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17th March 2023

**INET Oxford Working Paper No. 2023-04**

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**Summary**

Green hydrogen and ammonia are forecasted to have key roles in deep decarbonization, although national energy system models have yet to capture their full integration potential with sector coupling in future scenarios. In this study, the Power-to-X sector coupling potential of green hydrogen and ammonia is explored via a case study on the national-scale electricity grid of India in which the projected electricity demands for hydrogen and ammonia production account for nearly 25% of the total Indian electricity demand in 2050. Here we show that connecting the required fleets of electrolyzers to the grid and leveraging low-cost storage of ammonia with coupled sectors, such as shipping, steel, and agriculture, would provide valuable short-duration and long-duration load-shifting services. We find that this system design uses seasonal ammonia production patterns to reduce the levelized cost of hydrogen and ammonia, reduce curtailment, provide system resilience to interannual weather variations, and reduce the requirement for long duration energy storage or firm generating capacity while reducing total system cost.

**Keywords:** sector coupling, Power-to-X, ammonia, hydrogen, India

# 1 Introduction

Carbon-free green hydrogen and green ammonia have been recognized as essential technologies for achieving net-zero greenhouse gas emissions [1]. These energy dense fuels will play crucial roles in decarbonizing heavy-duty transport (i.e., trucking, aviation, and shipping), decarbonizing industrial processes such as fertilizer and steel production, providing long-duration storage and dispatchable electricity generation, and trading energy between regions [2]. Net zero targets have been set by over 130 countries to date [3] and hydrogen specific roadmaps, strategies, and policy have been announced in many countries, including India, United States of America, United Kingdom, Germany, France, Portugal, Spain, Denmark, Australia, Chile, Japan, and South Korea [4, 5]. Some of these targets make reference to green electrolysis capacity ambitions, such as 40 GW in the EU by 2030 [6] and 5 million tons of green hydrogen in India by 2030 [7].

Despite such clear signals, the relationship between new giga-scale fleets of electrolyzers and the grid has not been sufficiently explored in the literature. At a global level, the International Renewable Energy Agency (IRENA) forecasts that the production of green hydrogen and its derivatives (mostly green ammonia) will account for 30% of the global electricity demand in 2050 [8]. Yet, analyses published using Energy System Models (ESMs), the dominant tool for understanding different scenarios of decarbonization, have systematically overlooked the dynamic integration of sector coupling of green hydrogen and ammonia for industrial demands, such as steel and fertiliser, and for heavy-duty transport fuel, such as aviation and shipping, in net-zero decarbonised energy systems. Furthermore, simply including static demands in ESMs is not sufficient; the future potential for sector coupling is a dynamic give-and-take. Power-to-X (PtX) is useful for taking flexible amounts of electricity from the grid via short and long-duration load shifting as well as giving dispatchable electricity back to grids via re-electrification, for example in hydrogen or ammonia-fired gas turbines.

The main focus in the sector-coupled ESM literature is on short-duration, intra-daily load shifting predominantly in the light-duty vehicle transport sector and the thermal sector, such as coordinated charging of battery electric vehicle (BEV) fleets [9, 10], flexible heating and cooling demands [11, 12], and agricultural irrigation pumping [13]. He et al. [14] begin to capture the load-shifting potential of the hydrogen sector in an ESM-based analysis of the northeast USA grid; however, they only considered a flat weekly hydrogen demand for transport in light and heavy-duty fuel cell electric vehicles (FCEVs), omitting other key sectors such as chemicals, steel, and aviation and shipping fuels. Given the high costs of storing hydrogen above-ground, the sector coupling explored by He et al. only results in load-shifting benefits on an intra-daily level [14]. Several ESM-based analyses of parts of the European energy system have begun to investigate sector coupling of hydrogen for various sectors, such as aviation and shipping fuel, industry, and heating [15–17]. However, no analyses were found that adequately include the role of both hydrogen *and* ammonia flexible production and storage for intra-daily, weekly, seasonal, and interannual load-shifting. One potential reason this sector coupling potential is often overlooked is that the few models to date which include PtX sector coupling have focused on hydrogen, which is expensive to store in above-ground tanks, while ammonia is cheaper to store in large quantities above-ground (or trade overseas) for seasonal and interannual load-shifting. Additionally, the techno-economic potential of ammonia-to-power has been completely overlooked in almost all ESM to date, with the focus on synthetic methane and hydrogen gas turbines.

ESM studies based on variable renewable electricity (VRE) dominated systems have increasingly identified the need for long-duration storage [18] or firm generating capacity [19] for achieving zero emissions in the electricity grid. Many studies use significant nuclear and carbon capture and storage (CCS) technologies [1]; however, these technologies are likely to have higher costs in the long term than hydrogen or ammonia-fired gas turbines at the low capacity factors likely to be used in high renewable systems [20], and analyses are beginning to highlight the role of hydrogen and ammonia-based power generation in future electricity systems [21, 22]. However, by not including the role of load-shifting from these fuels in a sector coupled ESM, the requirement for long-duration storage is over-estimated. For example, Cole et al. find a least-cost, 100% decarbonized USA grid deploys over 500 GW of green hydrogen-based electricity generation via gas turbines [22]. Cole et al. do not consider grid connected electrolysis for any sector coupling load-shifting– not even for the hydrogen consumed in the model itself.

In this study, we build a state-of-the-art ESM to explore the full sector coupling potential of hydrogen and ammonia for both give-and-take services to the grid, i.e., load-shifting and dispatchable power generation. We build a national ESM of India's electricity grid to 2050 as a case study to explore the dynamic role of significant green hydrogen and ammonia production in a rapidly decarbonized electricity system. India is chosen as the case study due to its globally unmatched demand growth in all three relevant sectors: green electricity, green hydrogen (for steel and transport demands), and green ammonia (for fertilizer and shipping fuel demands). The decarbonization scenarios in this research are compiled from other sectoral level research (see Experimental Procedures) and find that by 2050 over 25% of electricity generated in India will be used for producing green hydrogen and ammonia, as shown in Figure 1. This forecast aligns well with the IRENA global forecast of 30% of the total electricity demand in 2050 used for the production of green hydrogen and its derivatives [8].

India is also pioneering in green hydrogen and ammonia focused policy. The Indian government announced a target to be Net-Zero by 2070 [23] as well as the National Hydrogen Mission (NHM) to accelerate the deployment of hydrogen technologies and to establish India as a global manufacturing hub for electrolyzers and fuel cells through green hydrogen obligations in industrial production of materials such as fertilizers, steel, and petrochemicals [24].

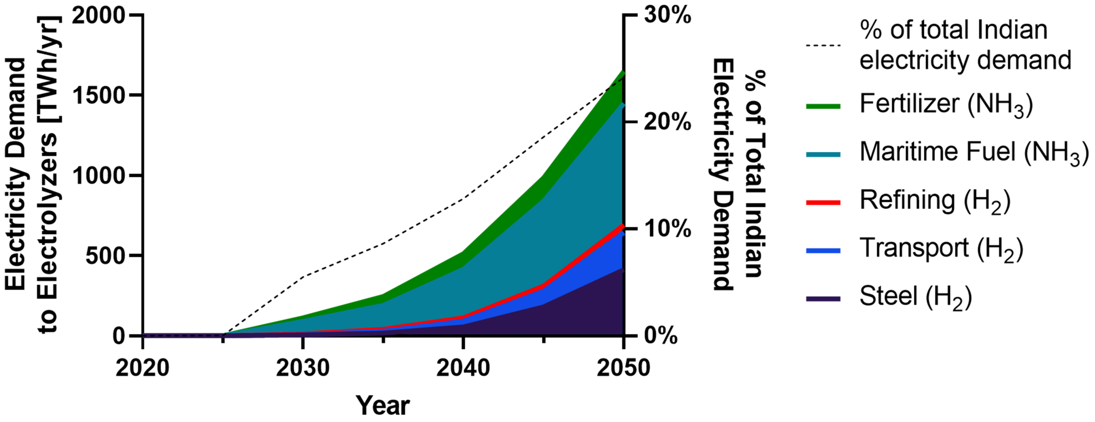


**Fig. 1** Green hydrogen and ammonia sector-level demand in India to 2050, including comparison to total final electricity demand. See Experimental Procedures for further detail on assumptions.

The proposed green ammonia obligations in the fertilizer sector alone would drive the world's fastest national green ammonia build out. This front-runner positioning has strong economic and political motivations. Today, India is the world's largest importer of fossil-fuel based ammonia, with ammonia imports equivalent to 1.3 billion USD [8]. Moreover, India imports Liquefied Natural Gas (LNG) to make over half of the domestically produced ammonia, thus being almost completely dependent on imports for the ammonia industry [25].

However, the transformation of the Indian energy system extends far beyond green ammonia for fertilizer, and thus creates an ideal case study on the cross-sector role of hydrogen and ammonia in decarbonized energy systems. The Indian economy is poised for rapid economic growth, rapid urbanization, rapid industrialization, and rapid decarbonization– all at the same time. In global models from the International Energy Agency (IEA), the soon-to-be most populous country on the planet is found to have the single largest increase in energy demand as well as single largest increase in $CO_2$ emissions to 2040 of any country [26]. Unsurprisingly, the IEA has firmly stated, **"Whichever way the global energy economy evolves from here, India will be firmly at its centre"** (IEA, 2021) [26].

Despite the scale of the required electrolyzer fleet, there has not been a modelling effort, to the best of our knowledge, that considers the dynamic role of industrial electrification and PtX sector coupling at this scale in India. There is a large body of recent work that evaluates the role of integrating VRE into the Indian electricity system [13, 26–33]. Many of these ESM analyze the development of new generation, transmission, and storage assets, as well as the best way to utilize existing assets. However, all of these studies overlook the significant role of PtX sector coupling on facilitating the integration of high levels of VRE, reducing the cost of decarbonization, and reducing the need for long-duration storage.

In summary, India is chosen as a case study because it is at the heart of the global energy transition, it has unmatched demand growth in hydrogen and ammonia end-use cases, and it has already established a willingness to move rapidly into deploying this technology with pioneering policy. However, the large upcoming role of green hydrogen and ammonia, and the overlooked potential of sector coupling are universally relevant across all regional ESMs in the literature.

# 2 Main

## 2.1 Beyond state-of-the-art energy system modelling

ESMs are a key tool for providing insights into energy system evolution for research institutions, policy makers, and energy companies. However, traditional ESM are lacking 1) a detailed dynamic integration of PtX sector coupling, (considering production, storage, transportation, industrial use and peak power generation), 2) empirically grounded technology cost forecasts, and 3) representation of system resilience to interannual weather variation at high VRE penetration. In this study, novel methodological approaches are added to a traditional capacity expansion ESM to better capture the transformational changes of an energy system (Figure 2).

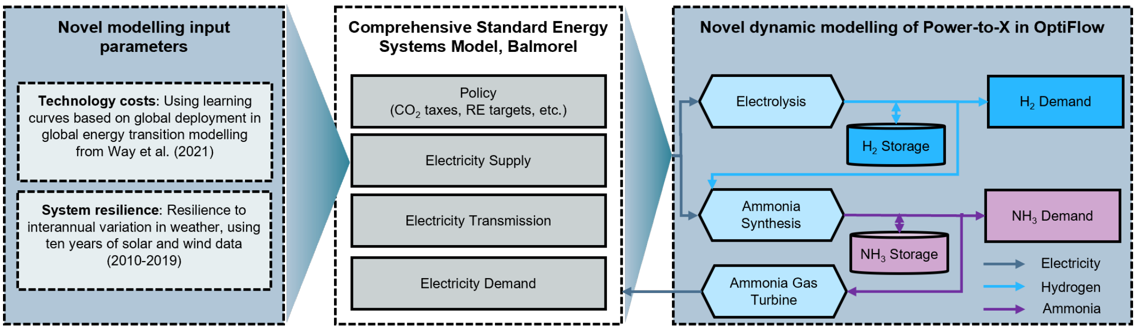

**Fig. 2** Overview of improvements to standard ESM.

The first innovation is a network model of PtX based on OptiFlow modelling from [34, 35], adapted to hydrogen and ammonia production, storage, transport, and use, including in the power sector itself.

The second innovation is using empirically grounded technology cost forecasts (experience curves) based on global energy transition scenarios from Way et al. [36]. Experience curves are a reliable forecasting tool for technology progress [37], and have been found to be significantly more reliable than expert forecasts in the context of the energy transition [38]. In this study, three global scenarios for the speed of the energy transition are considered (Historical Mix, Slow, Fast) from Way et al. [36] global transition modelling. Leading ESMs, such as those from the IEA [1, 39] use cost estimates which are systematically biased against progress in key clean energy technologies [40], with latest projections generally falling in between the Historical Mix and Slow scenarios (Figure 3). Reliable and coherent cost forecasts are essential for predicting the transformation of an energy system. For example, Lu et al. [33] forecast Indian solar capital costs to be \$550 to \$1650 kW$^{-1}$ by 2040, while the cost as of 2020 was \$596 kW$^{-1}$ and still rapidly dropping [41]. Unsurprisingly, Lu et al. design an Indian electricity system which is dominated by onshore wind, rather than solar PV, amongst other differences with our study.

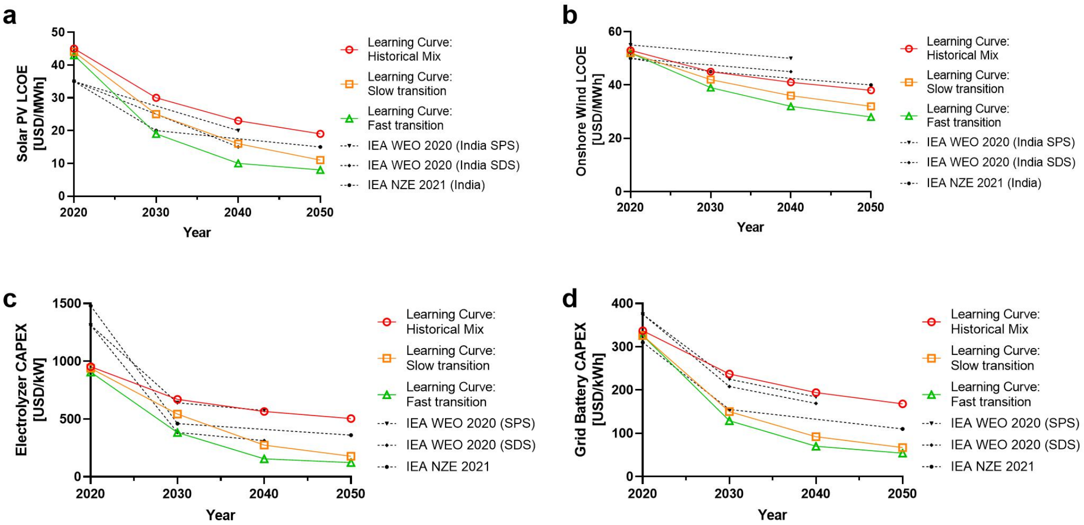


**Fig. 3** Cost reduction scenarios for key technologies, with comparisons to two scenarios from IEA World Energy Outlook (WEO), namely the Sustainable Development Scenario (SDS) and Stated Policy Scenario (SPS) [39], as well as comparison to the Net Zero Emissions by 2050 Scenario (NZE) [1]

The third innovation is system resilience to interannual weather variation by using 10 years of hourly wind and solar data rather than a typical meteorological year (TMY). Dowling et al. [18] find that including more years of weather data dramatically increases the need for long-duration storage in ESM results due to interannual variation.

## 2.2 Network Effects: Why connect to the grid?

The results show that there are significant benefits to connecting the hydrogen and ammonia production to the electricity grid rather than having islanded production sites. Grid integration reduces the Levelized Cost of Hydrogen (LCOH) and Ammonia (LCOA) by 10%-25% across the scenarios (Figure 4a,4b). The reduction in LCOH and LCOA is driven by lower electricity prices available to grid connected electrolyzers because they gain access to electricity that would otherwise be curtailed. In the islanded production scenarios, 15%-20% of electricity generated in India in 2050 is curtailed, while only 10%-14% is curtailed in the grid connected scenarios (Figure 4c). In absolute terms, this saves 350 to 460 TWh of electricity from being curtailed, and 200-300 GW less PV and wind needs to be installed by 2050.

By reducing curtailment, connecting electrolyzers to the grid reduces annual system costs by approximately 5% in 2050 across all scenarios (Figure

4d). Beyond reducing costs, benefits of grid connected electrolyzers include reducing material consumption and land-use associated with the extra solar PV that is no longer required.

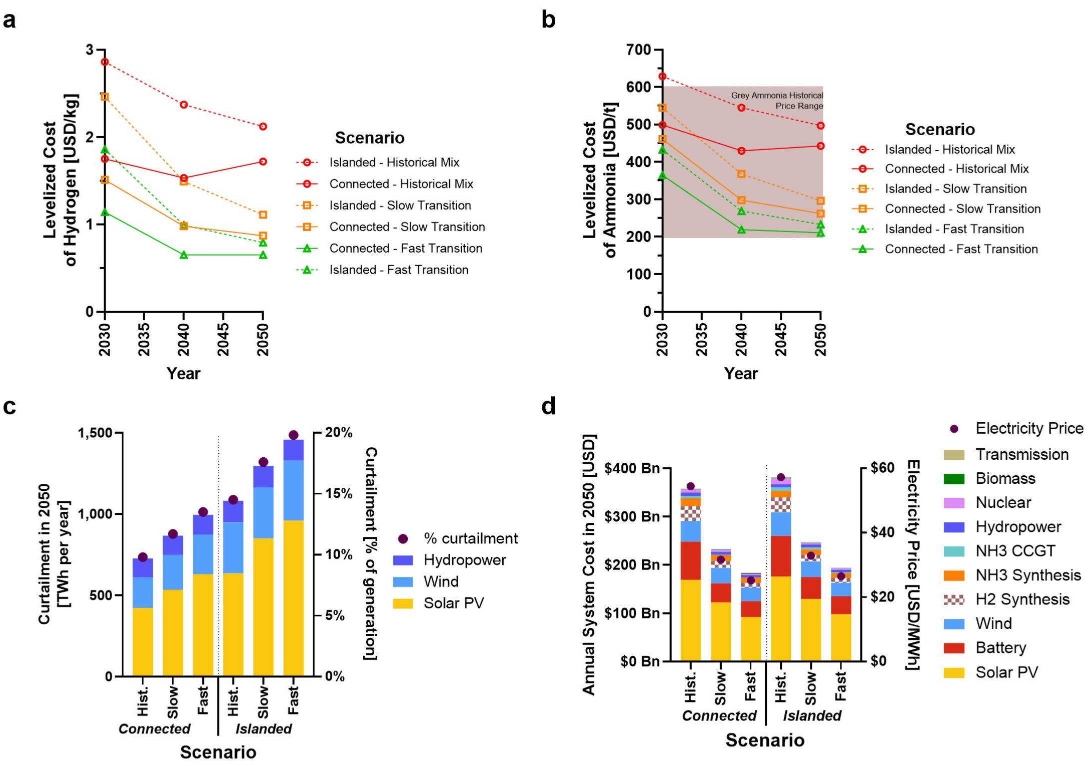


**Fig. 4** Key result metrics across grid connected and islanded system scenarios. a. LCOH across scenarios from 2030-2050, b. LCOA across scenarios from 2030-2050 with grey ammonia historical commodity price (Black Sea) from [42], c. Curtailment across scenarios in 2050, d. Annualized system costs across scenarios in 2050

Grid connected electrolyzers and ammonia synthesis plants are operated seasonally to access cheaper, otherwise curtailed electricity, with significant ammonia storage to manage seasonal and interannual variations (Figure 5). Across all scenarios, ammonia production mostly occurs from March until August, with plants' loads reduced to minimum technical levels outside of these months (Figure 5a). These months correspond to the strongest solar resource in the Northern Region, and strongest wind resource in the Western and Southern Regions due to the monsoon. Ammonia storage is required for the system to maintain a constant output of ammonia for fertilizer and shipping demand, ranging from 15 to 40 million metric tons (MMT) of ammonia storage (Figure 5b). Simulating the 2050 system with weather data from ten consecutive weather years (WY1-WY10), the system's storage levels are nearly emptied in January and reach their maximum in August. The difference in WY can be noted in the ammonia storage levels, with WY9 and WY10 being particularly good years compared to others, and thus having surplus storage levels at the end of the low production season (Figure 5b).

The Historical Mix cost scenario requires more storage than the Slow or Fast scenarios because it is lower cost to buffer ammonia rather than overbuild solar and wind. This is due to the higher technology costs of solar PV and wind in the Historical Mix scenario. Still, all scenarios, regardless of technology costs, find seasonal ammonia production with storage to be beneficial for a least-cost system. While significant ammonia storage was used, no scenarios utilized ammonia or hydrogen trading between regions via pipeline, truck, or ship for industrial demands (i.e., steel, fertilizer, transport, refining, maritime fuel). The ammonia production cost difference between regions was less than \$50 per metric ton, which is a relatively small difference, and justifies local production. Instead of moving energy-storing molecules, the results point towards moving electricity via an increase in grid connected transmission lines (Figure 7b).

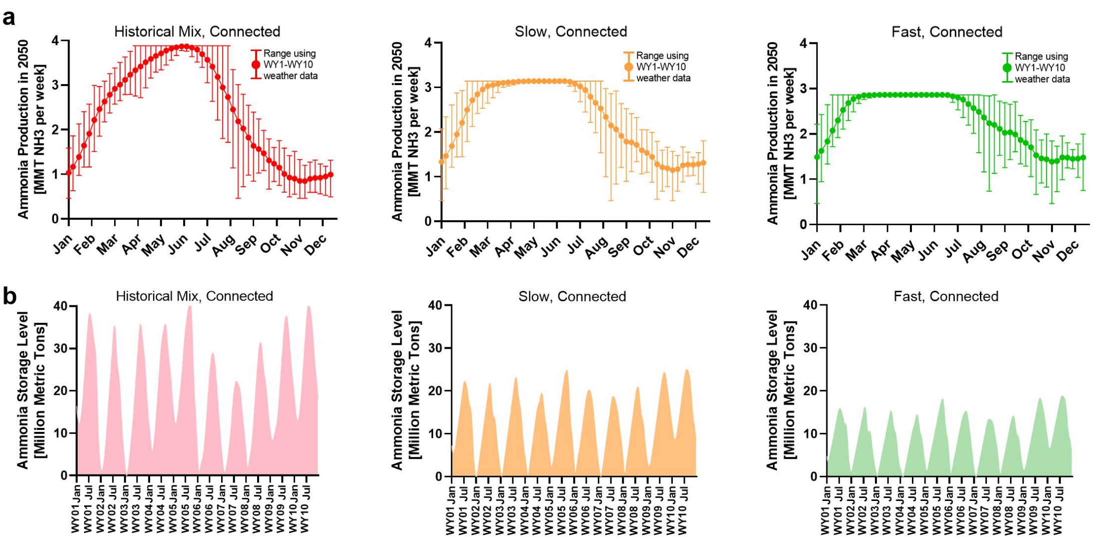


**Fig. 5** Seasonal and interannual variation in ammonia production and storage levels to meet a constant demand. a. Country-wide weekly ammonia production in 2050 across Connected scenarios, showing the range of weekly ammonia production depending on year of solar and wind data, b. Country-wide storage levels of ammonia in 2050 over 10 weather years (WY1-WY10) of solar and wind data in simulation.

## 2.3 Dispatchable electricity generation requirements for seasonal storage and system resilience

Across all scenarios, dispatchable electricity represents 3% to 6% of electricity consumption in 2050 (Figure 6a). Dispatchable electricity is mostly delivered via existing and planned hydro-power and nuclear power plants in India. Nevertheless, ammonia-to-power is still used to some extent in all scenarios except the Fast and Connected scenario to provide seasonal storage and resilience to unfavorable weather years. Green ammonia is used to generate up to 0.4% of consumed power, or 30 TWh per year based on 70 GW of installed capacity built from 2040 onwards. These plants have an average utilization factor of 2% to 5%, far lower than current power-plant utilization factors.

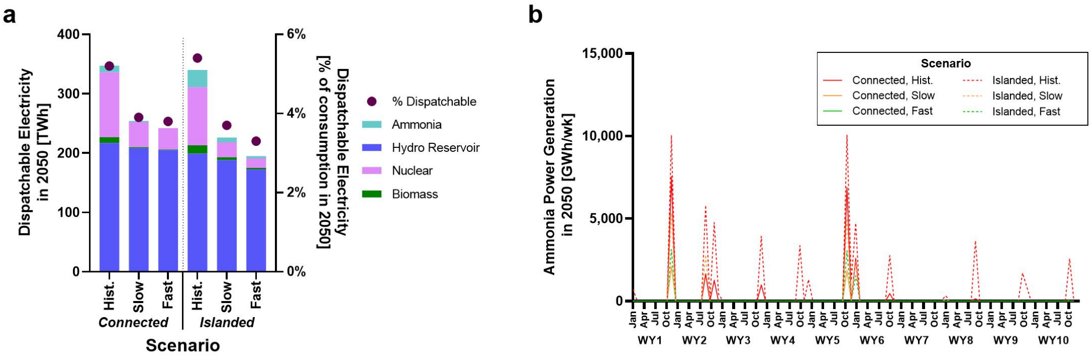


**Fig. 6** Dispatchable electricity requirements; a. Country-wide annual electricity generated from dispatchable assets in 2050 across scenarios, and relative percentage of total electricity consumed, b. Country-wide weekly ammonia GT power generation in 2050 over 10 simulated weather years (WY1-WY10) of solar and wind data.

In the Islanded scenarios, ammonia is used for seasonal power generation and system resilience in the Oct-Jan period (Figure 6b). In the Connected scenarios, the requirement for seasonal dispatchable electricity is reduced because of the demand-side flexibility gained from the ammonia production. In short, islanded scenarios use seasonal dispatchable power generation (i.e., supply-side flexibility) because they do not have the demand-side, load-shifting flexibility of grid connected electrolyzers to manage seasonality of the renewable resources. As shown in Figure 6b, WY1 and WY5 required the most dispatchable electricity via ammonia-to-power for providing system resilience.

## 2.4 Decarbonization Results

The evolution of the Indian power system depicted across our scenarios is dominated by solar power with battery storage (Figure 7a). Across scenarios, solar PV installed capacity reaches over 4,000 GW by 2050, with 1,000 GW of 4-hour battery storage. The installed capacity is concentrated in the Northern Region (NR), Western Region (WR), and Southern Region (SR) (Figure 8). Onshore wind power is mostly installed in the WR and SR, totaling 330 GW to 460 GW in the country by 2050. Electrolyzer capacity reaches nearly 600 GW by 2050, representing a source for load-shifting almost as large as batteries. Transmission infrastructure increases by over 60% in the Connected scenarios, while only up to 20% in the Islanded scenarios (Figure 7b).

Electricity generation rapidly shifts towards wind and solar, and increasingly to solar over time (Figure 7c). Carbon emissions begin rapidly declining to near-zero by 2040 and zero by 2050 across all scenarios (Figure 7d), driven by VRE technology cost declines, a gradual $CO_2$ tax to \$200 USD $t^{-1}$, and the phase out of existing coal and gas by 2040 and 2050, respectively (see Experimental Procedures Section for assumptions). No new nuclear, hydro-power, or biomass power plants are built beyond what is already under construction or planned. New ammonia-to-power plants come online in 2040, specifically in the SR, NER, and ER.

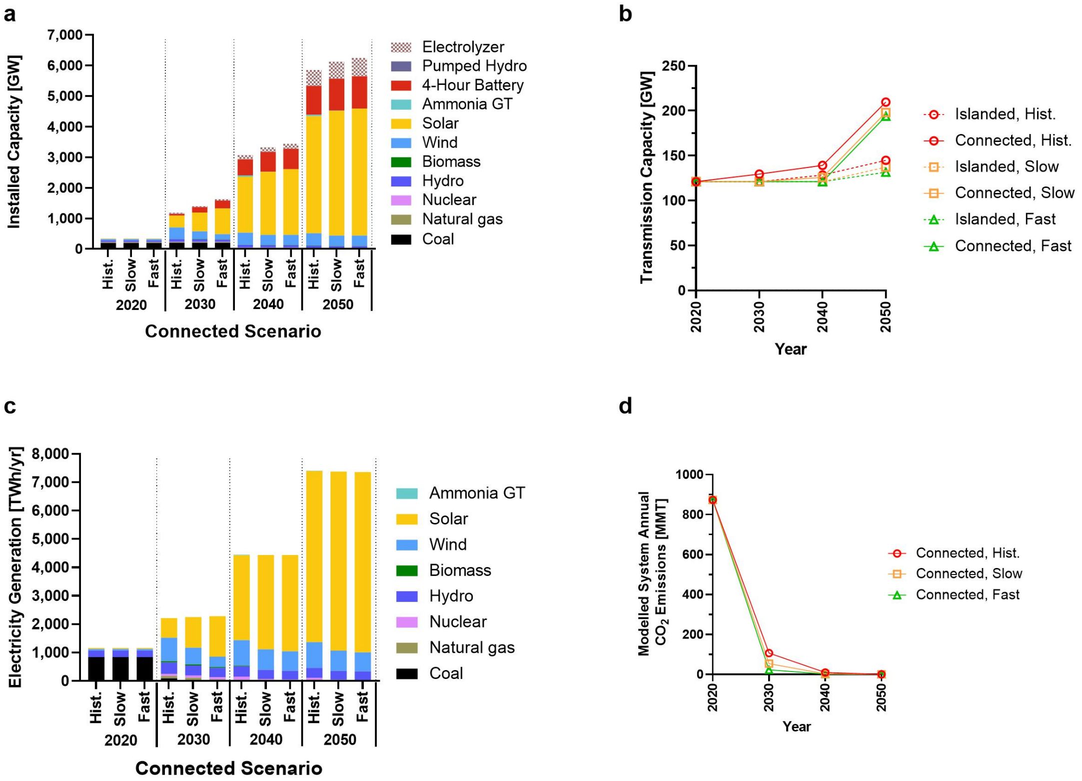


**Fig. 7** a. Installed capacity by year in the Connected scenarios, including grid connected electrolyzers. b. Installed transmission capacity by year. c. Electricity generation by year in the Connected scenarios. d. $CO_2$ emissions from modelled system from 2020-2050, excluding emissions from non-electrified sources.

# 3 Discussion

As the momentum builds with more societies transitioning towards net-zero, both Integrated Assessment Models (IAMs) and more temporally granular ESMs need to continue to expand their scenarios to enable explorations of new clean energy pathways available for deep decarbonization. In these models, the foundational role of green hydrogen and ammonia needs to be better integrated because it is increasingly clear that fleets of electrolyzers will be deployed at considerable scale starting this decade.

In our modelling, we find that connecting large fleets of electrolyzers into the grid infrastructure and load-shifting the industrial production, specifically green ammonia production for fertilizers and shipping fuel, is a plausible strategy towards a lower cost, more efficient, and more reliable electricity grid. This

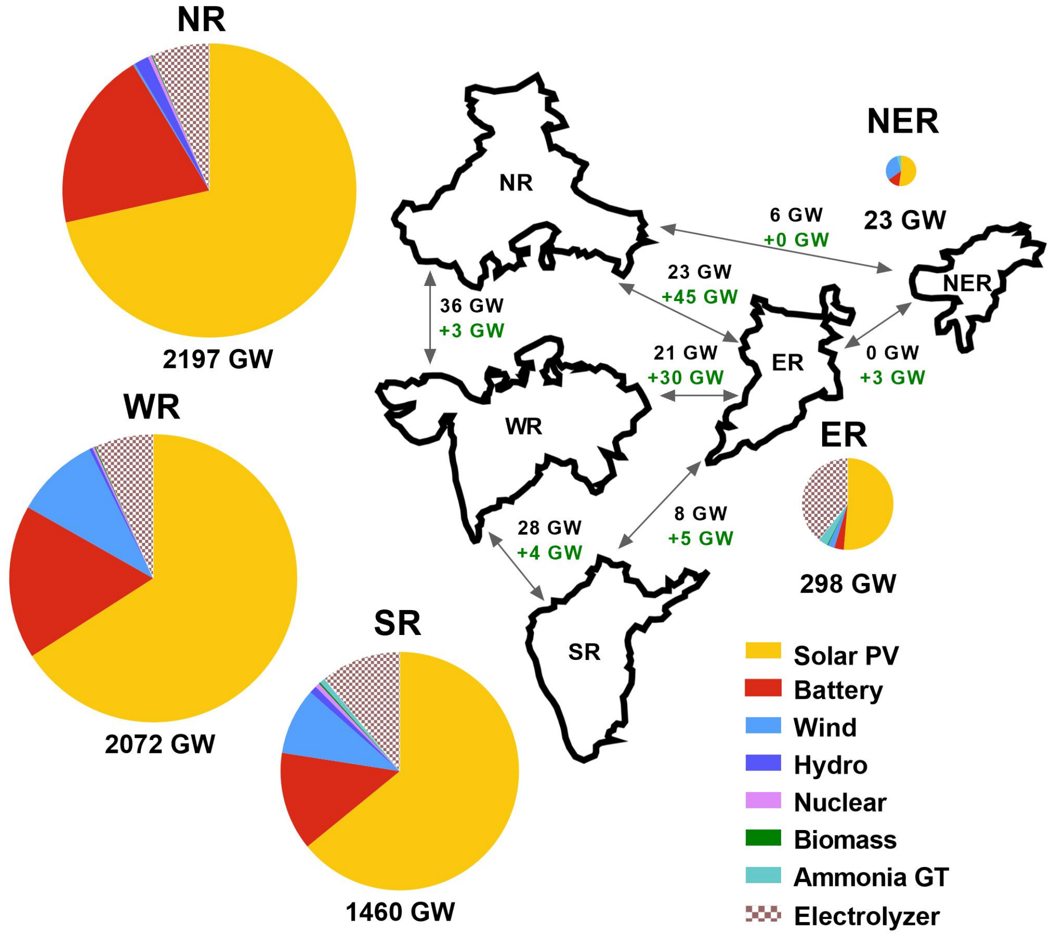


**Fig. 8** Generation capacity, battery capacity, electrolyzer capacity, and transmission (new transmission in green) by region in the Slow, Connected scenario in 2050.

envisioned least-cost system produces green hydrogen and ammonia in a seasonal pattern to match VRE surplus. Excess green ammonia is stockpiled in low-cost aboveground storage and then consumed in the seasons of lower green hydrogen and ammonia production to meet constant demands in the fertilizer and shipping sectors as well as to provide firm generating capacity. Smaller quantities of green hydrogen are stored aboveground for intra-daily load shifting. This PtX sector coupled system configuration is not only lower cost, but it is more resilient to unfavorable VRE weather years, as shown over ten years of weather data.

Unfortunately, the potential benefits on this system design will not be realized unless policy steers industry-grid relations away from its historical precedence. For industry, grid connection is often associated with high grid connection charges and unreliability, which warrant onsite power backup and complete "captive" power-plants in extreme scenarios. This historical path dependency is extremely evident in India, where captive power plants at commercial and industry users accounted for 17% of the country's generation in 2019-20, with over 78 GW of captive power generation installed [43]. These captive power plants are either fractionally or completely disconnected from the distribution and transmission grids to avoid the historically under-performing and expensive rates charged to industrial users.

As it stands today, electrolyzer fleets for industry would likely follow in the same footsteps, with islanded systems avoiding grid connection charges and other real or perceived disadvantages. However, based on our findings, policy should steer the system *towards* a new paradigm of industry-grid relations which synergistically benefit both parties in the transformation towards net-zero. Recent policies announced as part of India's NHM are a step towards grid connecting PtX. One policy aims to reduce grid costs for green hydrogen and ammonia plants by waiving interstate transmission charges among other incentives [7]. The suitability of these policies and further policy and market mechanisms need to be explored today, at the initiation of this transformation, in order to progress towards a more integrated future scenario.

Beyond India, the potential role of load shifting in green hydrogen and ammonia needs to be modelled for other countries and regions, which will have unique local VRE supply and demand mismatch as well as country specific PtX demands. Furthermore, the evolution of new technologies must be monitored, and the ESM adapted to best capture imminent changes, such as in aviation e-fuels demand or geographies with underground hydrogen storage capabilities. Further work should also investigate global trade of green ammonia to balance seasonal production [44], rather than only considering stockpiling in an isolated country. Moreover, we only consider resilience to ten years of historical weather data, while it is important for the system to be resilient to less frequent events as well as to consider the changing weather patterns due to climate change. These additional resilience requirements could significantly increase the role of dispatchable power and should be considered as climate models are able to provide this data.

Finally, there exist fundamental uncertainties and complexities that limit our ability to predict the exact mix of our future energy systems. The real value of models such as the one we present here is not the precise results of an ESM looking toward 2050, but rather to highlight leverage or sensitive intervention points [45] and bases of system designs which dramatically alter the end-state of the system transformation. We find that hydrogen and ammonia *can* be one point of leverage to change our electricity grids for the better, if they are fully integrated. We hope the analysis presented here motivates and accelerates the wider research community into expanding ESMs of various regions and associated assumptions to considering the potential impacts of PtX with sector coupling.

# 4 Experimental Procedures

## 4.1 Energy System Model setup and scenarios

### 4.1.1 Balmorel - a comprehensive long-term energy system model

Balmorel [46] is an open-source energy system model, with the objective of minimizing total power system costs. In its basic configuration, the Balmorel model linearly optimizes investment in generation and transmission using hourly dispatch simulation and multi-year scenario development. Essentially, Balmorel finds the least-cost economical dispatch and capacity expansion solution for the represented energy system, subject to the technical and economic assumptions and constraints provided. It is a deterministic model which assumes perfect market competition and economic rational decision-makers and end-consumers. Furthermore, Balmorel is demand driven and computes the conversion of primary energy to energy carriers in the form of electricity, whilst simultaneously optimizing investments and/or operational decisions, i.e. subject to policy and environmental restrictions.

The Balmorel version used in this study covers a large geographical area of the Indian power system, whilst allowing spatial analysis focusing on, for example, the production of green hydrogen and ammonia. India is divided into the historical five electricity grid regions. Electricity is allowed to be traded between adjacent market regions. Each region consists of one or more areas, which represent PtX networks or installations of local electricity technologies.

The temporal resolution in Balmorel is user-defined, allowing the system to be simulated using an hourly time-resolution or to be aggregated according to the research question.

Overall, Balmorel is a suitable tool for long-term planning of future energy system and has been extensively used world-wide. Advantages of Balmorel include that it is scalable from regional to international power systems, customizable, and open-source. Balmorel has recently been used to examine the energy transition in capacity building countries, including in China [47], Indonesia [48], and Vietnam [49].

The limitations of this Balmorel model include a simplified representation of transmission (a single capacity between regions), short-sighted investment optimization (i.e., no inter-year foresight to anticipate falling technology prices or rising $CO_2$ prices), full intra-year foresight (e.g., hydro use, storage, and fuel restrictions using perfect prediction of wind and solar), and perfect competition in a market of economic rationality. These limitations do not detract from the findings.

Balmorel has previously been used to model green ammonia for fertilizer and dispatchable power generation in Northern Europe to 2050 [50]; however, that analysis does not consider flexible HB plants, and thus no meaningful load-shifting can occur. Additionally, other hydrogen demands are not considered, such as steel or maritime fuel. Nevertheless, those results pointed towards the potential use of green ammonia for energy storage and energy transport, with significant aboveground ammonia storage.

### 4.1.2 OptiFlow - generalized spatio-temporal network optimisation model

OptiFlow [51] is an open-source spatio-temporal network optimization model which can be linked with Balmorel. OptiFlow uses node-arc relationships to represent flows such as energy, mass, economic, or environmental metrics. Nodes include storage, transport, and chemical processes, such as ammonia synthesis. Arcs in this model include electricity, hydrogen, and ammonia. In the linkage with Balmorel, the OptiFlow objective equation of minimizing cost is included inside Balmorel's cost optimization objective equation. Other linked equations include the electricity balance equations and ammonia balance for re-electrification in gas turbines. In this research, green hydrogen and ammonia production, storage, transport and use are modelled using OptiFlow linked with Balmorel, based off of the configuration used in [34, 35].

OptiFlow is deterministic, i.e., there is no probabilistic element, and a model run will reliably produce the same result based on a fixed set of inputs. The model is partial equilibrium, meaning it only considers the electricity sector while IAMs are usually general equilibrium, and consider multiple sectors of the economy and feedback between these sectors.

### 4.1.3 Scenarios

We investigate six scenarios which consider three different speeds of global transition (Historical Mix, Slow, Fast) across two network configurations (connected or islanded). Techno-economic assumptions for the scenarios are detailed in the Supplementary Material. There is no direct cost differential assumed for the RE power plants or PtX production sites used in the connected and islanded scenarios, such as a grid connection charge. Ultimately, this ESM does not capture the costs related to new investments in distribution grids, which could favor the islanded solution. However, the costs of the transmission grid capacity expansion are included, and indeed the connected scenario has a large increase in transmission grid infrastructure accounted for in the costs as presented.

### 4.1.4 Spatial and temporal aggregation

We consider 35 areas (Indian States and Union Territories excluding Andaman & Nicobar Islands and Lakshadweep) which are combined to form 5 Regions (East, North, South, West and Northeast). Unlimited transmission is assumed within regions and limited transmission between regions. Data for existing and planned generation and transmission was used for each area based on the NEP [52] and EPS [53].

We model the development of the system to 2050 in 10 year time-steps. We use ERA5 [54] climate data for generating hourly solar and wind profiles for 2010-2019 (see Supplementary Note 1). We aggregate every 5 hours and every 5 weeks, which we found captures interannual weather variation as well as hourly weather variation without causing untenable calculation times. The model runs took 3 to 72 hours on 256 GB RAM, 2.2 GHz.

## 4.2 Supply side technologies

Balmorel considers a range of available power generation technology options, such as coal, gas, wind, solar, nuclear, hydropower, batteries, and biomass, with country-specific cost forecasts and availability. Cost scenarios for all technologies are listed in Supplementary Tables S1-S3.

### 4.2.1 Technical potential for solar and wind

We use 48 wind locations and 33 solar locations across India which capture the spatial variation in profiles across areas of significant technical potential. The National Institute of Wind Energy (NIWE) estimates a maximum of 693 GW of onshore wind installed capacity at 120 m based on suitable land, divided into states [55]. The National Renewable Energy Laboratory (NREL) RED-E tool [56] was used to identify over 9,000 GW of solar PV potential capacity in India, using land identified as barren land, wasteland, and shrubland. This is the same technical potential used by TERI [25]. See see Supplementary Note 1 for further information.

### 4.2.2 Green hydrogen and ammonia production and storage

Green hydrogen and ammonia production was modelled used electrolysers, aboveground hydrogen storage in tanks, flexible Haber-Bosch (HB) ammonia synthesis and air separation units (i.e., nitrogen generation), and aboveground ammonia storage tanks. Underground hydrogen storage is possible in certain geologies, such as salt caverns; however, India does not likely have suitable formations, and further work is required to understand India's geological storage options in other formations such as rock caverns [25]. Therefore, aboveground hydrogen storage in tanks was the only technology considered in this analysis.

The production modelling of ammonia is typically modelled in islanded systems [57, 58], while more rarely modelled in grid connected scenarios [59]. We consider both configurations, with batteries and ammonia gas turbines available in the islanded case for providing reliability.

HB operation flexibility is a key assumption in this analysis which allows for seasonal load-shifting. HB plants in operation today do not have flexibility below 50-60% of minimum load [60] because the source of feedstock hydrogen is fossil fuel based, and thus the least cost strategy is to run continuously at maximum throughput to increase asset utilization. Given the numerous green ammonia commercial announcements since 2020, HB technology companies are also announcing much lower minimum loads in greenfield plants built to connect with VRE. Patents have been filed for as low as 10% minimum load [60], and chemical engineering modelling in the literature suggests minimum loads of 30% can be achieved by increasing the inerts in the synthesis loop and adjusting the ratio of hydrogen to nitrogen, all while maintaining current reactor design and auto-thermal operation [61]. This analysis assumes a 20% minimum load, which could be met by turning assets down or by designing plants with multiple smaller reactors and selectively shutting them down for periods at a time, i.e., seasonally. The other processes which demand substantial amounts of hydrogen, namely steel, refining, and transport, were not assumed to have any load-shifting capability.

No import or export of hydrogen or ammonia was considered. Imports will not have a significant cost advantage because India is likely to be a least cost location for green hydrogen and ammonia production [2]. Exporting green hydrogen and ammonia is a strategic target announced in the NHM [24], but is difficult to model at this point due to the unclear supply and demand relationship at a global level due to complexities such as countries' preferences for hydrogen and ammonia fuel security, subsidizing domestic industries such as steel and fertiliser, etc.

### 4.2.3 Green ammonia power generation

Green ammonia was included as a new fuel option to be used in combined cycle gas turbine (CCGT) power-plants based on [20]. Due to the high cost of above-ground hydrogen storage, ammonia has significant techno-economic advantages for use in dispatchable GTs [20] and there are clear signals from manufacturers to have ammonia-fired GTs on the market by 2024 [62]. New investments in ammonia CCGT were permitted alongside other power generation technology options from 2030. Any ammonia consumed in the power sector was an additional endogenous ammonia demand (i.e., generated within the model run) on top of the exogenous ammonia demands (i.e., fixed fertilizer and maritime fuel demands).

### 4.2.4 Fossil fuel generation and carbon tax

No new fossil fuel generation capacity additions were permitted after 2039. Existing coal plants were phased out by 2039 and gas plants by 2049. A linear $CO_2$ tax of \$45 (2025) to \$200 (2050) was used, in line with IEA forecasts for developing countries [39].

### 4.2.5 Dispatchable power

Dispatchable power is available on-demand regardless of weather conditions. This includes hydro-power equipped with large reservoirs, nuclear power, biomass power, coal or natural gas with CCS, and ammonia power plants. Short term storage of several hours in batteries, while crucial for the system, is not included in the classification of dispatchable electricity in this analysis; however, long-term storage in the form of ammonia is considered dispatchable.

## 4.3 Demand scenario

Based on scenarios from TERI [25] and the World Bank [63], we developed a decarbonization scenario where production of green hydrogen and ammonia could account for more than 25% of electricity demand by 2050 in India, as shown in Figure 1. These demands total 15 MMTPA of hydrogen and 120 MMPTA of ammonia by 2050, which is significantly larger than India's present-day fossil fuel-based hydrogen and ammonia production capacities of 6 MMTPA and 18 MMTPA, respectively. The modelling underpinning this low-carbon demand scenario by TERI [25] assumes 50% of steel, 60% of ammonia fertilizer, and 30% refining demand are met by green hydrogen. Shipping demand is based on supplying 10% of global shipping fuel (meeting 25% of Asia's fuel demand) based on the most conservative scenario for India from [63]. Indian electricity demand is modelled by TERI [25] based on detailed modelling of electricity growth in the Residential, Commercial, Transport, Industry and Agricultural sectors. Further data is available in Supplementary Note 2.

Exogenous demands for hydrogen and ammonia do not include long-duration storage needs (which are determined endogenously) or synthetic aviation fuel which is still technologically uncertain. No demand side flexibility in residential heating or vehicle charging was considered; however, these intra-daily load-shifting technologies would only affect the deployment of 4-hour battery storage, rather than this research's focus of seasonal load-shifting and storage requirements.

**Supplementary information.** See Supplementary information file.

**Acknowledgments.** The authors acknowledge Dr. Rupert Way for his support with learning curve forecasts.

This work was supported by the Oxford Martin School Post-Carbon Transitions Programme (grant number LDR00530) and the Economics of Energy Innovation and System Transition (EEIST) programme. The EEIST programme is jointly funded through UK Aid by the UK Government Department for Business, Energy and Industrial Strategy (BEIS), and the Children's Investment Fund Foundation (CIFF). The contents of this manuscript represent the views of the authors, and should not be taken to represent the views of the UK government or CIFF.

**Contributions.** Z.C. carried out the investigations and simulations, and wrote the original draft of the manuscript. Z.C. and R.B. developed and managed the model code. Z.C., R.B., M.I., and R.B-A. provided conceptualization of the project, contributed to simulation designs and editing of the manuscript. M.I. and R.B-A. supervised the project and acquired funding. All authors gave their final approval for publication.

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