenarios with and without use of 2030 grid electricity conditions. The 2020−2021 cost of natural-gas-based ammonia is around 0.4 $/kg,[52] while the levelized cost

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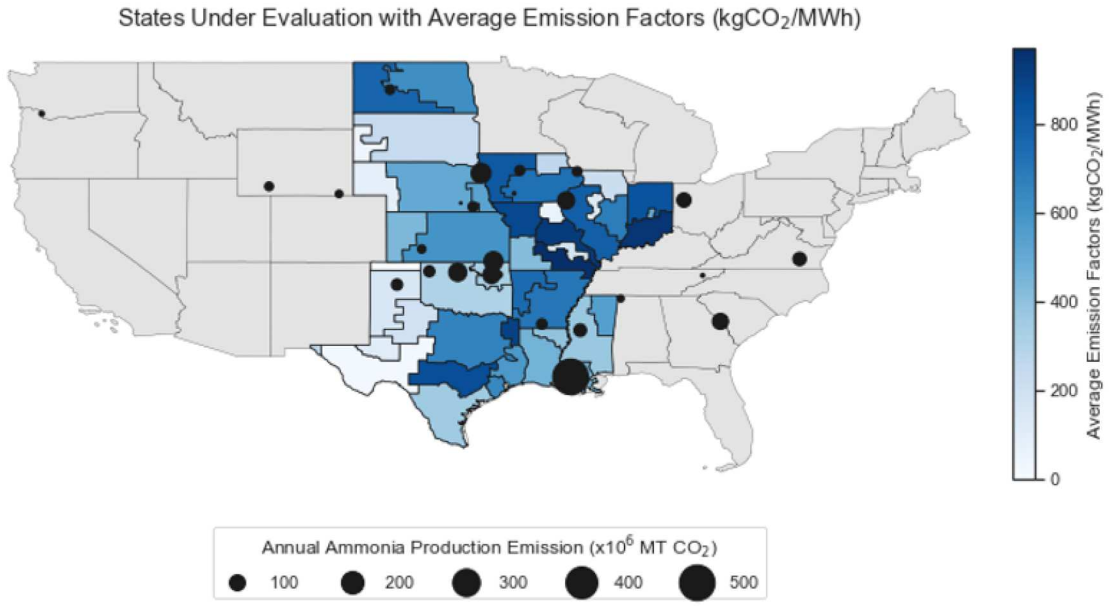

Figure 2. Time average of marginal CO_2 emissions intensity for 2030 projected by the National Renewable Energy Laboratory analysis under midrange renewables cost assumptions[48] for the focus area of study. Reported average emissions intensities are calculated as simple averages of hourly long-term marginal emissions factors reported for 8760 h of the year. Major ammonia production facilities are shown for reference, with the size of the bubble proportional to their annual CO_2 emissions in 2019.[51]

of ammonia ((LCOA) = (annualized CAPEX + OPEX)/(yearly NH_3 production)) of the grid-only case is 0.5−0.6 \$/kg and that of the completely VRE driven case (VRE only) is between 0.95 and 1.20 \$/kg at 2030 cost scenarios for the locations being evaluated (Figure 3). On the basis of simulated 2030 electricity prices and marginal emissions factors for the two locations, grid-electricity-derived ammonia production has a positive abatement cost of 85 \$/tonne of CO_2 and corresponds to 77% CO_2 emissions reduction in Amarillo, TX, while it has a negative abatement cost (−28 \$/tonne CO_2) and leads to 340% greater CO_2 emissions in Greenfield, IN. Here, the cost of carbon abatement (CoCA) is calculated via eq 1, where LCOA and CO_2 emissions intensity of the incumbent natural gas process and emissions intensity are assumed to be 0.4 \$/kg and 2.35 tonnes CO_2/tonne NH_3, respectively.[5] Here, we do not include upstream emissions associated with the natural gas supply chain that, if included, would further lower the CO_2 abatement costs estimated here.

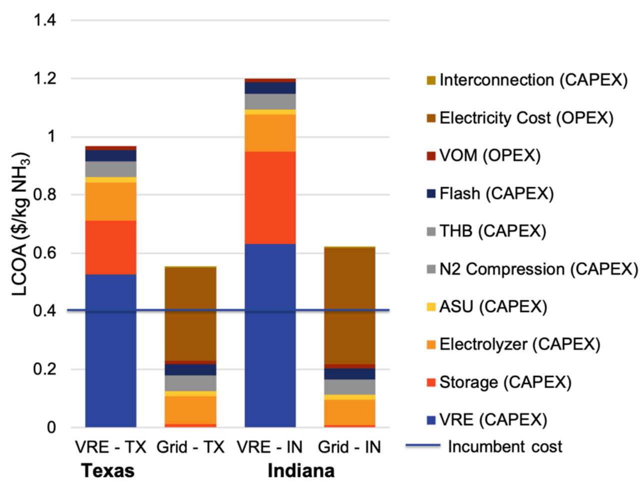

Figure 3. Levelized cost of ammonia (LCOA) comparison for VRE- and grid-driven ammonia production for sample locations in Texas (near Amarillo, TX) and Indiana (Greensfield, IN). The grid supply is modeled as per 2030 grid scenarios available from NREL Standard Scenarios.[48] The storage cost includes levelized costs of three types of storage—Li-ion battery, hydrogen (above ground), and nitrogen—see Figure S3 for details. The typical cost of natural-gas-based ammonia production in the US is shown as a horizontal line. Abbreviations; ASU, air separation unit; VRE, variable renewable electricity; THB, thermochemical Haber-Bosch synthesis loop; VOM, variable operating and maintenance cost.

$$\text{CoCA} = (\text{LCOA}_{\text{process}} - \text{LCOA}_{\text{incumbent}}) / (\text{emissions}_{\text{incumbent}} - \text{emissions}_{\text{process}}) \quad (1)$$

Thus, while it is possible to realize 80% CO_2 emission intensity reduction at a location with a low-emissions-intensity grid (average grid emissions intensity at Amarillo, TX 50 kg of CO_2/MWh), connecting to a high-emission grid (average grid emissions intensity at Greenfield, IN 856 kg of CO_2/MWh) results in higher emissions per tonne of ammonia and becomes a counterproductive solution in this case. A 100% process CO_2 emissions removal is achievable at the two locations using a VRE electricity supply and corresponds to a CO_2 abatement cost of 242 and 342 \$/tonne CO_2 on the basis of a dedicated VRE electricity supply for the locations in TX and IN, respectively.

In addition to the levelized cost comparisons for these scenarios, the developed model provides detailed information on the investment requirements for each of the components in the facility (Figure S4 in the Supporting Information) as well as the temporal dynamics of the system operation in response to electricity supply variability. We simulate the operations of the facility to run at a constant production flow rate, which results in a constant baseline power input for operating the H-B synthesis loop as well as a constant flow of the reactants into the H-B synthesis loop. Figure 4 highlights the operation of a

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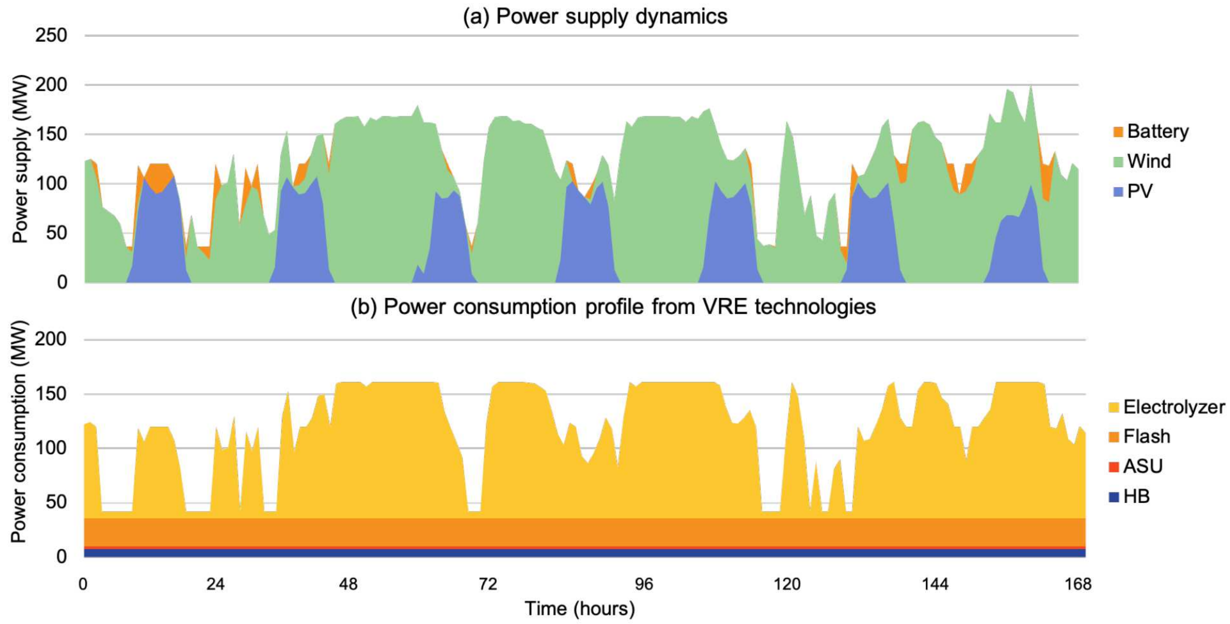

Figure 4. Plant operation over a representative week for a VRE-based ammonia production facility in Amarillo, TX: (a) power supply dynamics; (b) power consumption profile from VRE technologies

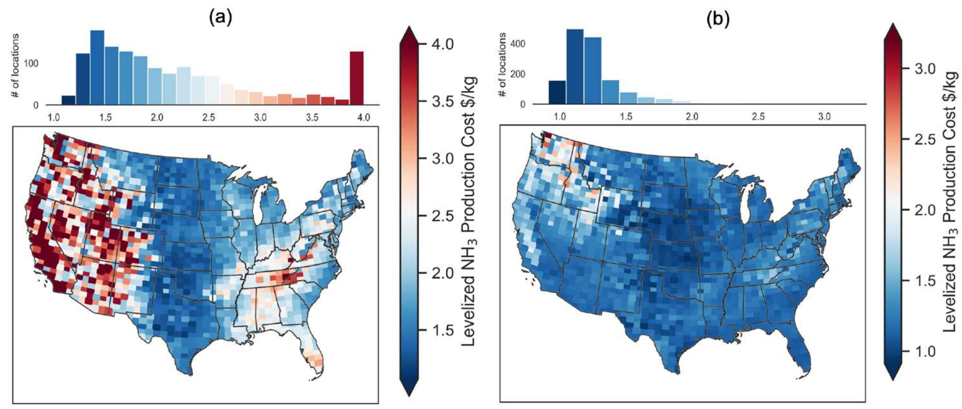

Figure 5. Spatial distribution in the levelized cost of ammonia map for (a) wind-driven (left) 5th, median, and 95th percentile CO_2 abatement costs 343, 665, 1873 \$/tonne CO_2, respectively, and (b) wind + PV driven electrolytic ammonia production 5th, median and 95th percentile CO_2 abatement costs 260, 340, and 596 \$/tonne CO_2 respectively.

VRE electricity-based plant, located in Amarillo, TX, under low-VRE-availability periods (hours 25−65). During these periods, the majority of energy-intensive and flexible processes (H_2 generation through the electrolyzer and ASU are turned down/off (Figure 4a) while discharging from physical storage (Figure 4b,c). Without a grid connection, Li-ion battery storage is the only feasible option to provide the baseline power requirement for the base H-B synthesis loop and ammonia liquefaction (flash) during low-VRE-availability periods and contributes 5−7% of the total ammonia cost in both the Texas and Indiana locations. Because of the availability of other lower cost forms of storage, Li-ion storage is not used for managing the seasonal variations in VRE supply.

Estimated Costs for Dedicated VRE-Based Ammonia Production in the United States. We evaluate the outcomes for both standalone solar (PV) and onshore-wind-driven ammonia production for the continental U.S. and find that the resulting LCOA distributions largely follow spatial patterns in VRE resource availability due to the dominant role of VRE capital cost in LCOA (results for PV-only-based facility configurations are shown in Figure S5). For PV-only systems, the key areas which provide the lowest LCOA are in the southwest U.S. These regions, however, lack existing agricultural demand for ammonia (as implied by the location of existing ammonia production facilities) and may also lack access to freshwater, which might limit their deployment value. At the same time, for the emerging uses of ammonia as an energy carrier or fuel, these regions could be favored to serve neighboring demand centers such as California or the Gulf of Mexico region, wherein water needs could be met using relatively inexpensive reverse osmosis of seawater.[53] In the case of wind-driven ammonia production (Figure 5a), the lowest cost regions align better with the existing ammonia consumption regions, primarily the U.S. Midwest, which accounts for more than 90% of the ammonia production capacity in the country (Figure 2) . The costs of wind-driven ammonia across the U.S. ranges from 1 to 12 \$/kg (5th, median, and 95th percentile costs of 1.28, 1.96, and 4.80 \$/kg,

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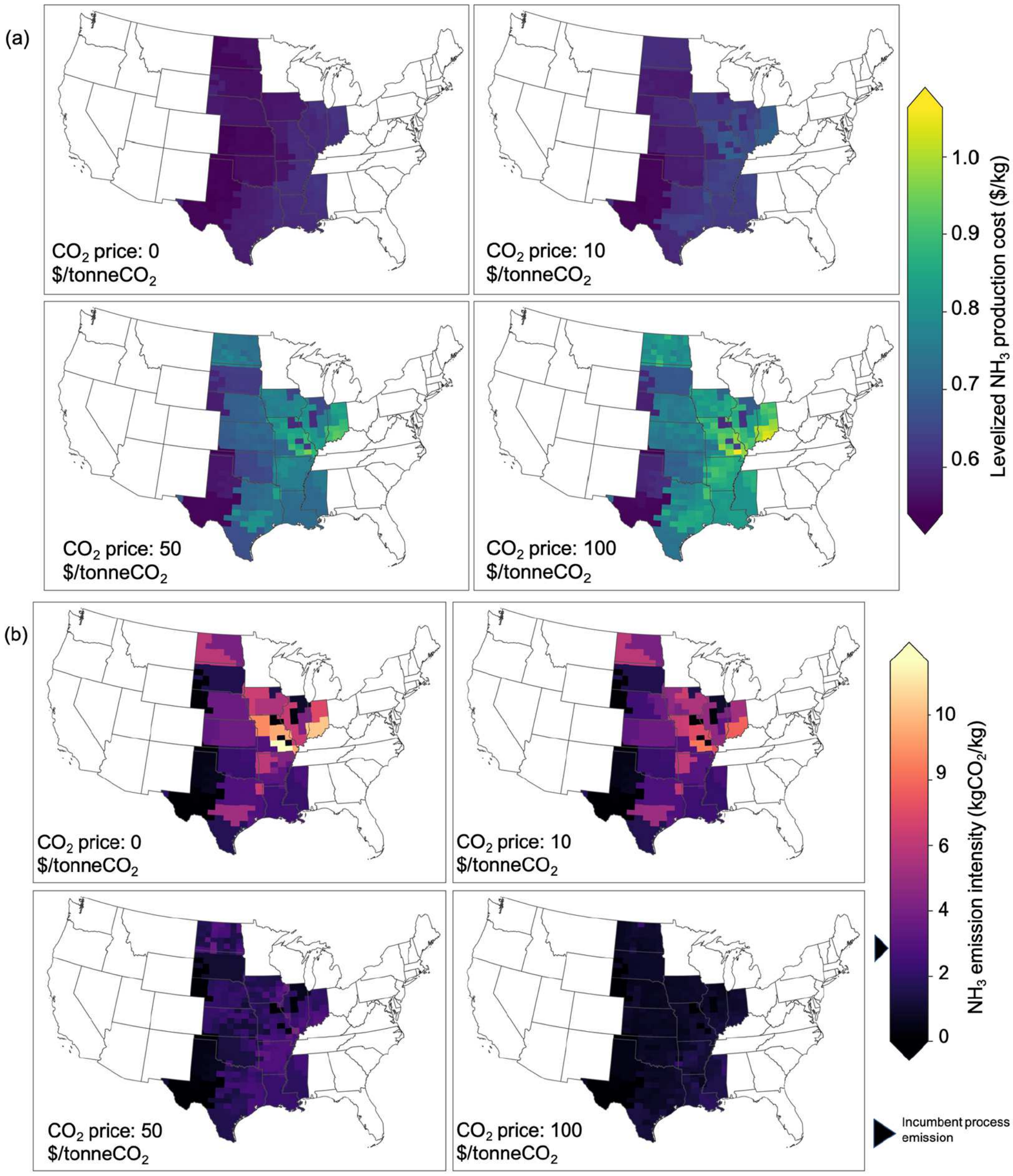

Figure 6. Spatial distribution in levelized cost of ammonia (LCOA) (a) and average CO_2 emission intensity of ammonia production (b) for PV + wind + grid connected electrolytic ammonia production under different CO_2 price scenarios. Grid emissions and cost profiles for each location are based on 2030 projections available from NREL standard scenarios modeling outcomes.[48,49]

respectively) with about 93% of locations with a cost of less than 4 \$/kg (more than 10× the cost of current fossil-fuel-driven ammonia production). Our modeling also reveals the distinctive dynamics and investment decisions driving the levelized cost outcomes for wind- and PV-driven systems. On comparison of high wind (NE) and PV (AZ) resource quality with similar LCOA (∼1.04 \$/kg), installed VRE capacity is almost twice as high for PV than for wind, given the lower capacity factor of solar resources. For the same reasons, the intermediate storage options (Li-ion, H_2 and N_2) are relatively smaller (around 10% lower) for wind sites along with a higher capacity utilization of the electrolyzer (60% capacity factor for lowest cost wind site vs 32% for lowest cost PV site) (see Figure S6 in the Supporting Information).

Figure 5b highlights how allowing for PV and wind resources to be used jointly results in lowering the cost of dedicated VRE-based ammonia production with a median cost of 1.20 \$/kg and 5th and 95th percentiles of 1.01 and 1.80 \$/kg, respectively. In fact, costs below 1 \$/kg levels are estimated for 4% (58 out of 1487) of the locations in the continental U.S. The complementary resource profiles for wind and PV lead to a reduced need for daily storage requirements for the on-site production facility (see Figure S6). While there is still a need for a round-the-clock electricity supply to operate the inflexible H-B synthesis loop which necessitates the deployment of Li-ion battery storage, the battery capacity required is reduced with simultaneous wind and PV utilization (Figure S6 in the Supporting Information). On average, battery energy capacity reduces by 10% for the locations with less than \$ 1/kg NH_3 identified in Figure 5b in comparison to the wind-only cases in Figure 5a. At each location, the relative contribution of wind and solar to the electricity supply capacity is dependent on the

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ACS Sustainable Chem. Eng. 2022, 10, 7862−7872

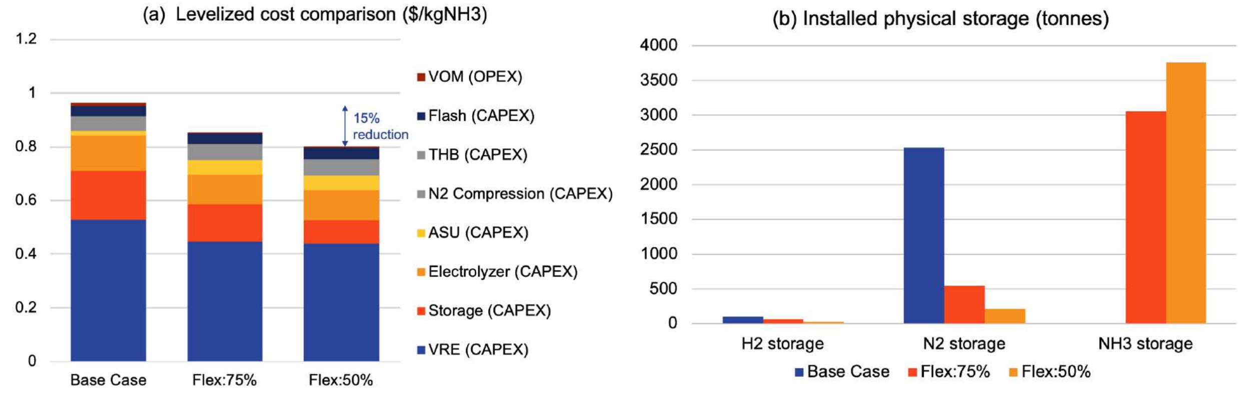

Figure 7. LCOA comparison for electricity-driven ammonia production with varying levels of flexibility for the thermochemical Haber-Bosch synthesis loop, ranging from no flexibility, H-B system turndown to 75% of design flow rate, and system turndown to 50% of design flow rate (a) and storage capacity installed for flexibility cases (b). Abbreviations: VOM, variable operation and maintenance cost; ASU, air separation unit; VRE, variable renewable energy; HB, Haber-Bosch unit.

dominant VRE resource in terms of resource quality for the region (Figure S7 in the Supporting Information).

Carbon Footprint and Cost of Ammonia Production Using Grid + VRE Electricity. The above analysis indicates that while dedicated VRE-based ammonia production can achieve full decarbonization, it is estimated to be more expensive than reliance on a grid-electricity-based supply even with 2030 technology cost assumptions that assume continued cost decreases from 2020 cost levels. Moreover, as the CO_2 emissions intensity of the electric grid is anticipated to decrease over time due to increasing VRE penetration, the relative CO_2 emissions benefits of pursuing a dedicated VRE electricity supply vs grid electricity use are likely to diminish while the cost differences will remain. To understand this tradeoff further, we explore the LCOA and process design outcomes for ammonia production using a grid + VRE electricity supply under various CO_2 price scenarios. As identified in the previous section, the key demand and supply hubs for ammonia currently are in the Midwestern states and Texas, and therefore we focus this part of our analysis on this region. To explore the cost and emissions tradeoffs of increasing VRE supply, we evaluate model outcomes for this region under the four CO_2 price scenarios: no policy, low CO_2 price (10 \$/tonne CO_2), medium price (50 \$/tonne CO_2) and high CO_2 price (100 \$/tonne CO_2). For the analysis, we model the grid in 2030 as per the standard scenario projections from the NREL for price and marginal CO_2 emissions for the system.[49]

Figure 6 shows that, under the no-policy scenario, grid connectivity leads to relatively small spatial differences in LCOA outcomes but significant spatial variations in CO_2 emissions intensity. For example, under the no-carbon price scenario, ammonia production in Oklahoma and Kansas is estimated to have 32−57% lower carbon intensity in comparison to ammonia production in Iowa or Illinois (Figure 6b, top left panel). Note that these states have existing production capacity (see Figure 2). A 50 \$/tonne CO_2 policy leads to a greater share of VRE electricity supply for ammonia production in regions where the grid electricity has relatively high CO_2 emissions intensity. This leads to more spatially uniform emissions outcomes for electricity-based ammonia production (Figure 6b, bottom left panel), which are generally below that of natural-gas-based ammonia production. As an example, CO_2 emissions of electricity-based ammonia production in Iowa are reduced by an average 64% in the 50 \$/tonne CO_2 case in comparison to the no CO_2 policy case, with a corresponding cost increase of 33%. Across locations of existing ammonia production facilities in the midcontinental U.S. (see Figure 2), we find that 2030 grid + VRE connected ammonia under a \$50/tonne CO_2 policy scenario can achieve 2−80% CO_2 emissions reduction per tonne of ammonia produced in comparison to natural-gas-based routes, which corresponds to an LCOA of 0.57−0.85 \$/kg.

In general, increasing VRE penetration in the electric grid tends to increase instances of low wholesale electricity prices due to the well-documented merit order effect.[54] Consequently, we find that locations with a low-emissions-intensity grid supply, synonymous with a greater share of grid-based VRE generation, tend to also have lower LCOAs. This explains why locations such as West Texas, Oklahoma, and Kansas with a low marginal CO_2 emissions intensity electricity supply tend to have lower LCOAs in comparison to higher marginal CO_2 emissions intensity grid locations in Indiana and Illinois across all CO_2 price scenarios (Figure 6). This observation and our scenario results indicate that favorable locations for electricity-based ammonia production, in terms of both cost and emissions, may overlap for different carbon policy scenarios. An important caveat to this finding is the price-taker assumption implicit in our calculation that assumes the industrial process represents a relatively small electricity demand and hence cannot influence electricity prices and marginal CO_2 emissions substantially.

Impact of Process Flexibility on Cost of VRE-Based Ammonia Production. As was noted earlier, for dedicated VRE-based ammonia production, round-the-clock operation of the H-B synthesis loop requires a continuous electricity supply that necessitates the need for deploying Li-ion battery storage. Here, we explore how innovations to introduce flexibility in the H-B synthesis loop operations can contribute toward lowering the cost of dedicated VRE-based ammonia production while still adhering to the same round-the-clock ammonia supply requirements. Specifically, we investigate the cost and design impacts of the following two modifications: (a) allowing the H-B synthesis to function at outputs below its nameplate capacity while constraining its ramp rate (10% change from previous hourly production level) and (b) allowing the storage of produced ammonia to enable producing more than nameplate capacity at times of high VRE availability to make up for less

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than nameplate production at low-VRE-availability periods. We consider two forms of ammonia storage—large-scale cryogenic ammonia storage at −33 °C, and 1 bar (larger than 20000 tonnes) and small-scale high-pressure storage systems (20 bar, 25 °C). It should be noted that ammonia is still modeled to be output at a constant rate from the facility, which now can be supplied by a combination of ammonia storage and the H-B synthesis loop, since the produced ammonia might be used in other inflexible industrial processes (e.g., urea production).

Figure 7 highlights that introducing the specified flexibility in the H-B synthesis loop (e.g., ability to turn down by 50% or 75% in comparison to the nameplate and stay at that level for 48 h) can enable a 10−15% decline in LCOA in comparison to the case of an inflexible H-B synthesis loop. Figure 7 shows that the reduction in cost results from shifting the storage requirement downstream into the production process, with decreasing N_2 and H_2 storage and increasing NH_3 storage with increasing process flexibility. Moreover, the relative decrease in storage costs more than offsets the slight increase in cost of the H-B synthesis loop that needs to be oversized in comparison to the case of the inflexible process to enable NH_3 storage. In both cases of flexible operations (50% and 75% flexibility cases), large-scale cryogenic ammonia storage is selected with a capacity capable of providing more than 12−15 days of continuous ammonia output for the plant for the design capacity of the plant at 250 tonnes/day. Overall, this framework can be used to study the maximum affordable cost impacts of innovations to improve process flexibility that are valued in terms of improving the process economics.

■ CONCLUSIONS

Here, we propose a systematic framework to explore the economics and CO_2 emissions impacts of commercially available electricity-driven ammonia production schemes while considering spatial and temporal variations in electricity supply from the grid as well as on-site production via VRE resources. Our findings are based on a design and operations modeling framework that allows for co-optimizing the size of various components, including grid connection, electricity, H_2, and N_2 generation capacity, and different types of on-site storage while enabling round-the-clock, steady ammonia production. On the basis of 2030 technology cost and electric grid projections, we find that ammonia produced solely via grid electricity could achieve lower CO_2 emissions intensity in comparison to natural gas based ammonia in some locations (e.g., Texas) but could also lead to higher CO_2 emissions intensity in other locations (e.g. Indiana) (CO_2 intensity of the grid drives which locations have higher or lower emissions). As is illustrated elsewhere (Figure S8 in the Supporting Information), the key drivers of the levelized cost is the cost of electricity, be it in the form of PV or wind, while variation in costs of other components such as electrolyzer or HB has a lower impact on the LCOA. In contrast to grid electricity use, dedicated wind- and solar-PV-based ammonia production can reduce process CO_2 emissions by 100% but have widely different process designs and abatement costs depending on location and configuration of the VRE supply. Across the U.S., we investigated the cost of VRE-based-electricity-driven ammonia production and estimated the 5th percentile, median, and 95th percentile values for the resulting CO_2 abatement cost to be (1) 343, 573, and 984 \$/tonne CO_2 for a PV-based electricity supply (LCOA: 1.21, 1.74, and 2.71 \$/kg NH_3), (2) 376, 665, and 1873 \$/tonne CO_2 for a wind-based electricity supply (LCOA: 1.28, 1.96, and 4.17 \$/kg NH_3), and (3) 260, 342, and 596 \$/tonne CO_2 for a PV + wind based electricity supply (LCOA: 1.01, 1.21, and 1.80 \$/kg NH_3), respectively. The combination of grid + colocated VRE electricity supply locations may be the most cost-effective way for reducing CO_2 emissions from ammonia production in the short term, since it reduces the on-site energy storage requirements for continuous ammonia production. This is particularly true for locations near existing ammonia production facilities in the midcontinental U.S. Finally, a key driver for the cost of dedicated VRE systems is the need for battery storage to enable a continuous power supply for the H-B synthesis loop and ammonia liquefaction systems. In this context, enabling operational flexibility in H-B synthesis to allow some ramping capability in ammonia production could be beneficial in reducing the cost of a VRE-based ammonia supply. This analysis also suggests that emerging ammonia production routes based on electrochemical rather than thermochemical synthesis schemes that are likely to be more flexible may be more synergistic and cost-effective for using VRE electricity input.

The methodological contributions of this paper in modeling the design and operation of electricity-driven chemical production can be extended to study other key industrial commodities with large carbon footprints such as steel, cement, ethylene, and methanol. In addition, there is a scope for incorporating alternative technology choices for each of the system components considered in the process, similar to the approach adopted by Palys and Daoutidis.[55] For instance, where feasible, utilization of underground hydrogen storage could be modeled with injection, withdrawal rates, and pressurization requirements dependent on the location. For a given location, the availability of underground H_2 storage, with lower capital cost per tonne than above-ground storage, could contribute toward reducing the LCOA for VRE-only systems (see Figure S3 in the Supporting Information for the H_2 storage cost contribution to LCOA).

The findings of this study should be interpreted by keeping in mind the following limitations, which also are interesting areas of future work. First, our assessment of process and grid interactions are based on a price-taker assumption that assumes no change in wholesale electricity prices or marginal grid emissions factors due to increasing grid electricity consumption by the ammonia production process. An interesting area of future work would be to represent such industrial electricity demand with flexibility constraints in grid operation models to understand the complete picture of large-scale electrification of industrial processes. Second, our spatial assessment of LCOA does not account for spatial variation in the cost of land or the cost of transporting ammonia from the production site to the point of consumption. The impact of ammonia shipping on the final landed costs can range from relatively small (5−7%)[2] for transport of the product in the continental US but can be higher for trans-ocean shipments. Accounting for these attributes may lead to some locations being more favorable than others in terms of the delivered cost of ammonia rather than the LCOA metric used here. These factors could be included in a detailed supply chain analysis that also considers the capital cost differences between distributed and centralized ammonia production as well as alternate energy transport modes (electricity, ammonia) to connect energy production and consumption sites.

Third, our analysis relied on characterizing VRE resource availability on the basis of a single weather year and, while this is reasonable for a screening analysis, further assessment is needed to understand the impacts of interannual variability in VRE output as well as the impacts of climate change on VRE variability on the LCOA of VRE-based ammonia production. Fourth, while our analysis has quantified the potential benefits of process flexibility, further analysis using dynamic simulations is necessary to understand the operational implications of flexible process operation.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.1c08032.

Additional results, detailed modeling assumptions, and description and simulation outputs (PDF)

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Notes

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